

# **Experimental and numerical assessment of H2 combustion potential : extreme events in laminar premixed burners and flame stability in non-premixed swirled injectors**

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# **To cite this version:**

Andrea Aniello,. Experimental and numerical assessment of H2 combustion potential : extreme events in laminar premixed burners and flame stability in non-premixed swirled injectors. Electric power. Université Paul Sabatier - Toulouse III, 2023. English. NNT : 2023TOU30024. tel-04213813

# **HAL Id: tel-04213813 <https://theses.hal.science/tel-04213813v1>**

Submitted on 21 Sep 2023

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THESE **A** 

**En vue de l'obtention du**

# **DOCTORAT DE L'UNIVERSITE DE TOULOUSE ´**

**Délivré par :** *l'Université Toulouse 3 Paul Sabatier (UT3 Paul Sabatier)* 

Présentée et soutenue le  $29/03/2023$  par : Andrea ANIELLO

Experimental and numerical assessment of H<sub>2</sub> combustion potential: **extreme events in laminar premixed burners and flame stability in non-premixed swirled injectors**

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**JURY**

 $\textbf{École}$  doctorale et spécialité :

*MEGEP : Energ´etique et transferts ´*

Unité de Recherche :

*Institut de M´ecanique des Fluides de Toulouse, IMFT, Universit´e de Toulouse, CNRS, France*  $Directeur(s)$  de Thèse :

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### <span id="page-3-2"></span><span id="page-3-0"></span>**Experimental and numerical assessment of H**2 **combustion potential: extreme events in laminar premixed burners and flame stability in non-premixed swirled injectors**

<span id="page-3-1"></span>Recent years have witnessed a raising alarm for climate change and predicted a potential lack of energy supply for the next future. In this respect, the combustion community is looking for affordable and sustainable solutions to solve these issues. Green-hydrogen can be potentially produced from renewable electricity and is a promising alternative to decarbonize the current energy mix. Nevertheless, its exploitation in combustion systems remains limited due to its unique combustion characteristics and most applications are generally limited to 20%*vol* of H<sub>2</sub> in the fuel blend. Only very recently we assisted to the spread of new technologies that allow to sustain greater hydrogen content. In view of that, this work focuses on fundamental aspects of hydrogen combustion as part of  $\text{CH}_4/\text{H}_2$  blends or for pure hydrogen-air mixtures either in laminar premixed flames or in turbulent non-premixed conditions. The analysis of these configurations is performed via both experimental and numerical tools to shed light on fundamental mechanisms related to  $H_2$  combustion.

Experiments are conducted on two multi-perforated premixed burners, originally designed for methane-air mixtures, to assess the limits of  $H_2$  substitution and investigate potential risks associated to it. Results are presented by means of stability maps and the impact of hydrogen addition on blow-out and flashback limits is then analyzed. Measurements unveil different flashback regimes and several triggering mechanisms are put in evidence as function of the  $H_2$  content.

Second, high fidelity Large Eddy Simulation is used to investigate the impact of a central pilot hydrogen injection on the Flame Transfer Function (FTF) of a swirled premixed methane-air flame. This study, validated on experimental results, show that the central recirculation zone responds to specific oscillation frequencies, undergoing a pronounced axial movement that modulates the penetration of the hydrogen central jet that, in turn, affects the flame structure and the position of the flame root. This dynamics interferes with the perturbation generated by the hydrodynamic eddies shed at the injector rim, explaining the trend of the FTF.

Finally, high-fidelity LES are presented for non-premixed H2-air flames stabilized on a novel injector for gas turbine applications named HYLON. Two flame archetypes are investigated: one attached to the injector lip and the second one aerodynamically stabilized. A modeling approach for non-premixed flames is proposed and validated against experimental results. The flame structure and the flame stabilization mechanisms leading to the two flame types are scrutinized. The transition between the lifted and the attached flames is investigated.





### Évaluation expérimentale et numérique du potentiel de combustion du H2 : événements extrêmes dans des brûleurs prémélangés laminaires et stabilité de flamme dans des injecteurs swirlé nonprémélangé

### RÉSUMÉ

Ces dernières années, le changement climatique a fait l'objet d'un cri d'alarme et on a prédit un manque potentiel d'approvisionnement en énergie pour l'avenir. À cet égard, la communauté de la combustion est à la recherche de solutions abordables et durables pour résoudre ces problèmes. L'hydrogène vert est une alternative prometteuse pour décarboniser le mix énergétique actuel, puisqu'il peut être produit à partir d'électricité renouvelable. Néanmoins, son exploitation reste limitée en raison de ses caractéristiques de combustion uniques et la plupart des applications sont généralement limitées à 20%vol de H2 dans le mélange de carburant. Ce n'est que très récemment que nous avons assisté à la diffusion de nouvelles technologies qui permettent de maintenir une plus grande teneur en hydrogène. Dans cette optique, ce travail se concentre sur les aspects fondamentaux de la combustion de l'hydrogène en tant que partie de mélanges CH4/H2 ou pour des mélanges hydrogène-air purs, soit dans des flammes laminaires prémélangées, soit dans des conditions turbulentes non prémélangées. L'analyse de ces configurations est réalisée à l'aide d'outils expérimentaux et numériques afin de mettre en lumière les mécanismes fondamentaux liés à la combustion de l'hydrogène. Des expériences sont menées sur deux brûleurs pré-mélangés multiperforés, conçus à l'origine pour des mélanges méthane-air, afin d'évaluer les limites de la substitution de H2 et d'étudier les risques potentiels qui y sont associés. Les résultats sont présentés au moyen de cartes de stabilité et l'impact de l'ajout d'hydrogène sur les limites de blow-off et de retour de flamme est ensuite analysé. Les mesures révèlent différents régimes de retour de flamme et plusieurs mécanismes de déclenchement en fonction de la teneur en H2. Deuxièmement, une LES haute fidélité est utilisée pour étudier l'impact d'une injection centrale d'hydrogène sur la fonction de transfert de flamme d'une flamme tourbillonnaire prémélangée méthane-air. Cette étude, validée sur des résultats expérimentaux, montre que la zone de recirculation centrale (CRZ) répond à des fréquences d'oscillation spécifiques, subissant un mouvement axial prononcé qui module la pénétration du jet central d'hydrogène. Cette interaction avec la structure de la flamme et la position de la racine de la flamme interfère avec la perturbation générée par les tourbillons hydrodynamiques versés au bord de l'injecteur, expliquant la tendance du FTF. Enfin, des LES haute-fidélité sont présentées pour des flammes H2-air non-prémélangées stabilisées sur un nouvel injecteur pour turbine à gaz nommé HYLON. Deux archétypes de flammes sont étudiés: l'un attaché à la lèvre de l'injecteur et le second stabilisé de manière aérodynamique. Une approche de modélisation pour les flammes non prémélangées est proposée et validée par rapport aux résultats expérimentaux. La structure de la flamme et les mécanismes de stabilisation de la flamme conduisant aux deux types de flammes sont examinés. La transition entre les flammes soulevées et les flammes attachées est étudiée.

#### **Preface**

This work has been performed at the Institut de Mécanique des Fluides de Toulouse (IMFT) from October 2019 to December 2022. It has been supervised by Dr. Thierry Poinsot, Research Director at CNRS, and Prof. Thierry Schuller, professor at University Paul Sabatier. I was also deeply supported by Dr. Davide Laera, now Associate Professor at Polythechnic of Bari, and Dr. Laurent Selle, Research Director at CNRS.

During this period there have been fruitful collaborations with the Centre Européen de Recherche et de Formation Avancée en Calcul Scientique (CERFACS). I was also Co-Principal Investigator of the awarded PRACE project "WONDER", which granted in 2021 an allocation of 16 M CPUh. Furthermore, part of this work was performed in occasion of the CTR summer program of 2022 at Stanford University.

This led me to the following scientific production in peer reviewed international journals and a proceeding from the CTR summer program 2022:

- **–** A. Aniello, D. Schuster, P. Werner, J. F. Boussuge, M. Gatti, C. Mirat, L. Selle, T. Schuller, T. Poinsot, U. Rüde, **Comparison of a finite volume and two Lattice Boltzmann solvers for swirled confined flows**, *Computers and Fluids*, vol. 241, p. 105463, 2022.
- **–** A. Aniello, T. Poinsot, L. Selle, T. Schuller, **Hydrogen substitution of natural-gas in premixed burners and implications for blow-off and flashback limits**, *International Journal of Hydrogen Energy*, vol. 47, p.33067- 33081, 2022.
- **–** S. Marragou, H. Magnes, A. Aniello, L. Selle, T. Poinsot, T. Schuller, **Experimental analysis and theoretical lift-off criterion for H**2**/air flames stabilized on a dual swirl injector**, *Proceeding of the Combustion Institute*, 2022, https://doi.org/10.1016/j.proci.2022.07.255, in Press.
- **–** A. Aniello, D. Laera, L. Berger, A. Attili, T. Poinsot, **Introducing thermodiffusive effects in LES of turbulent combustion for lean hydrogen-air flames**, *Proceedings of the summer program*, 2022.
- **–** H. Pers, A. Aniello, F. Morisseau, T. Schuller, **Autoignition-induced flashback in hydrogen-enriched laminar premixed burners**, *International Journal of Hydrogen Energy*, 2022, https://doi.org/10.1016/j.ijhydene.2022.12.041, in Press.
- **–** A. Aniello, D. Laera, S. Marragou, H. Magnes, L. Selle, T. Schuller, T. Poinsot, **Experimental and numerical investigation of two flame stabilization regimes observed in a dual swirl H**2**-air coaxial injector**, *Combustion and Flame*, vol. 249, 112595, 2023.
- **–** A. Aniello, D. Laera, S. Marragou, T. Poinsot, T. Schuller, L. Selle, **Influence of pilot H**2 **injection on methane-air swirled flame stabilization and acoustic response**, *Combustion and Flame*, 2022, Submitted.
- **–** S. Marragou, H. Magnes, A. Aniello, T. Guiberti, L. Selle, T. Poinsot, T. Schuller, **Modeling the stabilization regime of**  $H_2$ **/air flames above a coaxial dual swirl injector**, *Combustion and Flame*, 2023, Submitted.

# <span id="page-8-0"></span>**Acknowledgements**

First of all, I want thank Prof. Heinz Pitsch and Dr. Benedetta Franzelli for reviewing this manuscript and for their valuable feedbacks. I want to thank also Prof. Luc Vervisch for being part of the examination committee.

I must express my gratitude to my directors and supervisors, who deeply supported me during the last three years. First of all, Dr. Thierry Poinsot, who believed in me and gave me the chance to join the research group at IMFT in the first place. Prof. Thierry Schuller, whose passion and commitment have been always contagious and inspirational. I am glad I had him on my side through this entire period at the laboratory. I must also thank Dr. Laurent Selle for the uncountable discussions that helped me improving all along this experience as person and as researcher. Last but not least, a special thank goes to Prof. Davide Laera, who has been an example to follow and who supported my work with relentless dedication. Overall, I feel lucky and proud I had the occasion to establish ordinary relations with extraordinary people.

A great thank to my colleagues and friends, with whom I had memorable experiences and that contributed to make my stay at IMFT unique! They have been a family far from home and I will always feel part of this group.

My stay at the lab could not be so special without the guys at the workshop and the entire IMFT staff, who have supported me with extreme professionalism since the beginning.

This work is dedicated to my family and especially to my loved grandfather.

# **Contents**







# <span id="page-14-1"></span>CHAPTER

# **Introduction**

#### **Overview**



## **1.1. Context of the work**

Combustion indicates the global exothermic chemical reactions that release heat and electromagnetic radiation starting from a mixture of fuel and oxidizer after the addition of an energy source. In the simplest case this reaction zone determines the existence of a well-defined flame front which separates unburnt and burnt gases. The reactants (eg.  $H_2$ ,  $CH_4$  and air) are characterized by a thermodynamic state and a certain degree of mixing, while the combustion products (e.g.,  $H_2O$ ,  $CO_2$ , NO*x*, soot) are at a temperature that depends on the initial mixture conditions and composition [\[1\]](#page-153-0).

#### **1.1.1. Combustion and society**

<span id="page-14-0"></span>Combustion processes have been exploited for more than a million years under different forms and have changed the course of humanity ever since. The turning point was the development of the efficient Watt steam engine in 1769, through which the transformation from thermal to mechanical energy drove the industrial revolution of the XIX century. These machines accelerated the development of the industrial and agricultural sectors posing the basis for the modern civilization. The availability of energy provided by fossil fuels coupled with technological improvements led to the economical *boom* after the second world war, allowed the countries with solid economies to thrive from generation to generation increasing exponentially their needs. As claimed by the International Energy Agency (IEA) this continuous growth was (and is) affected by several drivers like: the rise of the global population. gross domestic product (GDP) and the type of energy supply [\[2\]](#page-153-1). To this respect, Fig. [1.1\(](#page-14-1)a) shows the global primary energy consumption since 1800 underlining its

<span id="page-15-0"></span>

**Figure 1.1.** – (a) Evolution in time of the global primary energy demand by source with-out considering any efficiency factor for fossil fuel production [\[3\]](#page-153-2). (b) Evolution of  $CO<sub>2</sub>$  concentration during the last 800 000 years obtained via ice core gas analysis. Figures adapted from https://ourworldindata.org and https://climate.nasa.gov

strong reliance on hydrocarbons [\[3\]](#page-153-2). Till 1950 coal was the main fuel (other than traditional biomass) supporting the energy request, while both oil and gas increased their share of the market afterwards. Figure  $1.1(a)$  $1.1(a)$  shows also that the current rate of growth of the renewable energies (and nuclear power) is insufficient to balance the annual raise of the global energy demand and fossil fuels keep contributing to roughly 90% of it. According to the report published by the World Resources Institute in 2016, 33% of this consumption is attributed to the industrial sector. Aviation, shipping and road transport account for 2.6%, 2.3% and 16.3% respectively. Finally, the use of fossil fuels in residential and commercial buildings contribute for an additional 23.9% and the remaining part consists of fugitive emissions and unallocated fuel combustion.

#### **1.1.2. Global warming**

The combustion of fossil fuels is responsible of roughly 80% of the global Green House Gases (GHG) emissions. Figure [1.1\(](#page-14-1)b) shows the evolution of the  $CO<sub>2</sub>$  concentration in the atmosphere during the last 800 000 years. Measurements have been obtained considering ice core analysis on samples belonging to different geo-



<span id="page-16-1"></span>**Figure 1.2.** – Consumption-based  $CO<sub>2</sub>$  emissions per capita vs GDP per capita in 2020. GDP per capita is adjusted for price differences between countries and over time (https://ourworldindata.org)

logical eras. The results show that the level of  $CO<sub>2</sub>$  emissions has always remained constant before increasing relentlessly since the industrial revolution. This accumulation of  $CO<sub>2</sub>$  driven by the combustion of fossil fuels is promoting irreversible global warming.

Moreover, it is worth noting that the contribution of the single nations to the environmental problem is not equally distributed. Figure [1.2](#page-15-0) shows the relation between the per capita consumption-based  $CO<sub>2</sub>$  emissions against the GDP per capita in US dollar (\$) for several countries. These data are based on the research conducted by Global Carbon Project, UN Population, World Bank (2017) and put in evidence a dual problem. On one hand, rich countries  $(GDP > $ 15,000)$  with free access to energy produce much more equivalent  $CO<sub>2</sub>$  with respect to the global average of  $4.8t$  CO<sub>2</sub> per capita. In this case emissions increase linearly with the GDP and the comparison between rich and poor countries is shocking: the richest  $1\%$  in the EU contribute roughly 9 times more to the global emissions than the average. In other words, the easy access to energy is a driver for its exploitation to guarantee comforts of the modern life, demonstrating that richer countries are responsible for endangering the ecosystem and wellbeing of current and future generations. In fact, despite countries like France or Sweden (bottom part of the rich side in Fig. [1.2\)](#page-15-0) have decarbonized their energy mix significantly thanks to renewable sources or nuclear energy, the majority of the dominant economies are still heavily based on fossil fuels.

<span id="page-16-0"></span>On the other hand of the problem, poor countries are affected by financial, structural and technological limitations that prevent the access to energy (see left side of Fig. [1.2\)](#page-15-0). The minimum services are not granted and the populations rely on primitive solid energy source (e.g., wood) without any control on the localized indoor air pollution, which is considered responsible for 1.6 millions deaths each year worldwide. Clearly, the only solution to these problems are represented by scalable alternatives to fossil fuels that are sustainable, safe and affordable.

Recent years have seen unprecedented political and economical actions to cooperate globally in the framework of a sustainable development, without forgetting the necessity to support under-developed countries and eliminate poverty in the long <span id="page-17-0"></span>term scenario. One example is the Paris agreement signed in 2015 by 196 Countries around the world with the objective to limit the mean world temperature increase below 1.5  $\degree$ C with respect to the pre-industrialization period. The combined effort of governments, industrial partners and research community defined the initiatives and the milestones needed to limit GHG emissions, like: the ban of future development based on fossil fuel, decarbonization of energy carriers, electrification of heating and transports, funding for renewables and zero-carbon-ready technologies. Unfortunately, limiting the global warming to 1.5  $\rm{^{\circ}C}$  would require negative  $\rm{CO}_2$  emissions by 2070, which seems more utopic than realistic. The only encouraging counterpart of the current situation, though, is that several countries that pollute the most such as China and Australia, are also the countries that invest the most in technological innovation to limit GHG emissions, like shown in Fig. [1.3.](#page-16-1) It shows the change in low-carbon intensity of the energy generated in different countries with respect to the previous year.



**Figure 1.3. –** Annual percentage change in low-carbon energy generation, 2021 (https://ourworldindata.org).

### **1.1.3. Renewable energy carriers**

The decarbonization of the energy sector translates in the necessity to develop sustainable energy mix for the future. To this regard, the [International Renewable](https://www.irena.org) [Energy Agency \(IRENA\)](https://www.irena.org) considered established socio-economic, technological and geopolitical trends around the world to predict the shifts in the value of trade in energy commodities between 2020 and 2050 (see Fig. [1.4\)](#page-17-0). According to it, coal will disappear and the trading market for oil and gas are expected to shrink substantially in the next 30 years. Bioenergy will cover the largest chunk of the global trading, while the electricity market will triple with respect to 2020. Nevertheless, combustion will play an essential role in the future of the energy consumption and both ammonia and *green* hydrogen are expected to play a central role from this perspective.

*Green* hydrogen, in particular, is a carbon-free fuel that could be produced from



**Figure 1.4.** – Figure taken from IRENA: Geopolitics of the energy transformation. Shifts in the value of trade in energy commodities, 2020 to 2050.

<span id="page-18-0"></span>renewable energies via electrolysis in order to eliminate both direct and indirect  $CO<sub>2</sub>$ equivalent emissions. It can be produced from peaks of renewable energy production and use it as energy vector for later exploitation. For many countries it is also very attractive as a pure economical asset. In fact, while the fossil fuels trading is led by the few countries that own the natural sources, *green* hydrogen could be produced and sold by any country with an optimal combination of abundant renewable energy production and access to water. The production chain, in this case, would not be based on extraction but on conversion. Hence, developed countries that are massively dependent on external supply of fossil fuels see it as an opportunity to reduce their energetic dependence that could be catastrophic in case of political and social instabilities.

<span id="page-18-1"></span>EU, rather dependent on external energy supply, is particularly active from this perspective with an average annual funding of 4.56 USD Billion potentially available for  $H_2$  projects in the next decades. According to BloombergNEF, this corresponds to twice the investment claimed in Australia and almost ten times the one forecasted in US. To this respect, one of the main initiative in Europe is the [Clean Hydro](https://european-union.europa.eu/institutions-law-budget/institutions-and-bodies/institutions-and-bodies-profiles/clean-hydrogen-joint-undertaking_en)[gen Joint Undertaking \(FCH JU\),](https://european-union.europa.eu/institutions-law-budget/institutions-and-bodies/institutions-and-bodies-profiles/clean-hydrogen-joint-undertaking_en) a european public-private partnership made of research organization and industry that aims at supporting the technological development and demonstration activities to enable  $H_2$  technologies and accelerating their market introduction since 2008. Sectors of interest include residential and commercial heating, transport and electric power generation which, as described above, have a large contribution to the global GHG emissions. The [Testing Hydrogen ad](https://thyga-project.eu)[mixture for Gas Applications \(Thyga\)](https://thyga-project.eu) project, for instance, has the objective to set benchmarks and certification protocols in order to increase the  $H<sub>2</sub>$  volume content in natural gas appliances for domestic and commercial use. As discussed in the following chapters, hydrogen cannot simply replace standard hydrocarbons and clear recommendation for manufacturers and end-users are needed. This is relevant in the context of Power to Gas (PTG) where  $H_2$  is injected in the current gas network to provide a direct decarbonization of combustion processes (i.e., Hy-Net project in UK). Another European ambitious project is [Clean Sky,](https://clean-aviation.eu/clean-sky-2/programme-overview-and-structure) a feasibility study to adopt  $H_2$  thermal propulsion for the aviation sector based on the collaboration among international partners. Results underlined that medium and long range aircraft are the better suited for  $H_2$  turbine propulsion and that a shift from kerosene to hydro-

<span id="page-19-1"></span>gen would provide a climate impact reduction around 55% with a cost penalty of approximately 35%. Following this momentum, Airbus launched the [Zeroe](https://www.airbus.com/en/innovation/zero-emission/hydrogen/zeroe) project announcing a multi-year demonstrator program to produce the first  $H_2$  powered zero-emissions commercial aircraft by 2035. Furthermore, since aeronautical and land-based gas turbine applications rely on similar combustion technologies, it is not surprising that the main manufacturers for electric power generation compete with each other to deliver the first full-H<sub>2</sub> system compliant with safety and pollution standards. On one side we assist to the retrofit of existing concepts with alternative combustion strategies and additional aftertreatment systems [\[4,](#page-153-3) [5,](#page-153-4) [6\]](#page-153-5) in order to accomodate high  $H_2$  additions in the fuel blend. On the other side there is a push for new technologies suitable for pure-hydrogen combustion for a medium-long term implementation [\[7,](#page-153-6) [8\]](#page-153-7).

To sum up, combustion remains crucial to supply the energy demand worldwide. For this reason, it urges decarbonizing these processes to contrast climate change, to guarantee energetic independence and to support sustainable developments of emerging countries without compromising the wellbeing of future generations. In this context, *green* hydrogen is one of the most promising alternative since its production can be integrated to renewables to eliminate direct and passive  $CO<sub>2</sub>$  emissions. However, there is still a long way to go. In the following sections the complexity of its use will be highlighted putting in evidence the importance of investing in research and innovations to favor its exploitation.

### **1.2. Challenges of H<sub>2</sub> combustion**

This section introduces the main characteristics of hydrogen combustion that distinguish it from other fuels.

#### **1.2.1. Low density fuel**

An important quality of fuels is their Lower Heating Value (LHV), which is the measure of the heat produced by the complete adiabatic combustion of unit mass of fuel. The LHV of hydrogen is about  $121 \text{ MJ/Kg}$ , roughly three times larger than methane (50 MJ/Kg) or kerosene (43 MJ/Kg). This means that in principle it has the potential to deliver a greater amount of energy than classic fuels. However, in normal conditions the  $H_2$  density is only 0.08375 Kg/m<sup>3</sup> and its energy density drops below the one of standard hydrocarbons (see Fig. [1.5\)](#page-19-1).

<span id="page-19-0"></span>For this reason, in applications that require to minimize the energy density, hydrogen is stored in liquid phase under cryogenic conditions (i.e. spacecraft tanks [\[9,](#page-153-8) [10\]](#page-153-9)). However, this process is too difficult and expensive to be used in large scale applications. Hence, when hydrogen needs to be distributed over long distances, this would be rather done using the existing gas network (i.e. Power-to-Gas approach). Even in this case though, the exploitation of hydrogen raises several concerns. One of the main issues is related to the composition of the gas itself. In this regard, EU laws and regulations standardize the limit of relative density for gases that are transmitted, injected into/from storages, distributed and utilized [\(EN16726\).](https://www.cdfa.ca.gov/dms/pdfs/regulations/NG-AnnexA_Title_and_pp9-30.pdf) The injection of hydrogen into the gas network reduces the relative density of the fuel blend modifying the *quality* of the gaseous mixture, which may not fulfill the requirement of the legislation. To prevent this risk, the Wobbe index  $I_W$  is generally used to determine the fuel interchangeability in existing burners without compromising their correct functionality [\[11,](#page-153-10) [12\]](#page-153-11). A constant  $I_W$  ensures that the same injector with fixed pres-

<span id="page-20-1"></span>

**Figure 1.5.** – Relations between energy density and specific energy for metal fuels (red), hydrocarbon (black) and hydrogen (blue).

sure drop delivers the same energy content through the same exit nozzle diameter, irrespective of the mixture composition. It is for this reason that the EASEE-gas Common Business Practice from 2005 fixes the minimum and maximum allowable Wobbe index  $I_W$  to 48.96 MJ/Kg and 56.92 MJ/Kg, respectively in EU. According to these thresholds, the amount of hydrogen that can be safely added to natural gas network without requiring any modification of the systems [\[13\]](#page-154-0) varies normally between 15%vol and 20%vol. Nevertheless, it must be said that the Wobbe index is only a global parameter, not sufficient to guarantee the correct operability of a generic burner. In fact, it does not consider the specific combustion characteristics of the different fuels that can be blended together. This simple approach can be tolerated when similar hydrocarbons are mixed together, but  $H_2$  properties deviate consistently from the ones of common fuels [\[14\]](#page-154-1) and could lead to unexpected issues independently of the Wobbe Index [\[15\]](#page-154-2). In the following some of these specific aspects of  $H_2$  combustion are briefly introduced.

#### **1.2.2. Large burning rate**

<span id="page-20-0"></span>Hydrogen is characterized by a greater reactivity with respect to common hydrocarbons and this is illustrated for example in Fig. [1.6.](#page-20-1) It shows the laminar burning velocity  $S<sup>0</sup><sub>L</sub>$  (a) and the flame adiabatic temperature  $T<sub>ad</sub>$  (b) against the equivalence ratio for  $\mathrm{H}_2/\mathrm{CH}_4$ -air mixtures varying the hydrogen content in the fuel blend  $\mathrm{P}_{H_2}^{-1}$  $\mathrm{P}_{H_2}^{-1}$  $\mathrm{P}_{H_2}^{-1}$ . Data are obtained using the 1D free-flame solver CANTERA with GRI3.0 chemical mechanism including 53 species and 325 reactions. As widely demonstrated in literature [\[16,](#page-154-3) [17,](#page-154-4) [18,](#page-154-5) [19,](#page-154-6) [20\]](#page-154-7), hydrogen admixture to hydrocarbon fuels increases greatly the laminar burning velocity and the adiabatic flame temperature. At stoichiometric conditions, for example, the consumption speed of H<sub>2</sub>-air mixtures is an order of magnitude larger than the methane case and the adiabatic flame temperature increases by more than 150 K (see Fig. [1.6](#page-20-1) (b)).

Moreover, Fig. [1.6](#page-20-1) shows that increasing the hydrogen content  $P_{H_2}$  in the fuel blend, shifts gradually the maximum  $S<sub>L</sub><sup>0</sup>$  towards higher equivalence ratios. This

<sup>1.</sup>  $P_{H_2}$  defines the percentage of the total thermal power  $P_{th}$  provided by hydrogen oxydation and will be discussed extensively in the next chapter of the manuscript

<span id="page-21-0"></span>

**Figure 1.6.** – Laminar burning velocity  $S_L^0$  (a) and adiabatic flame temperature  $T_{ad}$  (b) against the equivalence ratio  $\phi_g$  from pure CH<sub>4</sub>-air to pure H<sub>2</sub>-air mixtures.

trend is accompanied by a continuous broadening of the flammability limits with  $H_2$ enrichment: CH<sub>4</sub>-air mixtures ( $P_{H_2}=0\%$ ) can burn up to the equivalence ratio  $\phi =$ 2.5, while pure hydrogen flames ( $P_{H_2}=100\%$ ) allow to sustain combustion above  $\phi =$ 8. These results are corroborated by several experimental studies [\[18,](#page-154-5) [20,](#page-154-7) [21,](#page-154-8) [22\]](#page-154-9) that proposed empirical relations to describe the variation of  $S<sup>0</sup><sub>L</sub>$  as function of the H<sub>2</sub>enrichment in hydrocarbon mixtures. It must be underlined that all these properties correspond to freely propagating 1D adiabatic flames and, despite they do not take into account multi-dimensional effects, they are extremely useful to understand the global characteristics of a combustible mixture.

From a practical perspective, the growth of the mixture reactivity due to hydrogen addition must be considered and understood to anticipate potential problems that could arise in combustion systems. For instance, the addition of hydrogen in premixed burners increases the risk of flashback [\[23,](#page-154-10) [24\]](#page-154-11), which could cause the system failure [\[25,](#page-154-12) [26,](#page-154-13) [27\]](#page-155-0) like the ones seen in Fig  $1.7(a)$  $1.7(a)$ , and represents today one of the main safety concerns that limits the spreading of hydrogen premixed combustion technologies. Moreover, due to this general enhancement of the flame speed, H2 enriched flames are more compact [\[28\]](#page-155-1) than hydrocarbon flames at comparable flow Reynolds numbers. This reduction of the flame length affects the flame dynamics and can potentially change the thermo-acoustic behavior of the combustor [\[29,](#page-155-2) [30\]](#page-155-3). These modifications could lead to destructive consequences on the systems as shown for instance in Fig [1.7\(](#page-21-0)b-c). Also, the increased reactivity of  $H_2$  facilitates the anchoring of the flame to the nozzle and concur to increase the thermal stress on the burner components. All these aspects affect both the shape and the stabilization mechanism of the flames, which may affect the burner performances in terms of durability, stability and pollutant emissions [\[31\]](#page-155-4).

#### **1.2.3. Low Lewis number**

Another specific characteristic of hydrogen is the large difference between the molecular diffusivity and the thermal diffusivity, which results in a fuel Lewis number smaller than unity. This is a crucial variation with respect to classical hydrocarbons, which generally exhibit Lewis numbers near unity or above [\[33\]](#page-155-5). Molecular transport properties play an important role in multi-dimensional combustion problems and can influence the flame characteristics. In this respect, literature proposes different relations to define an effective Lewis number  $Le<sub>eff</sub>$  of the mixtures [\[34,](#page-155-6) [35,](#page-155-7) [36\]](#page-155-8) in order to predict and interpret these variations of the flame behavior as function of

<span id="page-22-1"></span>

**Figure 1.7.** – Figures taken from [\[32\]](#page-155-9). Damaged injector due to high temperatures generated by flame flashback (a). Combustion instabilities create pressure and velocity oscillations that can ruin either the injection system (b) or the 1st turbine stage downstream the combustion chamber (c).

the transport properties. The latter can influence the flame extinction [\[37,](#page-155-10) [38\]](#page-155-11), local burning rate and stretch response [\[39\]](#page-155-12). For example, it is well known that the flame response to stretch  $\kappa$  in lean premixed flames depends directly on the Lewis number of the deficient reactant (fuel) and asymptotic developments in the low stretch limit demonstrated the following relation [\[40\]](#page-155-13):

$$
\frac{S_L^{str}}{S_L^0} = 1 - Ma_b Ka.
$$
\n(1.1)

where the extent of the stretch is represented by a reduced Karlovitz number *Ka* and the type of response of the flame to the stretch is governed by the Markstein number  $M_{a}$ <sup>[2](#page-3-2)</sup>. The linear relation suggests that, under the hypothesis of positive stretch, the flame speed increases with stretch for  $Le_{eff} < 1$  ( $Ma_b < 0$ ) and it is reduced in case of  $Le_{eff} > 1$  ( $Ma_b > 0$ ). Considering for example that the Lewis number of  $H_2$  and  $CH_4$  are approximately 0.3 and 1.0 respectively, a variation of the flame behavior must be expected.

Despite the simplification of the analytical development, this tendency of hydrogen mixture has been corroborated by experiments for several types of flame and for different fuel blends. For example,  $H_2$ -air outwardly propagating flames at different equivalence ratios (i.e for different effective Lewis number  $Le_{eff}$ ) were investigated to put in evidence the influence of the stretch on the flame structure [\[42\]](#page-156-0). Results show that at  $\phi = 0.4$  (*Le<sub>eff</sub>* < 1) a positive stretch promotes higher flame speed, greater adiabatic flame temperature T*ad* and larger production of OH, H and O radicals in comparison to the planar unstretched flame. The reaction rate is boosted in this case. When the  $Le_{eff}$  is higher than 1 ( $\phi = 1.4$ ), instead, the flame speed, the burnt gas temperature and the radicals production decrease under positive stretch. Similar results were found in a combined experimental-numerical study [\[43\]](#page-156-1), confirming the global results of the asymptotic analysis. These effects were also observed in turbulent swirled premixed flames powered by  $\rm CH_4/H_2$  blends [\[44\]](#page-156-2). In this particular case, the increased stretch resistance due to  $H_2$  addition was considered responsible for the transition from V-shape to M-shape flames. The enhancement of the stretch resistance due to  $H_2$  enrichment of  $CH_4$ -air mixtures is also determinant in autoignition measurements [\[45\]](#page-156-3). Hydrogen flame response to stretch can be highly different from standard fuels at comparable equivalence ratio and this can affect

<span id="page-22-0"></span><sup>2.</sup> Markestein number are indicated as  $Ma_b$  and  $Ma_u$  when calculated with respect to the burnt or unburnt gases, respectively

<span id="page-23-0"></span>

**Figure 1.8.** – Figure taken from [\[41\]](#page-155-14). Direct photographs of bunsen flames stabilized over a 10 mm diameter tube for different air-fuel mixtures: (a) rich propane-air at  $\phi_g = 1.38$ ; (b) lean propane-air at  $\phi_g = 0.53$ ; (c) rich methane-air at  $\phi_g = 1.52$ ; (d) lean methane-air at  $\phi_g = 0.58$ . Rich and lean methane-air flames are characterized by  $Le_{eff} \approx 1$ , hence there is not any specific burning rate variation between the flame tip and the flame sides. Propane mixtures exhibit  $Le_{eff}$  < 1 when rich and  $Le_{eff}$  > 1 when lean, reason for which it results in tip opening in the first case.

flame stabilization and the flame behavior.

The non-equidiffusion in hydrogen mixtures also makes the flame structure dependent on the curvature of the reaction front. Note that this is not the case for fuels characterized by unity *Le* number such as methane. For example, in lean premixed H<sub>2</sub>-air bunsen flames, the preferential diffusion can generate *tip-opening*. When the flame is concave with respect to the reactants, the high molecular mass diffusion defocuses hydrogen from the concave tip towards the nearby convex region, reducing the local fuel concentration. If the local conditions fall off the flammability region, the flame quenches locally [\[46\]](#page-156-4). Note that this phenomenon is piloted by the Lewis number of the deficient reactant and has been both in lean  $H_2$  flames, but also for rich  $C_3H_8$ -air mixtures ( $Le_{eff}$  < 1) [\[41\]](#page-155-14) as illustrated in Fig. [1.8.](#page-22-1) This phenomenon is then of interest even for other fuels than hydrogen. However, while rich propane mixtures are not of critical technical interest, lean hydrogen-air flames seem to be crucial for a wide range of future applications.

#### **1.2.4. Intrinsic instabilities**

Lewis number effects are also responsible for the occurrence of thermo-diffusive instabilities undergone by propagating non-planar flame fronts. According to this phenomenon, the initial corrugation of a planar reaction layer is self-amplified. The driving mechanism is the same leading to the flame *tip-opening* described above. When the planar flame gets wrinkled by local and transient disturbances, the concave parts reduce their reactivity, while the convex ones increase the burning rate and the initial perturbation of the flame front grows. On the other side, mixtures at  $Le<sub>eff</sub>$  > 1 suppress this growth acting in the exact opposite way. In the first case the propagating flame develops a cellular structure, while in the second case the flame



**Figure 1.9.** – Figure adapted from [\[35\]](#page-155-7). Schlieren pictures of hydrogen ( $\alpha = 0.00$ ), hydrogen–propane mixtures ( $\alpha$  equals 0.25, 0.50, and 0.75), and propane ( $\alpha$  = 1.00) in air at 5 atm and at an overall equivalence ratio of 0.80. Important flame properties are tabulated, and  $t_{\alpha}$  indicates the time in microseconds for different  $\alpha$ .

<span id="page-24-0"></span>front remains flat. This phenomenon has been largely investigated in outwardly propagating flames and Fig. [1.9,](#page-23-0) taken from [\[35\]](#page-155-7), shows an example of spherical expanding flames for three combustible mixtures characterized by different effective Lewis number lower than unity. Initially the flame surface shows big cracks provoked by the ignition and when the radius reaches the critical length R*cr*, we assist to the formation of cellular structure due to thermo-diffusive instabilities  $[35, 47]$  $[35, 47]$ . It was also shown that small flame thicknesses promote the onset of thermodiffusive insta-bilities [\[35\]](#page-155-7), while increasing the stretch may have a stabilization effect, inhibiting the formation of cellular structures [\[48\]](#page-156-6). These cellular structures increase the flame surface, excercising similar effects as turbulence. In view of these similarities, Law et al. [\[35\]](#page-155-7) proposed to define this capacity of the flame surface to wrinkle itself in absence of turbulence as *autoturbulization*.

Recent Direct Numerical Simulations (DNS) of laminar hydrogen flames [\[49,](#page-156-7) [50\]](#page-156-8) have been performed with the objective to study the effect of thermo-diffusive instabilities on flame speed propagation and evaluate the growth of the instabilities for different mixture, temperature and pressure. The results correlate qualitatively well with previous theoretical results describing the growth rate of reaction layer instabilities as function of the wavenumber of the initial perturbation [\[51\]](#page-156-9). These numerical works also unveiled the dependence of thermodiffusive instabilities on fundamental flame properties like: the Zeldovich number *Ze*, the volumetric expansion ratio  $\sigma$  between burnt and fresh gas, the Markstein length  $L_{Ma}$ , effective Lewis number *Leeff* and Peclet number *Pe*. In light of these results the authors exploit DNS results to propose a relation to describe the dependence of the effective laminar flame consumption speed on these parameters [\[49,](#page-156-7) [50,](#page-156-8) [52\]](#page-156-10). A parallel numerical work [\[53\]](#page-156-11) demonstrated that the destabilizing parameters proposed in asymptotic theory [\[51\]](#page-156-9) correlate well with the onset of the thermodiffusive instabilities found in DNS of lean laminar  $H_2$  flames. This set of simulations also identified a pressure ridge: fixing the equivalence ratio  $\phi$  and the temperature of the unburned mixture  $T_u$ , there exists a preferential pressure at which these intrinsic instabilities are maximized. Interestingly both numerical works have shown that low Lewis number effects may increase the laminar unstretched consumption speed by a factor  $2$ , which is of interest from practical perspective. Extracting data from 2D DNS allows to expand the knowledge of such phenomena under controlled conditions. Moreover, they can contribute to build Large Eddy Simulations combustion models that embed the physics of these intrinsic instabilities to simulate with accuracy cases that are too expensive to be computed via DNS. This is extremely relevant since several studies demonstrated that thermodiffusive instabilities might play a primary role even in turbulent flows [\[54,](#page-156-12) [55\]](#page-156-13) and this is somehow counterintuitive. In fact, thermodiffusive effects arise from a disparity between the molecular mass diffusion and molecular thermal diffusion. In high Reynolds number flow, molecular transport should be negligible with respect to the transport generated by turbulence and the Lewis effects should vanish. Nevertheless, results seem to go in the opposite direction and recent studies suggest a non linear interaction between turbulence induced wrinkling and intrinsic instabilities [\[55\]](#page-156-13). Note that the manner with which small turbulent scales should interact with thermo-diffusive scales is still an open issue in the combustion community and further work will be needed.

#### <span id="page-25-0"></span>**1.2.5. Low activation energy**

The large reactivity of hydrogen also favors spontaneous ignition [\[14,](#page-154-1) [56,](#page-157-0) [57\]](#page-157-1). Understanding the physical details of this phenomenon under different thermodynamic and chemical conditions is essential to prevent accidents that could potentially lead to flame detonation. In case of hydrogen the crossover temperature  $(T_c \approx 950 \text{ K})$ , defined as the value at which the rate of consumption of H radicals by third body reactions is compensated by the production of H radicals by the main chain branching reactions, defines which kind of autoignition mechanism would prevail. Above this temperature the ignition is driven by chain branching explosion reactions involving H, O and OH radicals [\[14,](#page-154-1) [58,](#page-157-2) [59\]](#page-157-3) and is characterized by a vigorous uniform ignition that can potentially lead to detonation. Below the cross-over temperature, instead, autoignition is governed by low activation energy reactions involving  $HO_2$  and  $H_2O_2$  [\[14,](#page-154-1) [60\]](#page-157-4) and autoignition is mainly non-homogeneous [\[59\]](#page-157-3). With the objective of developing practical relations to predict autoignition of  $H_2$ -air mixtures, several theoretical works attempted to derive explicit formula to estimate the autoignition time delay (induction time) of hydrogen-oxygen-inert mixtures for temperatures below [\[61\]](#page-157-5) and above [\[58\]](#page-157-2) the crossover.

Moreover, experiments have demonstrated that the flow conditions, the turbulence level, the heat flux at the wall as well as the local molecular diffusion can affect the final result and they are not all included in these formulations. From safety perspective is certainly interesting to understand the characteristics of ignition when H2-air mixtures are exposed to a hot surface, which is a practical situation that is encountered in several burner and combustion chamber designs. Experiments on H2 air mixtures evidence that, contrary to standard fossil fuels, lean mixtures require lower surface temperature for ignition [\[62\]](#page-157-6) and that reducing the equivalence ratio towards the low flammability limits can trigger different ignition mechanisms [\[63\]](#page-157-7). In view of the high hydrogen reactivity, one could think to use it in order to promote ignition of slower reacting mixtures [\[45,](#page-156-3) [64\]](#page-157-8). Interestingly though, this is not always the case. At high pressure (above  $5 \text{ bar}$ ), hydrogen exhibits an inhibitive effect on the ignition of methane-air mixtures [\[45\]](#page-156-3). Pressure, in fact, promotes third body reactions that increase the crossover temperature, retarding the ignition of pure H2 flames [\[14\]](#page-154-1). This result is particularly relevant considering that some real applications work above atmospheric pressure and should always be considered to examine this type of problems.

# **1.3. Contribution of the thesis**

This work focuses on the fundamentals of  $H_2$  combustion, either as part of  $CH_4/H_2$ blends or for pure hydrogen-air mixtures in laminar premixed flames or in turbulent non-premixed flames resulting from a separated injection of hydrogen and oxidizer into the combustion chamber. The first are relevant for example in condensing boiler applications, the second ones are of technical interest for gas turbines. The analysis of these configurations is performed via both experimental and numerical tools to shed light on H2-related combustion mechanisms encountered in lab-scale configurations. The main contributions can be synthesized as:

- **Development of the experimental bench CoMix:** the bench was developed in the framework of the ERC grant SCIROCCO to investigate violent dynamics (i.e. flashback) in  $H_2$ -enriched and pure- $H_2$  laminar flames. The bench, designed to maximize its flexibility in terms of geometry and operating conditions, is suitable to: (1) test the impact of  $H_2$  addition in commercial burners, (2) run fundamental experiments to analyze flashback events, (3) investigate the thermo-acoustic behavior of  $H_2$  laminar premixed flames.
- **Impact of H**2 **substitution on premixed burner operability:** the objective is to identify the physical mechanisms that limit the  $H_2$  volume fraction that can be safely injected in existing systems. This work tackles the problem of firing two premixed multi-perforated burners, designed for natural gas, with increasing  $H_2$  content. On one side, experiments show that Lewis effects may contribute to extend the blow-off limit towards ultra-lean mixtures when the H2 content increases. On the other side, several flashback regimes are identified and analyzed, putting in evidence factors of practical importance to limit risks associated to the use of  $H_2$  in commercial application and providing a novel insight for future developments.
- $-$  Impact of  $\mathbf{H}_2$  on the flame response to acoustic disturbances: pilot  $\mathbf{H}_2$ injection changes the acoustic response of perfectly premixed CH4-air swirling flames. A numerical setup is developed in order to reproduce accurately the gain and phase of the Flame Transfer Function of a fully premixed CH4-air

<span id="page-27-0"></span>flame and with the addition of a central  $H_2$  injection. It was shown that the Central Recirculation Zone responds to specific oscillation frequencies undergoing a pronounced axial oscillation that modulates the penetration of the hydrogen central jet. This interaction affects the structure and the position of the flame root and it interferes with the the perturbation generated by the hydrodynamic eddies shedded at the injector rim, affecting the resulting FTF gain. The analysis shows that, while the perfectly premixed  $CH<sub>4</sub>$ -air flame is entirely dominated by the flame tip dynamics, the H<sub>2</sub> piloted flames exhibit an out-of-phase contribution of several flame regions at specific frequencies that weakens its response to incoming flow disturbances.

**– Stabilization mechanisms in H**2**-air non-premixed swirling flames:** simulations have been performed to support and optimize the design of the HYdrogen LOw  $NO<sub>x</sub>$  injector [\[65\]](#page-157-9), in which different flame archetypes were observed. LES put in evidence the mechanisms governing two different flame stabilizations, (1) a flame attached to the injector lips and (2) an aerodynamicallystabilized flame. The analysis of the flame structures highlights that diffusion, rich premixed and lean premixed flame branches coexist.

# **1.4. Outline of the manuscript**

The manuscript is organized in three main parts. The first one (I) considers experimental activities on condensing boiler burners. The rest of the work focuses on high-fidelity LES: part II investigates the effect of  $H_2$  pilot injection on flame dynamics of methane-air swirled flames and part III analyzes flame stabilization in a novel H2-air swirling injector.



**Figure 1.10.** – Visual outline of the manuscript.

# **Part I.**

# **Experimental investigation of laminar premixed flames: CoMIX burner.**

# <span id="page-32-0"></span>**Presentation of the test rig CoMix**

This section describes the characteristics of the CoMix test bench, which has been developed in the framework of the ERC grant SCIROCCO at IMFT with the objective to study  $H_2$ -enriched flames in laminar premixed conditions. The design of the rig was thought to maximize the flexibility of the system in terms of geometry, operating conditions, probes location and optical access allowing then to test several types of burners and injectors. The test rig is used in the next chapter to assess the stabilization limits of laminar premixed burners for different levels of hydrogen substitution focusing on flashback and blow-off phenomena.

Even though not described in this manuscript, this test rig has been used as basis in companion works to scrutinize several flashback regimes identified in Chapter [3](#page-37-0) and to analyze thermo-acoustic instabilities in condensing boiler applications.

#### **Overview**



# **2.1. Description of the test bench**

The CoMix test bench can be adapted to different kinds of injectors and burners depending on the targeted application. It is used in part I of the manuscript to investigate the impact of H<sub>2</sub>-enrichment on the stability of laminar premixed burners normally used in condensing boiler applications. The bench can be divided in two main parts, as illustrated in the axial cross section of Fig. [2.1:](#page-32-0) the lower one consists of the *main housing* and the upper one is made of the *bench head*. The *main housing* has a cylindrical shape with internal diameter of 100 mm, which is large enough to limit the flow Reynolds number even for high volumetric flow rates. Fuel and oxidizer mix directly into the supply lines, ensuring the injection of a fully premixed charge at the bottom of the bench. Here, there are 6 *injection holes* with a diameter of 20 mm to avoid compressibility effects (aerodynamic noise) inside the gas lines and through the nozzles. Entering the bottom part of the plenum, the mixture encounters a *perforated plate* with a substantial pressure drop that favors the homogenization of the flow over its entire cross section. Then, the mixture goes through a *honeycomb* element, which has the objective to brake the largest flow turbulent structures remaining downstream the *perforated plate*. In Fig. [2.1](#page-32-0) the *honeycomb* is located nearby an *adjustable component* with a length of 35 mm. This part can be also removed or replaced by another one of different length to add further probes or modify the acoustic properties of the plenum. The top part of



<span id="page-33-0"></span>**Figure 2.1.** – Axial section of the CoMix test bench comprehensive of the main housing and the bench head with the description of the components (a) and the main dimensions (b).

<span id="page-33-1"></span>the bench, named *main plenum* in Fig. [2.1\(](#page-32-0)a), offers different probe accesses: four are placed 50 mm below the *upper flange*, equally spaced by an angular distance of 90°. In the specific example of Fig. [2.1](#page-32-0) two diametrically opposed probes are named *probe 1* and *probe 2*. A third one is labeled in Fig. [2.1](#page-32-0) as *thermocouple* and could be used for example to control the local inlet temperature in case of mixture preheating. Additional ports are also located 50 mm below like the *probe 3*. The type of instrumentation can be changed using specific fittings according to the necessities of the experimental campaign. At the top of the *main plenum* is placed a metallic *porous disk* that acts as flame arrestor in case of flashback. This component can eventually be removed depending on the experiments conducted.

The *bench head* is made of a *convergent inlet* that supports the *burner* and the combustion chamber shown in the upper part of Fig. [2.1.](#page-32-0) The *convergent inlet* has the first objective to provide a smooth geometrical transition between the large cross section of the *main plenum* and the cylindrical cross section of the burner with a diameter of roughly 30 mm. The *convergent* is roughly 55 mm high with an external diameter of 80 mm, sufficiently large to support a squared combustion chamber. Moreover, this element offers four additional inclined ports equally spaced along the azimuthal direction to provide probe access to the combustion chamber. Two of these passages are displayed in Fig. [2.1](#page-32-0) and named *in-chamber probes*. These accesses allow to collect experimental signals such as acoustic pressure and temperature, which are used to characterize the thermal state of the burner or its acoustic behavior in case of

thermo-acoustic instabilities. On top of the *convergent* element is placed a squared combustion chamber that is 144 mm wide and 211.5 mm long. These dimensions are chosen because they are comparable to the ones of heat exchangers used in some commercial applications. The chamber outlet exhibits a contraction of the cross section area to increase the bulk flow velocity and prevent any reverse flow from the outlet. This avoids the entrainment of external air, which would bias temperature and emissions measurements at the burner outlet. The confinement is made of 4 quartz windows, which ensure a full optical access to the combustion region. The *quartz* components are sustained by 4 stainless steel pillars that can be equipped with additional ports to insert further probes along the vertical direction of the burner.

In addition to that, the bottom plate of the bench in Fig. [2.1](#page-32-0) can be replaced by a support for *loudspeaker* to study the acoustic response of the flow and the flames. This additional configuration, not shown here, is used in companion studies and it is not considered in this manuscript.

### <span id="page-34-0"></span>**2.2. Control of the gas supply**

The rig is designed to control independently the  $H_2$  substitution of methane, the global equivalence ratio and the total thermal power over a wide range of operating conditions. Four gases are used:

- $-$  Air, dried and filtered with a Atlas Copco filter with size equal to  $0.01 \mu m$ . Pumped at 7 bar via a GA 30 VSD compressor.
- **–** CH4, with a purity of 99.999% and stored in a bottle at 200 bar
- $-$  H<sub>2</sub>, with a purity of 99.995% and stored in a bottle at 200 bar
- **–** N2, with a purity of 99.999% and stored in a bottle at 200 bar

The mass flow rate of  $H_2$ , CH<sub>4</sub> and air are controlled separately using three Bronkhorst EL-FLOW mass flow controllers. Hydrogen and methane flow regulators are limited



**Figure 2.2.** – Schematic of the gas supply system with 4 external solenoid valves used for safety purposes, three flow regulators to control the mass flow rates of the reactants and the piping that redirect the combustible mixture towards the test bench.

<span id="page-35-1"></span>to 90 nL/min and 50 nL/min, respectively. These values correspond to a total input thermal power  $P_{th} = 42.5$  kW, of which 15 kW are supplied by  $H_2$  and 27.5 kW from  $CH<sub>4</sub>$ . The air mass flow regulator supplies a maximum flow rate of 700 nL/min, which is necessary to operate the burner at high air-excess ratio. Upstream each flow regulator there is a solenoid valve to provide a double security system in case of incident. These valves are "normally opened" and they are automatically closed if the system detect a risk such as flashback or high temperature of a critical component of the setup, inhibiting the supply of reactants. Simultaneously, the solenoid valve on the nitrogen line, "normally closed", would open in case of danger injecting inert gas to quench the reactions. A "T" element is used to mix fuels before being injected into a *mixing box* depicted in Fig. [2.2.](#page-33-1) Here, the fuel blend mixes with air and the flammable mixture is redirected towards the bench. For safety reasons, the mixture goes through an additional flame arrestor located between the *mixing box* in Fig. [2.2](#page-33-1) and the bench shown in Fig. [2.1,](#page-32-0) which acts as additional security measure to avoid upstream flame propagation. The pipe is then divided into six to feed the bottom of the burner. These additional systems are not shown here.

### <span id="page-35-0"></span>**2.3. Geometries of the burners**

The burners are installed on top of the convergent element as shown in Fig. [2.1.](#page-32-0) Figure [2.3](#page-35-0) illustrates two examples of the burners that can be tested with the CoMix test bench. These are used in condensing boiler applications and feature a cylindrical shape with a specific distribution of the holes above which a multitude of small flames can be stabilized. The two technologies presented here differ mainly because of the porosity of the external surface, the distribution and the size of the holes and their internal structure schematically represented in Fig. [2.3.](#page-35-0) It will be demonstrated in Chapter [3,](#page-37-0) that their internal structure and the geometry of the small outlets have a substantial impact on the flame stabilization and on the limit of the hydrogen substitution in the fuel blend.

The forced draft burners *B*1 and *B*2 used in this study are representative of two technologies used in residential condensing boilers and are designed to operate between 2 and 30 kW with natural gas. Figures [2.3\(](#page-35-0)a-b) display photos of the two burners with a sketch of their internal structure. They are made of stainless steel and feature similar sizes as shown in Tab. [2.1.](#page-35-1) They are roughly 90 mm high with an external diameter of roughly 70 mm. Nevertheless, the shape of the exit holes and their distribution over the multi-perforated surface are different. As illustrated in Fig. [2.3\(](#page-35-0)a), burner *B*1 is characterized by both round and slit holes. The first ones have 0.5 mm diameter with a pitch distance  $l = 2.5$  mm, while the slits are 4.0 mm long and 0.5 mm wide. Moreover, Fig. [2.3\(](#page-35-0)a) shows that the burner *B*1 features a double metallic internal layer that creates a U-turn at the upper side of the burner, which guides the flow through the exit holes.

For the burner *B*2 in Fig. [2.3\(](#page-35-0)b), instead, the exit holes are distributed following the repetition of the same geometrical pattern: two circular holes of 0.7 mm diameter and two lateral hollow slots. This pattern is reproduced periodically along the burner azimuthal and axial directions with a step of 6.7 mm and 7.2 mm, respectively. Since the apertures of the hollow slots point towards the circular holes, the structure of the flow at the flame base is more complex for the burner *B*2 than burner *B*1, but this aspect is not considered in the present study. Also, a swirler is used at the inlet of burner *B*2 that helps to homogenize the flow at the hole outlets all along the burner.
	$h_t$	R	
	(mm)	$\text{(mm)}$	
B1	95.0	70.4	
B2	92.0	69.7	

**Table 2.1.** – Dimensions  $(h_t, R)$  and external surface porosity  $(\sigma)$  values of burners B1 and B2 shown in Fig. [2.3.](#page-35-0)

These two designs result in different burner porosities  $\sigma_{B_1} = 8\%$  and  $\sigma_{B_2} = 3\%$ which, considering constant volumetric flow rate and gas inlet temperature, leads to



**Figure 2.3. –** Illustration of external and internal designs of the burners *B*1 (a) and *B*2 (b) with qualitative description of the evolution of the gas stream temperature inside the burners. The two zoom-boxes at the bottom of each image represent a detailed view of the exit hole pattern for each burner.

<span id="page-36-0"></span>

**Figure 2.4.** – Sketch of flame shape and stabilization when a single hole of the condensing boiler burner is submitted to increasing mean bulk flow velocity  $U_b$ . When  $U_b$  is relatively high (a) with respect to the laminar burning velocity  $S_L$ , the flame is elongated  $L_{fl}$  and the distance between the flame and the wall  $\eta$ increases. The heat load is moderate with a relatively low wall temperature. If the volumetric flow rate reduces (b) the flame gets shorter and closer to the burner wall. In this case the wall temperature  $T_w$  increases. When the bulk flow velocity decreases even more (c) the flame interaction with the wall becomes stronger, the flame is almost flat and the burner wall temperature raises.

<span id="page-37-0"></span>a strong difference in bulk flow velocities  $U_b^{B_1}$  $U_b^{B_1}$  and  $U_b^{B_2}$  $b^B$ <sup>through</sup> the holes:

$$
U_b^{B_2} = \frac{\sigma_{B_1}}{\sigma_{B_2}} U_b^{B_1} \simeq 2.7 U_b^{B_1}
$$
\n(2.1)

This definition of the bulk flow velocity does not account for the non-uniformity of the flow field along the burner or for the specific geometry of the outlets and must be considered as an average value. Furthermore, the porosity of the burner is a key parameter of its design since the it affects the volumetric flow rate through a single hole and ultimately changes the flame stabilization. As sketched in Fig. [2.4\(](#page-35-1)a), the length  $L_f$  of the flame and its distance  $\eta$  from the flame holder is mainly regulated by the competition between the mean bulk velocity  $U_b$  in a single hole and the laminar burning velocity  $S_L^0$ . When  $U_b$  reduces with respect to  $S_L^0$ , the flame gets shorter and closer to the burner wall, as in Fig. [2.4\(](#page-35-1)b). In this case the gap between the flame and the wall diminishes and the heat load on the wall grows, so that the temperature of the flame holder must increase. This raises the heat transfer between the hot flame holder and the combustible mixture, resulting in a double effect: on one side it increases the volumetric flow rate through the hole, on the other side it increases the reactivity of the combustible mixture flowing through the hole. The first increases  $U_b$  and the latter boosts the  $S_L^0$ , favoring also spontaneous ignition. It is demonstrated in Chapter [3](#page-37-0) that the wall temperature  $T_w$  is a key parameter to evaluate the flame stability and a controlling parameter for flashback in premixed systems.

Over the conditions investigated here, the pressure losses characterizing the two burners are comparable and limited between 20 Pa and 50 Pa for the operating conditions explored.

Eventually, Fig. [2.5](#page-36-0) shows an horizontal view of the burner *B*2 with a white arrow indicating a weld that develops all along the the axial direction of the burner. This weld is a result of the manifacturing process and produces a local increase of the azimuthal spacing among the columns of holes. The impact of this geometrical discontinuity of the burner outlets is also discussed in Chapter [3.](#page-37-0)



**Figure 2.5. –** Figure taken from [\[66\]](#page-157-0). of the burner *B*2 with a white arrow that put in evidence the location of the weld in the center of the image.

# CHAPTER  $\bullet$

# <span id="page-38-0"></span>**H**2 **substitution of natural-gas in multiperforated burners and implications for blow-off and flashback limits**

Two multi-perforated premixed burners, designed for natural gas, are fueled with increasing hydrogen content to assess the limits of  $H_2$  substitution and investigate potential risks associated to it. The burners feature a different design that affects flame stabilization and heat exchange between the fresh mixture and the hot burner walls. First, results are presented by means of stability maps that were collected at constant power and over a wide range of equivalence ratios, from pure methane-air to pure hydrogen-air mixtures. The impact of hydrogen substitution on blow-o and flashback limits is then analyzed. On one side, it is observed that hydrogen addition increases blow off resistance, extending the operating range towards ultralean conditions. On the other side, increasing the hydrogen enrichment of the fuel mixture raises the thermal load on the burner favoring flashback. It is shown that the competition between the bulk velocity through the burner holes and the laminar burning velocity is not a reliable parameter to predict flashback occurrence, while the thermal state of the burner represents a determining factor. An analysis of the thermal transient from ignition to flashback reveals a strict correspondence between the onset of flashback for a given mixture composition and the burner surface temperature. Results highlight the challenges linked to the design of fuelflexible systems, pointing out practical limits of  $H_2$  substitution in burners designed for natural gas.

# **Overview**





# **3.1. Motivations of the study**

In Chapter [1,](#page-13-0) it has been shown that, adding hydrogen to standard fuels modifies fundamental combustion characteristics [\[14\]](#page-154-0) and can compromise the fulfillment of safety and pollution standards [\[23,](#page-154-1) [24\]](#page-154-2). It was also mentioned that the burners designed for natural gas, can only sustain hydrogen concentrations from 5 to 20 %*vol* in the fuel blend. Even in the best scenarios, a hydrogen volume fraction of  $20\%$  would represent only 7% of specific mass reduction of  $CO<sub>2</sub>$  with respect to natural gas. Hence, to develop new burners able to accommodate higher hydrogen concentrations, there is a need for more fundamental studies to understand critical issues associated to its addition.

Commercial systems are not designed for research purposes and it is difficult to monitor and control separately basic variables to generalize results, such as the thermal power  $P_{th}$  and equivalence ratio  $\phi_q$ . Moreover, the variety of hardware and control systems available on the market adds further complexity to the evaluation of hydrogen effects. For example, several self-aspirating burners have been tested with increasing hydrogen content showing a variable  $H_2$  tolerance with a burner temperature that was barely affected in one case and augmented by more than  $60\%$ in the other [\[13,](#page-154-3) [67,](#page-157-1) [68\]](#page-157-2). In self-aspirating burners the mixture composition depends on the air velocity at the fuel nozzle outlet, which creates a negative static pressure that sucks fuel into the oxidizer stream. As result, the equivalence ratio of the combustible mixture could not be controlled independently, so that the results are only valuable for the specific operating conditions tested.

<span id="page-39-0"></span>Pioneering studies on unconfined laminar premixed Bunsen flames [\[69,](#page-157-3) [70\]](#page-157-4) demonstrated that flame fronts stabilize where the flow velocity component perpendicular to the reaction front equals the laminar burning velocity, leading to a conical shaped flame. In particular, lowering the bulk velocity  $U_b$  in premixed system promotes flashbacks  $[71, 72]$  $[71, 72]$ , while higher values favor blow-off  $[69, 73]$  $[69, 73]$  $[69, 73]$ . These fundamental features have been studied since the early 1940s but, in spite of the empirical and numerical models proposed, they are not completely understood in practical configurations. Moreover, the flame structure is influenced by the local flow velocity, local strain and flame curvature and thermodiffusive properties of the mixture [\[74,](#page-158-3) [75,](#page-158-4) [76,](#page-158-5) [77\]](#page-158-6), which are particularly important for hydrogen [\[78,](#page-158-7) [79\]](#page-158-8). In addition, both measurements [\[80,](#page-158-9) [81,](#page-158-10) [82\]](#page-158-11) and numerical simulations [\[83,](#page-158-12) [84\]](#page-158-13) prove that heat losses towards the flame holder also affect flame stabilization and flame dynamics. A direct dependency between flame stand-off distance  $\eta$ , laminar burning velocity *SL*, heat losses and flame temperature is demonstrated in [\[85,](#page-158-14) [86\]](#page-158-15) for example. Heat recirculation has also been shown to alter flame stabilization by preheating the incoming gases [\[85,](#page-158-14) [87,](#page-159-0) [88\]](#page-159-1). In order to explore the impact of all parameters, the gas mass flow rates, fuel composition and equivalence ratio must be controlled separately.

Several works performed on multi-perforated cylindrical burners, already outlined

<span id="page-40-2"></span>the effects of burner porosity  $\sigma$  and wall surface temperature  $T_w$  [\[89,](#page-159-2) [90\]](#page-159-3). Tests on the heat exchanger efficiency also demonstrated that the risk of flashback increases at lower thermal power [\[91\]](#page-159-4), although experiments were not conducted at fixed equivalence ratio in that study. Further work dedicated to full-scale burners highlighted that pollutant concentrations depend on the temperature distribution inside the combustion chamber [\[92\]](#page-159-5). The critical role of flame heat losses on  $NO_x$ production was also analyzed in [\[93\]](#page-159-6). Recent studies revealed the impact of hydrogen enrichment in commercial devices in terms of flame stabilization and pollutant emissions  $[94, 95, 96, 97]$  $[94, 95, 96, 97]$  $[94, 95, 96, 97]$  $[94, 95, 96, 97]$  $[94, 95, 96, 97]$  $[94, 95, 96, 97]$ , but they do not consider flashback and blow off issues.

In this Chapter, the physical parameters that drive flame stabilization in cylindrical mullti-perforated premixed burners are identified and controlled, so that the impact of hydrogen addition on the operability of the systems is investigated. Two cylindrical premixed burners featuring different designs and used in condensing boilers are considered. The analysis is limited to forced draft burners, in which fresh reactants are maintained above atmospheric pressure. Only the low power range is investigated, since low volumetric flow rates favor flashback and increase the thermal stress on the burner, which are two main concerns related to  $H_2$  enrichment. First, the hydrogen and methane concentrations in the global mixtures are defined in Section [3.2.](#page-39-0) The description of the two burners and of the methodologies used to analyze the effect of hydrogen enrichment are provided in Section **??**. The burners response to dual fuel methane-hydrogen mixtures is then illustrated in Section [3.4](#page-44-0) for two different thermal powers via stability maps collected in steady state conditions. The effects of  $H_2$  addition on blow-off, thermal load on the burner and flashback are also evaluated. Finally, in Section [3.5](#page-55-0) two different flashback mechanisms are unveiled.

# **3.2. Definition of H**2**-enriched system**

In this work, methane is used as a surrogate for natural gas. Methane and hydrogen are perfectly premixed with air before injection and the combustible mixture is defined by its equivalence ratio  $\phi_q$  and by the molar fraction of hydrogen  $X_{H_2}$ in the fuel blend. The global balance equation for lean combustion ( $\phi_q$  <1) of this multi-component fuel blend is:

<span id="page-40-1"></span><span id="page-40-0"></span>
$$
\phi_g(X_{CH_4}CH_4 + X_{H_2}H_2) + (2 - \frac{3}{2}X_{H_2})(O_2 + aN_2) \to
$$
  

$$
\to \phi_g(X_{CH_4}CO_2 + (2 - X_{H_2})H_2O) + (2 - \frac{3}{2}X_{H_2})((1 - \phi_g)O_2 + aN_2)
$$
(3.1)

The global equivalence ratio  $\phi_q$  is defined as  $\alpha/\alpha_s$  in which  $\alpha$  is the ratio between the actual mass flow rates of fuel and air, while  $\alpha_s$  represents its value at stoichiometry:

$$
\alpha_s = \frac{X_{CH_4}W_{CH_4} + X_{H_2}W_{H_2}}{(2 - \frac{3}{2}X_{H_2})(W_{O_2} + aW_{N_2})}
$$
(3.2)

in which  $a = 3.76$  and  $W_k$  is the molar weight of species k. The molar fraction of  $H_2$  in the fuel mixture is given by:

$$
X_{H_2} = \frac{\dot{n}_{H_2}}{\dot{n}_{H_2} + \dot{n}_{CH_4}}\tag{3.3}
$$

<span id="page-41-1"></span>

**Figure 3.1.** – The solid line ( ––– ) illustrates the relation between the percentage of the total thermal power  $P_{th}$  provided by hydrogen oxidation  $P_{H_2}$  and the molar fraction of hydrogen  $X_{H_2}$  in the fuel blend. The dashed line  $(----)$  shows the reduction percentage of the emission factor EF  $(kg_{CO_2}/J)$  of hydrogen enriched mixtures with respect to pure methane combustion.

<span id="page-41-0"></span>where  $\dot{n}_{H_2}$  and  $\dot{n}_{CH_4}$  are the molar flow rates of hydrogen and methane. Since the fuel is a binary mixture, the methane molar fraction corresponds to  $X_{CH_4} = 1 - X_{H_2}$ .

It is also useful to define the amount of hydrogen in the fuel considering the percentage of the total thermal power  $P_{th}$  provided by hydrogen oxidation:

$$
P_{H_2} = \frac{X_{H_2} Q_{H_2}}{X_{CH_4} Q_{CH_4} + X_{H_2} Q_{H_2}}
$$
(3.4)

where  $Q_{H_2}$  and  $Q_{CH_4}$  are the molar lower heating values of hydrogen and methane. On one hand, this definition allows to compare operating conditions at constant power, which is a critical design parameter. On the other hand,  $P_{H_2}$  is equal to the reduction in *CO*2 emission associated to hybridization. The nonlinear relations between  $P_{H_2}$  and  $X_{H_2}$ , as well as the reduction percentage in  $CO_2$  mass emission per energy unit caused by hydrogen enrichment  $EF / EF_{CO_2}$ , are plotted in Fig. [3.1.](#page-40-2)

Note that the definitions introduced here are kept in the entire manuscript.

# <span id="page-41-2"></span>**3.3. Experimental Setup and Diagnostics**

#### **3.3.1. The CoMix configuration**

The configuration of the CoMix bench used in this Chapter is presented in Fig. [3.2.](#page-41-1) It corresponds to the system described in Chapter [2,](#page-31-0) but the combustion chamber is not used, and the entire set of data and measurements presented are gathered without any confinement of the cylindrical burners to avoid thermo-acoustic instabilities and investigate the largest possible range of operating conditions. The premixed burner *B*1 and *B*2, presented in Section [2.3](#page-34-0) are investigated. The two burners differ in terms of porosity, hole patterns and internal structure. These geometric discrepancies make the two burners ideal candidate to test the limit of  $H_2$  substitution in this kind of applications. Before analyzing the impact of hydrogen addition on the burner stability and flashback, the next Chapter provides a thermal characterization of the two burners, which will be used to interpret experimental results.



<span id="page-42-0"></span>**Figure 3.2. –** Illustration of the test rig adopted in Chapter [3.](#page-37-0) The CoMix bench described in Chapter [2](#page-31-0) is used without combustion chamber.

#### **3.3.2. Wall and gas temperature**

<span id="page-42-1"></span>A two-color infrared pyrometer FLUKE Endurance series (see Fig [3.2\)](#page-41-1) with spectral response between 1.5  $\mu$ m and 1.6  $\mu$ m is used to measure the surface temperature  $T_w$  of the burner to avoid overheating and verify convergence towards steady state condition in order to have repeatable measurements. With the double wavelength approach the temperature measurements can be performed irrespective of the surface emissivity, which depends on material surface properties and temperature. The pyrometer operates between 250 $^{\circ}$ C and 1200 $^{\circ}$ C, with a precision equal to  $\pm$  0.3%.

In order to account for the preheating of the reactants by the hot burner wall, flow temperature measurements in front of the small burner holes are performed following the technique presented in [\[87\]](#page-159-0): the burner operates in steady state condition when the fuel mass flow rate is shut forcing the flame quenching. This instant corresponds to the initial time of data acquisition and a movable K-type thermocouple

<span id="page-42-2"></span>

**Figure 3.3.** – Example of the exponential fitting for experimental data to evaluate the reactants preheating due to heat transfer from the burner hot walls. Three independent gas temperature measurements over time are shown using the burner *B*1 at 4 kW for  $P_{H_2} = 40 \%$  and  $\phi_g = 0.6$ .

<span id="page-43-0"></span>is placed near the external multi-perforated surface of the burner to measure the gas flow temperature exhausting the burner. After a certain time delay, related to the thermal inertia of the thermocouple itself, the measured temperature decreases exponentially following the gas temperature reduction and data are collected with 5 seconds interval. Finally an extrapolation between the time corresponding to the first valid signal acquisition and initial instant  $t = 0$  is performed to retrieve the preheating temperature of the reactants at the instant preceding quenching. Figure [3.3](#page-41-2) shows the result of the extrapolation obtained from three independent gas temperature  $T_u$  measurements performed with the burner  $B1$  at 4 kW for  $P_{H_2} = 40$ % and  $\phi_g = 0.6$ . It shows that the method yields repeatable results with a uncertainty of about  $\pm$  10 K, and this repeatability of the results holds for all operating conditions that were tested.

# **3.3.3. Velocity profile**

A hot wire (MiniCTA - Dantec Dynamics) is used to determine the velocity component in the radial direction, perpendicular to the burner holes. The probe is positioned at a distance  $d = 0.5$  mm from the burner wall, while the hot wire is moved along the burner longitudinal direction, like in Fig. [3.9\(](#page-50-0)b). Velocity measurements are taken with a spatial resolution of 0.1 mm, ensuring at least 4 points inside the diameter of a single burner hole. Each value is the average of measurements performed with a sampling frequency of 1 Hz over a duration of 5 seconds.

#### <span id="page-43-1"></span>**3.3.4. Flame imaging**

A Nikon D7500 camera, equipped with a lens AF-S VR Micro-Nikkor 105 mm f/2.8G is used to collect direct visualization of the flames anchored along the burner external surface. The same camera is also used to gather images of the entire burners under different operating conditions, like for instance in Fig. [3.4.](#page-43-0)

A Phantom V1612 equipped with a Micro-Nikkor 105 mm UV lens is used to gather flame images and identify the location where flashback initiate, as shown in Section [3.5.](#page-55-0) A band pass filter centered on the  $OH^*$  peak emission is used as marker for the flame front position during its propagation and a Lambert HiCATT intensifier is used to amplify the signal-to-noise ratio of  $H_2$  flames emission.

#### **3.3.5. Heat recirculation in burners** *B*1 **and** *B*2

Figure [3.4\(](#page-43-0)a-b) displays direct views of flames taken with the NIKON camera in both burners at the same operating condition:  $\phi_q = 0.6$  and  $P_{H_2} = 40\%$ . They show that the surface of burner *B*1 produces a stronger thermal radiation than *B*2, since flames stabilize closer to the metallic surface of *B*1 leading to higher temperatures of the burner walls. Figure  $3.4(c)$  $3.4(c)$  shows the mean normalized axial temperature distribution along the vertical direction for both burners. Temperature profiles were normalized by the maximum wall temperature  $T_w$  for each operating condition listed in Tab. [3.1](#page-43-1) and then averaged separately for burner *B*1 and *B*2. For each burner, the normalized temperature distribution remains roughly the same for all conditions explored. Measurements taken for locations 1 to 6 as indicated in Fig. [3.4\(](#page-43-0)a-b) also show that the temperature is more uniform along the burner *B*1 than the burner *B*2. For both burners the highest temperature occurs between locations 4 and 5. At the top and at the bottom of the burner, the wall temperature decreases due to

<span id="page-44-2"></span>

<span id="page-44-1"></span><span id="page-44-0"></span>**Figure 3.4.** – Photos collected with a Nikon camera yielding a qualitative insight of the burner surface temperature at steady state conditions for burners *B*1 and *B*2 at the same operating condition:  $\phi_q = 0.60$ ,  $P_{H_2} = 40\%$  and 4 kW. Burner *B*1 (a) exhibits higher surface temperatures and higher thermal radiation than *B*2 (b). The mean normalized wall temperature distribution from locations 1 to 6 along the axial direction is shown in (c). The white arrow puts in evidence the small flames anchored at the burner wall.

B1		B <sub>2</sub>		
$\phi_q$ - $P_{H_2}$	$T_{max}$ [K]	$\phi_q$ - $P_{H_2}$	$T_{max}$ [K]	
$0.6 - 40\%$	635	$0.6 - 70\%$	658	
$0.7 - 20\%$	698	$0.7 - 50\%$	695	
$0.8 - 0\%$	718	$0.8 - 30\%$	714	

**Table 3.1. –** List of operating conditions at 4 kW used to provide the average normalized axial wall temperature profile for burners *B*1 and *B*2 in Fig. [3.4\(](#page-43-0)c) .

heat losses. Moreover, Fig. [3.4\(](#page-43-0)c) shows that the relative temperature reduction at the bottom of burner *B*2 is much stronger than in burner *B*1.

Another aspect to be considered is the gas residence time inside the burner. This is dictated by the internal structure of the burners (see Fig.  $2.3$ ) and it can affect the temperature  $T_u$  at which the reactants exit the burner holes. As sketched in Fig. [2.3,](#page-35-0) burner *B*1 favors preheating, since the fresh mixture makes a U-turn at the top of the burner resulting in a longer residence time of the reactants. Inside *B*2, instead, the mixture is directly distributed over the external surface limiting the heat transfer to the flow. This effect is isolated in Tab. [3.2,](#page-44-2) where the wall temperature  $T_w$  is kept constant and the heating of the fresh reactants is measured for the burner  $B1$   $(T_u^{B1})$  and  $B2$   $(T_u^{B2})$ . The temperature  $T_w$  is adjusted by tuning the hydrogen content  $P_{H_2}$  at constant equivalence ratio, minimizing the variation on the total mass flow rate. Data in Table [3.2](#page-44-2) shows that burner *B*1 promotes larger heat transfer to the reactants than burner *B*2. In fact, the same wall temperature results in greater preheating of the reactants with burner *B*1 and this will be shown to have an influence on the flame stabilization. In the rest of the study  $T_w$  must be considered as the wall temperature measured at location 4 in Figs. [3.4\(](#page-43-0)a-b).

<span id="page-45-0"></span>CHAPTER  $3: H_2$  substitution of natural-gas in multiperforated burners and implications for blow-off and flashback limits

$\phi_g$			$\overline{PH_2^{B1} \quad PH_2^{B2} \quad T_w \text{ (K)}}$	$T_u^{B1}$ (K) $T_u^{B2}$ (K)	
0.6	$16\%$	48\%	$750 \pm 2.3$	$531 + 5$	$466 + 11$
0.6	28\%	$67\%$	$850 + 2.6$	$568 + 22$ $475 + 16$	
0.7	$15\%$	$50\%$	$950 + 2.9$	$652 + 13$ $555 + 10$	

**Table 3.2.** – Preheated gas temperatures  $T_u$  for burners  $B1$ ,  $T_u^{B1}$ , and  $B2$ ,  $T_u^{B2}$ , are compared at fixed wall temperature  $T_w$ . The burners are operated at the same equivalence ratio to minimize the mass flow variations. The hydrogen content is tuned to match the targeted wall temperature  $T_w$  with the different burners.

# **3.4. H**<sup>2</sup> **effect on the burner operability**

In this section the range of stability of the two burners is analysed over several operating conditions, which allows to evaluate the performance of the burners *B*1 and *B*2 varying independently the hydrogen content and the equivalence ratio at different thermal powers.

#### **3.4.1. Stability maps**

Figures [3.5\(](#page-45-0)a-d) present burners stability maps performed at constant power of 2 kW (at the bottom) and 4 kW (at the top) for burner *B*1 and burner *B*2 as a function of the hydrogen enrichment  $P_{H_2}$  and global equivalence ratio  $\phi_g$ . At constant hydrogen content  $P_{H_2}$  the equivalence ratio  $\phi_g$  is changed by modulating the air mass flow rate and, due to limitations of the air mass flow controllers, its minimum value is  $\phi_g = 0.45$  at 4 kW and  $\phi_g = 0.30$  at 2 kW. Three isolines representative of the ratio  $U_b/S_l = 1$ , calculated for mixture temperatures  $T_u = 300 \text{ K (red)}$ , 500 K (green) and 700 K (blue), are superposed on the maps and will be discussed in Sec. [3.4.4.](#page-52-0) The maps illustrate the combinations of  $P_{H_2}$  and  $\phi_g$  that allow to operate the burners without facing undesirable events, namely blow-off, overheating and flashback:

- Blow-off is defined here as the condition at which the flames detach from the lower side of the burner, leading to incomplete combustion.
- Overheating occurs when the burner surface temperature  $T_w$  overcomes 1050 K, which is the one measured for burner *B*1 when operated at the reference condition of  $P_{H_2} = 0\%$ ,  $\phi_q = 0.8$  and  $P_{th} = 4$  kW.
- **–** Flashback happens when the flame front propagates upstream through the injection system [\[25\]](#page-154-4).

Figures [3.5\(](#page-45-0)a-d) show that stable operating conditions, regardless of the burner and the power investigated, are limited by two main boundaries: one at the bottom-left side of the maps and the other one at the top-right side. The first corresponds to the blow-off ( $---$ ). For a given hydrogen content  $P_{H_2}$ , the reduction of the equivalence ratio  $\phi_g$  decreases the reactivity of the mixture and the flames blow-out. Interestingly, increasing the hydrogen content  $P_{H_2}$  the blow-off limit occurs at lower equivalence ratios and it is possible to sustain leaner combustion for both burners. For instance, Fig. [3.5\(](#page-45-0)a) shows that, increasing  $P_{H_2}$  from 0% to 40%, the equivalence ratio  $\phi_q$  can be reduced from 0.60 to 0.45. The other limits are overheating (  $\ldots$ , and flashback  $($  —  $)$ . Figures [3.5\(](#page-45-0)a-d) indicate that the highest achievable hydrogen enrichment  $P_{H_2}$  is reduced by increasing the equivalence ratio  $\phi_g$ , independently of the burner and thermal power. Closer to stoichiometry, the limiting factor



<span id="page-46-0"></span>**Figure 3.5.** – Steady-state stabilization maps displaying stable operating conditions as function of equivalence ratio  $\phi_g$  and  $H_2$  content  $P_{H_2}$ . Plots refer to burner *B*1 operated at 4 kW (a) and 2 kW (c) and to burner *B*2 operated at 4 kW (b) and 2 kW (d), showing the operating limits associated to blow-off  $(----$ ), flashback (  $\textcolor{red}{\overline{\phantom{a}}}$  ) overheating (  $\cdots\cdots\cdots$  ). The red, green and blue curves on each plot identify the isolines at  $U_b/S_l=1$  for reactants temperature of  $T_u{=}300$  K, 500 K and 700 K respectively.

<span id="page-47-0"></span>is the thermal resistance of the material because, thanks to the greater reactivity of the mixture, flames stabilize closer to the burner surface promoting heat transfer to the wall with higher wall surface temperatures  $T_w$ . At leaner conditions, instead, the maximum hydrogen enrichment  $P_{H_2}$  is dictated by flashback, which occurs for burner surface temperatures  $T_w$  below 1050 K. Nevertheless, Figs. [3.5\(](#page-45-0)a-d) show that  $H_2$  addition does not widen the range of achievable operating conditions. An improvement of the lean blow-off limit is systematically accompanied by a reduction of the highest achievable equivalence ratio due to overheating or flashback.

The aforementioned conclusions apply qualitatively to both burners. However, from a quantitative standpoint, several differences are found comparing the burners *B*1 and *B*2 when operated at the same power. On one hand, *B*2 exhibits a greater flashback resistance, allowing for higher hydrogen content at the same equivalence ratio. For example, at  $P_{th} = 4$  kW and  $\phi_q = 0.6$ , flashback appears at  $P_{H_2} = 50\%$ and  $P_{H_2}$  = 80% for *B*1 and *B*2, respectively. On the other hand, *B*2 is more prone to blow-off and a series of low- $\phi_g$  low- $P_{H_2}$  operating conditions are only achievable with *B*1, as for example  $P_{H_2} = 0\%$  and  $\phi_g = 0.6$ .

To sum up, there are operating conditions that are stable for one burner and not even achievable with the other, independently of power. Since the range of operating conditions is the same for both burners, these differences must be related to their specific design. It is demonstrated in Section [3.3](#page-40-0) that the burner *B*2 generates higher bulk flow velocities  $U_b$  at the hole outlets and features a lower influence on the unburned gas temperature  $T_u$  than burner  $B1$ . As a matter of fact these aspects facilitate flame detachment from the wall, hindering flashback and eventually favoring blow-off. Thus, the hole pattern of the multi-perforated surface and the internal path of the flow along hot solid walls influence the performances of the burner in terms of  $H_2$  substitution. Nevertheless, improving flashback tolerance worsens the blow-off resistance, limiting the effective fuel flexibility at fixed equivalence ratio.

#### **3.4.2. Blow-off limit**

Hydrogen addition is known for improving the blow-off resistance  $[28, 98]$  $[28, 98]$ . In this section, flame images are used to investigate the differences in the mechanisms leading to blow-off for different fuel blends in both burners. Images are taken with the Nikon camera from a direction tangent to the cylindrical surface of the burner (see for instance Fig.  $2.3(a)$  $2.3(a)$ ).

First, the effect of  $H_2$  substitution is considered and, secondly, the impact of the ports distribution is discussed.

#### **3.4.2.1. Effect of H**<sup>2</sup> **substitution**

Figures [3.6\(](#page-47-0)b-d) and [3.7\(](#page-47-0)b-d) correspond to specific operating conditions presented in Fig. [3.5\(](#page-45-0)a) for burner *B*1. The windows of investigation are illustrated in Figs.  $3.6(a)$  $3.6(a)$  and  $3.7(a)$  $3.7(a)$ , while the white-dotted lines represent the axis of two adjacent burner holes along the radial direction.

First, Figures [3.6\(](#page-47-0)b-d) show pure-CH<sub>4</sub> flames for equivalence ratios  $\phi_q = 0.70$ , 0.65 and 0.55. In Fig. [3.6\(](#page-47-0)b), flames are attached to the burner surface at  $\phi_q = 0.70$ and a series of independent conical reaction fronts develop beyond each slit hole. The small differences among the several flames along the radial direction of the burner are due to local inhomogeneities of the flow. Reducing  $\phi_q$  to 0.65, keeping a constant power, results in a simultaneous increase of the bulk flow velocity  $U_b$ and a reduction of the adiabatic laminar burning velocity *SL*, which concomitantly

<span id="page-48-0"></span>

**Figure 3.6. –** Flame shape along the longitudinal side of the burner *B*1, captured from a direction tangential to the burner surface above the slit holes as shown in (a). Operation at 4 kW with pure methane flames  $P_{H_2} = 0\%$  at equivalence ratios (b) 0.70, (c) 0.65 and (d) 0.55, respectively.



**Figure 3.7. –** Flame shape along the longitudinal side of the burner *B*1, captured from a direction tangential to the burner surface above the slit holes as shown in (a). Operation at 4 kW with a hydrogen content  $P_{H_2} = 50\%$  at equivalence ratios (b) 0.50, (c) 0.45 and (d) 0.40.

leads to a gradual increase in the flame length and a coalescence of adjacent conical flame fronts as shown in Fig.  $3.6(c)$  $3.6(c)$ . This phenomenon is exacerbated in Fig.  $3.6(d)$ , where the entire reaction layer detaches from the burner surface resulting in a severe blow-off.

Second, Figs.  $3.7(b-d)$  $3.7(b-d)$  show for the same burner  $B1$  H<sub>2</sub>-enriched flame images  $(P_{H_2} = 50\%)$  at  $\phi_g = 0.50, 0.45$  and 0.40, respectively. Figure [3.7\(](#page-47-0)b), similar to Fig. [3.6\(](#page-47-0)b), illustrates well-anchored flames and stable combustion. Note that, for the same equivalence ratio  $\phi_g = 0.5$ , the pure methane flame is blown off. Moreover, a reduction of  $\phi_q$  to 0.45 marks a strong difference with respect to pure methane case: the flames lengthen and their curvatures increase leading to flame tip-opening as in Fig. [3.7\(](#page-47-0)c). This effect is due to the low Lewis number *Le* of molecular  $H_2$  [\[46,](#page-156-0) [76,](#page-158-5) [99\]](#page-159-12) which, as discussed in Section [1.2,](#page-18-0) alters the properties of the mixture leading to a preferential diffusion within the flame front. According to [\[33\]](#page-155-1) and considering the *Le* number of CH<sub>4</sub> (H<sub>2</sub>) equal to  $Le = 1.0$  ( $Le = 0.3$ ), the characteristic Lewis

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**Figure 3.8. –** Flame shape along the longitudinal side of the burner *B*2, captured from a direction tangential to the burner surface above round holes as shown in (a). Operation at 4 kW with an hydrogen content  $P_{H_2} = 50\%$  at equivalence ratios (b) 0.60, (c) 0.55 and (d) 0.50.

number<sup>[1](#page-3-0)</sup> of the fuel blend at  $P_{H_2} = 50\%$  drops to  $Le_f = 0.46$  according to [\[33\]](#page-155-1), justifying the observation of thermodiffusive effects  $[49, 53]$  $[49, 53]$ . As a consequence, the flame tip is quenched while the reaction rate strengthens at the base of the conical flames. For that reason the reaction front shifts towards the periphery of the burner outlets promoting interactions among adjacent flames. Fig.  $3.7(d)$  $3.7(d)$  shows also that this trend is intensified at blow-off conditions, in which the reaction zones lie entirely between burner ports.

To sum up, preferential diffusion effects due to hydrogen addition promote a different flame stabilization at very lean conditions (i.e. close to blow-off). For CH4-air mixtures the flames detach from the burner surface as a continuous reactive layer. In case of hydrogen enrichment, instead, single flames stabilize in the low velocity region between two adjacent burner outlets, where combustion is sustained thanks to the interaction among several holes.

#### **3.4.2.2. Impact of holes distribution**

<span id="page-49-0"></span>The mechanism leading to a different flame stabilization near blow off conditions is stronger when the hydrogen content increases, but it is reasonable to expect that it also depends on the ports distribution over the burner surface. This is further discussed in Fig. [3.8\(](#page-48-0)b-d), in which burner *B*2 is considered. This figure shows the blow-off transition for  $P_{H_2} = 50\%$  and equivalence ratios  $\phi_g = 0.60, 0.55, 0.50$ . Figure [3.8\(](#page-48-0)b) shows M flames stabilized along the burner wall, where each lobe corresponds to a single outlet of the burner. In analogy with Fig. [3.7,](#page-47-0) when the equivalence ratio is reduced, hydrogen preferential diffusion effects make the reaction rate stronger at the flame base and weaker at the flame tip (see Fig.  $3.8(c)$  $3.8(c)$ ). A further reduction of the equivalence ratio to 0.50 in Fig. [3.8\(](#page-48-0)d) produces a stabilization of the flame fronts only between the two circular holes separated by a distance of 2.0 mm, while the reaction is quenched when the vertical distance between two adjacent ports increases to 4.5 mm (see Fig.  $(2.3(b))$  $(2.3(b))$  $(2.3(b))$ ). On one side, this observation confirms that the molecular diffusivity of hydrogen favors a change of flame stabilization that increases the blow-off resistance. On the other side, Fig.  $3.8(d)$  $3.8(d)$  shows that this

<sup>1.</sup> The effective Lewis number  $Le<sub>f</sub>$  here is weighted by the volume fractions of CH<sub>4</sub> and H<sub>2</sub> according to [\[33\]](#page-155-1).

<span id="page-50-0"></span>mechanism is promoted by the proximity of the the burner holes and it is shown that  $H_2$ -enriched flames stabilize in between holes only if these are sufficiently close to each other. In the latter case, hydrogen diffuses laterally encountering a relatively high-temperature and low-velocity region that enables flame stabilization. When the distance between two holes overcomes a critical value, instead, this mechanism is inhibited. One could also speculate on the fact that limiting the distance between adjacent holes inhibits dilution by external air engulfment, which normally acts at the base of isolated Bunsen flames favoring local quenching [\[100,](#page-160-0) [101\]](#page-160-1).

#### **3.4.2.3. Competition between convection and diffusion velocities**

The previous conjecture last interpretation requires the local flow velocity between the holes to be comparable to the hydrogen diffusion velocity in air at these thermodynamic conditions. This is verified considering the burner *B*1. In this setup, the hydrogen diffusion velocity  $V_{d,H_2}$  into air can be evaluated using Fick's law, under the hypothesis of constant mass fraction gradient of  $H_2$  over the distance  $l = 2.5$ mm between the hole axis and the mid point between two consecutive holes (see Fig. [3.9\(](#page-50-0)b)). If the mass fraction of  $H_2$  is considered to be equal to the value of the incoming premixed gases at the burner hole axis and linearly decreases to zero at the mid point between two consecutive holes, then  $V_{d,H_2}$  is of the order of 0.25 m/s. The flow velocity component  $U_r$  along the burner radial direction is measured in non-reactive conditions with a hot wire, imposing a volumetric flow rate representative of reactive operating conditions at  $4 \text{ kW}$ . Figure [3.9](#page-50-0) shows  $U_r$  with respect to the axial direction of the burner, taken at a distance  $d = 0.5$  mm above the burner surface. Note that the velocity profile changes moving the hot-wire closer to the burner wall. Here, *d* is chosen equal to the holes diameter.

Interestingly, despite the maximum velocity being around 3 m/s, *U<sup>r</sup>* drops below 0.3 m/s between two adjacent holes, reaching similar values as the  $H_2$  diffusion velocity  $V_{d,H_2}$  evaluated previously. Hence, the local flow velocity is comparable with the diffusion velocity of hydrogen in air and therefore, compatible with the conjectured mechanism of preferential diffusion.

<span id="page-50-1"></span>Overall, the discussion above suggests that either  $H_2$ -enrichment and a specific hole pattern must be considered to interpret flame stabilization, since both are necessary but not sufficient conditions to allow different flame stabilizations. These experiments also suggest that, in addition to the increased reactivity of  $H_2$ -enriched mixtures, a specific distribution of the burner holes can reinforce the blow-off resistance when  $H_2$  is involved thanks to its large molecular diffusion.

#### **3.4.3. Effect of flame stabilization on the burner thermal load**

The burner surface temperature  $T_w$  controls the lifetime of materials and it affects the mixture reactivity, since fresh gases are heated by the hot walls. The impact of the wall temperature  $T_w$  on flame stabilization is explored in this Section. Figures [3.10\(](#page-50-1)a-b) display the contour maps of surface temperature  $T_w$  at 4 kW for both burners. Data are retrieved by interpolating the temperature measurements collected with the pyrometer at steady state conditions over the operating points covered in Figs. [3.5\(](#page-45-0)a-b). Here  $T_w$  represents the temperature at location 4 displayed in Fig. [3.4\(](#page-43-0)a-b).

The wall temperature  $T_w$  depends on the adiabatic flame temperature  $T_{ad}$  and on the distance *η* between the flame root and the flame holder. As demonstrated for example in case of flat flames [\[85,](#page-158-14) [86\]](#page-158-15), these two parameters generally control the heat

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<span id="page-51-0"></span>

**Figure 3.9.** – The radial velocity profile  $U_r$ , measured along the axial direction of burner *B*1 at  $d = 0.5$  mm above the external surface ( $\longrightarrow$ ), is compared to an estimation of the hydrogen diffusion velocity at the burner outlets  $($  ----(a). Axial and radial directions are indicated in (b), as well as the distance *d* at which the velocity profile is determined.

load on the burner. However, data listed in Tab. [3.3](#page-51-0) demonstrate that the adiabatic flame temperature  $T_{ad}$  does not correlate to the wall temperature  $T_w$ , at least for the conditions investigated. For instance, for operating conditions 3 and 5  $T_w$  reaches comparable values but the corresponding adiabatic flame temperatures  $T_{ad}$  differ by 130 K. An additional example is given considering operating conditions 1 and 5. In this case the adiabatic flame temperature  $T_{ad}$  is similar for both conditions, while  $T_w$ differs by more than  $150$  K. Interestingly, Table [3.3](#page-51-0) shows that the wall temperature  $T_w$  results in a better correlation with the laminar burning velocity  $S_L^{T_u}$ , rather than with  $T_{ad}$ . In fact, as the laminar burning velocity increases with both equivalence ratio  $\phi_g$  and fraction of hydrogen  $P_{H_2}$  in the fuel blend, the burner surface temperature  $\tilde{T}_w$  increases consistently. Here  $S_L^{T_u}$  is retrieved from CANTERA 1D



**Figure 3.10.** – Wall temperature  $T_w$  contour maps as function of the hydrogen content  $P_{H_2}$  and equivalence ratio  $\phi_g$  for burner *B*1 (a) and *B*2 (b) at power of 4 kW.

<span id="page-52-1"></span>

	$\phi_q$ - $P_{H_2}$	$T_u$ (K)	$S_L^{T_{ad}}$ $\rm (cm/s)$	$S_L^{T_u}$ $\rm (cm/s)$	$T_w$ (K)	$T_{ad}^{I_u}$ (K)
	$0.6 - 10\%$	$407 \pm 10$	14.4	28.9	$710 \pm 2.1$	1765
2.	$0.6 - 20\%$	$481 \pm 12$	17.8	54.1	$813 \pm 2.4$	1838
3.	$0.6 - 30\%$	$512 \pm 9$	22.1	78.2	$883 \pm 2.6$	1878
	$0.6 - 40\%$	$530 \pm 8$	26.8	105.0	$943 \pm 2.8$	1909
5.	$0.5 - 62\%$	$521 \pm 11$	20.0	91.6	$863 \pm 2.6$	1748

**Table 3.3. –** Five operating conditions obtained with burner *B*1 at 4 kW are compared in terms of wall temperature  $T_w$ , adiabatic flame temperature  $T_{ad}$  and laminar burning velocity  $S_L$ , which is calculated considering fresh gases at  $T_a = 300$  K and at  $T_u$ . The laminar burning velocity is highly affected by the fresh gas temperature  $T_u$ .  $T_w$  results in good correlation with  $S_L^{T_u}$ , rather than  $T_{ad}^{T_u}$ .

simulations imposing  $T_u$  as unburnt gas temperature. Table [3.3,](#page-51-0) for instance, shows the impact of the fresh gas temperature  $T_u$  on the laminar burning velocity  $S_L^{T_u}$ that is between 2 to 4 times higher than considering ambient conditions, when *S<sup>L</sup>* is calculated at  $T_u = T_a: S_L^{T_a}$ .

One must consider that the flame stabilization is subjected to a positive feedback loop. An increase of the wall temperature  $T_w$  enhances the heating of the reactants from ambient condition to temperature  $T_u$ , that in turn generates larger  $S_L^{T_u}$ . As consequence, the flames get closer to the wall increasing  $T_w$  even more. This also means that the mixture composition and the thermal state of the burner are strictly coupled, which needs to be taken into account in view of the fact that this interaction directly affects flashback  $[100, 101, 102]$  $[100, 101, 102]$  $[100, 101, 102]$  $[100, 101, 102]$ .

To highlight the actual variation of the distance between the flame and the wall when the  $H_2$  substitution is increased, Figs. [3.11](#page-52-1) and [3.12](#page-52-1) illustrate the evolution of the flame front position at constant equivalence ratio for burners *B*1 and *B*2 at 4  $kW$ . Figures [3.11\(](#page-52-1)a) and [3.12\(](#page-52-1)a) depict the windows of investigation of the burners (as in section [3.4.2\)](#page-46-0). Figures [3.11\(](#page-52-1)b-d) refer to burner *B*1 at 4 kW and  $\phi_g = 0.6$ , varying the hydrogen power content  $P_{H_2}$  from 0% to 46%. In case of pure methane flames, the reaction front is detached from the burner surface (Fig. [3.11\(](#page-52-1)b)) because this operating condition is close to the blow-off limit (Fig.  $3.5(a)$  $3.5(a)$ ). An increment of  $P_{H_2}$  to 25% results in shorter flames, confirming the  $H_2$  stabilization effect against blow-off. In Fig. [3.11\(](#page-52-1)d), the hydrogen power content  $P_{H_2}$  is augmented to 46% and the  $H_2$ -enhanced flame reactivity drives the flame closer to the burner surface. The conical laminar flames in Fig.  $3.11(c)$  $3.11(c)$  transform into independent nearly flat flames anchored at the edges of the burner holes in Fig. [3.11\(](#page-52-1)d) and the heat load on the burner reaches its maximum.

<span id="page-52-0"></span>Similar observations are made in Figs. [3.12\(](#page-52-1)b-d), when the burner *B*2 is fueled with a growing hydrogen content at  $\phi_q = 0.7$ . The flame shapes differ with respect to those shown for burner *B*1 because of the distribution of the exit holes. Flames of burner *B*2 exhibit a "M" shape, where each lobe forms in the wake of a single burner hole. Boosting the hydrogen content  $P_{H_2}$  from 20% to 55%, the flames shorten continuously and the burner surface temperature  $T_w$  raises from 750 K to 1020 K. In both burners the reaction front approaches dangerously the burner hole outlets when the hydrogen content is increased (Figs.  $3.11(d)$  $3.11(d)$  and  $3.12(d)$  $3.12(d)$ ). An exacerbation of this phenomenon leads to flashback.

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**Figure 3.11. –** Flame shape evolution along the longitudinal side of the burner *B*1, captured from a direction tangential to the burner surface (a). Images correspond to steady state conditions for  $\phi_g = 0.6$  and  $P_{H_2}$  equals to 0% (b), 25% (c) and 46% (d).

<span id="page-53-0"></span>

**Figure 3.12. –** Flame shape evolution along the longitudinal side of the burner *B*2 , captured from a direction tangential to the burner surface (a). Images correspond to steady state conditions for  $\phi_g = 0.7$  and  $P_{H_2}$  equals to 20% (b), 40% (c) and 55% (d).

#### **3.4.4. Identification of different flashback regimes**

Flashback occurs in premixed burners when the flame propagates upstream through the injection system  $[25]$ , which can be the result of different mechanisms. The simplest criterion to interpret flashback is based on premixed flame kinematics: since a premixed flame lies where the component of the flow velocity perpendicular to the flame front matches the local flame speed, flashback is expected when the laminar burning velocity  $S_L$  overcomes the incoming bulk flow velocity  $U_b$ . This can be seen as a particular case of the general theory of the velocity gradient [\[69,](#page-157-3) [73\]](#page-158-2). According to that and considering a laminar flow with a given velocity profile, flashback occurs when the flow velocity gradient at the wall equals the ratio between the laminar flame speed and the flame thickness.

However, if a flame stabilizes above small holes or narrow tubes, the velocity gradient theory tends to lose its validity. In this case, heat losses increase lowering the flame reactivity and ultimately hindering its passage towards the injection system. In these conditions, the main governing parameters become the wall temperature <span id="page-54-0"></span> $T_w$  and the flame holder diameter [\[100,](#page-160-0) [101,](#page-160-1) [103\]](#page-160-3). Because of the high temperature reached by the burner walls and the substantial preheating of the fresh mixture, autoignition close to the hot metallic burner surfaces inside the burner should also be taken into consideration. In fact, depending on the mixture composition and flow field at the exit holes, the burner wall temperature may potentially serve as source of energy to ignite the mixture [\[63\]](#page-157-5), triggering flashback.

Considering now the present study, Figs. [3.5\(](#page-45-0)a-d) show three isolines representative of  $U_b/S_L = 1$  calculated for three different gas temperatures  $T_u = 300$  K (red), 500 K (green) and 700 K (blue). The slope of the isolines is in good agreement with the one of the experimental flashback limits, but it does not mean that flashback occurs for a unity value of  $U_b/S_L$ . In fact, the measured gas temperature  $T_u$  for the points that belong to the flashback lines (Figs.  $3.5(a-d)$  $3.5(a-d)$ ) is not constant and the ratio between the bulk flow velocity through a burner hole  $U_b$  and the laminar burning velocity *S<sup>L</sup>* varies substantially along the flashback line. Hence, the flashback limit cannot be simply explained in terms of kinematic equilibrium between the flow velocity and the flame speed. Table [3.4](#page-53-0) lists five operating points for burner *B*1

Description	$\phi_q$ ; $P_{H_2}$	$T_u(K)$	$T_w(\mathrm{K})$	$(U_b/S_L)_{T_u}$
$Stable*$	$1.0;0\%$	$771 \pm 4$	$1100 \pm 3.3$	1.1
Stable	$0.8:0\%$	$692 \pm 6$	$1060 \pm 3.2$	1.9
Flashback	$0.6:45\%$	$594 \pm 5$	$973 \pm 2.9$	1.8
Flashback	$0.5:62\%$	$521 \pm 11$	$863 \pm 2.6$	2.8
Flashback	$0.45:76\%$	$499 \pm 11$	$820 \pm 2.5$	3.3

**Table 3.4. –** List of operating conditions used to investigate the role of the ratio between the bulk flow velocity  $U_b$  and the laminar burning velocity  $S_L$  with respect to flashback occurrence. This ratio is calculated for the gas temperature *Tu*(after being heated by the combustor walls), showing the decisive role of the unburned mixture temperature. The first stable condition identified by \* is not included in the stabilization map since the wall temperature  $T_w$ overcomes the overheating threshold of 1500 K, but is specifically considered in this table because of the low value of the ratio  $(U_b / S_L)_{T_u}$ .

at 4 kW, where two stable operating points are compared to three conditions representative of flashback events. The ratio  $U_b/S_L$  is calculated considering flow and laminar burning velocity at the measured gas temperature  $T_u$ , showing that  $(U_b)$  $(S_L)_{T_u}$  increases considerably with the hydrogen content  $P_{H_2}$  at different flashback conditions. Hence, the  $H_2$ -induced flashback cannot be simply predicted in view of the competition between the bulk velocity  $U_b$  and the laminar burning velocity  $S_L$ .

With the goal of broadening the number of operating conditions subjected to flashback and investigate this phenomenon, a different measurement procedure is adopted. At the beginning, the burner is in thermal equilibrium with ambient. Then, the targeted mixture composition is imposed. After a few seconds, the burner is ignited and the evolution of wall temperature with time is monitored. Three distinct regimes are identified after ignition:

- Regime I: Combustion remains stable and the burner evolves naturally towards thermal equilibrium. Flashback does not occur.
- Regime II: Initially the flame stabilizes on the multi-perforated burner surface but, as  $T_w$  reaches a certain threshold, flashback occurs. This value of the wall temperature is defined as  $T_{w,fb}$ .

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**Figure 3.13. –** Description of the region of influence of regimes I, II and III with respect to the hydrogen power content  $P_{H_2}$  and equivalence ratio  $\phi_q$  for burners *B*1 (a) and *B*2 (b). Operating conditions belonging to regime II are sized and colored considering the value of  $T_{w,fb}$ .



<span id="page-55-0"></span>**Figure 3.14.** – Burner surface temperature  $T_w$  time evolution from ignition to the instant at which flashback occurs is illustrated for three different mixtures and the  $\,$ two burners *B*1 (a) and *B*2 (b). Each curve shows the heating process of the burner till the condition  $T_w = T_{w,fb}$  is attained.

Regime III: Ignition itself generates a sudden flashback. In this circumstance the flame is never stabilized on the burner, which remains at ambient temperature.

<span id="page-55-1"></span>The maps presented in Figs.  $3.13(a-b)$  $3.13(a-b)$  show the regions of influence of the three different regimes for both burners when operated at  $4 \,$  kW. Most of the mixture compositions investigated in these additional unsteady experiments do not belong to the stabilization maps in Figs.  $3.5(a-b)$  $3.5(a-b)$ . In fact, it would be impossible to gather this level of insight operating the burner in quasi-steady state mode. As expected, only the operating conditions leading to regime I correspond to the ones displayed in Figs. [3.5\(](#page-45-0)a-b). At high equivalence ratio  $\phi_g$  and large hydrogen power content  $P_{H_2}$ , instead, the burners undergo flashback during ignition corresponding to regime III in Figs.  $3.13(a-b)$  $3.13(a-b)$ . For this pool of operating points, the reactivity of the mixture increases so much that it is impossible to operate the burners. In between these two regimes, there is a range of mixtures for which flashback is thermally activated by a specific burner surface temperature  $T_{w,fb}$ . This mechanism is here defined regime <span id="page-56-1"></span>II. Both maps in Fig. [3.3](#page-41-2) show that this limit can be attained from regime I either by increasing the hydrogen power content  $P_{H_2}$  or raising the equivalence ratio  $\phi_g$ towards stoichiometry. Moreover, results reveal that this transition depends on the burner design.

Regime II identifies a strict dependence between flashback and the thermal state of the burner. Figures  $3.14(a-b)$  $3.14(a-b)$  display the evolution of the burner surface temperature  $T_w$ , after ignition, for three different mixture compositions with burners *B*1 and *B*2. In each case the wall temperature  $T_w$  increases up to a peculiar value  $T_{w,fb}$  at which flashback occurs. It was verified that this value only depends on the mixture composition and it is not related to the time needed to attain  $T_{w,fb}$ . As shown in Fig. [3.14,](#page-54-0) by increasing either the hydrogen power content  $P_{H_2}$  or equivalence ratio  $\phi_g$  leads to a reduction of this activation threshold, presumably due to the boosted reactivity of the mixture. Figure [3.14\(](#page-54-0)b), for instance, puts in evidence that increasing  $P_{H_2}$  from 80% to 90% at constant  $\phi_g = 0.6$ , reduces  $T_{w,fb}$  from 967 K to 912 K. On the other side, increasing  $\phi_g$  to 0.7 keeping  $P_{H_2}$  constant to 80%, reduces  $T_{w,fb}$  to 880 K. Measurements have been repeated at least three times for each condition and the variation of  $T_w^{fb}$  lies within  $\pm 5$  K, which is below the instrumentation error. Furthermore, Figs. [3.13\(](#page-54-0)a-b) illustrate that burner *B*1 undergoes flashback for a wall temperature that is lower than for burner *B*2. This is particularly evident for a hydrogen power content  $P_{H_2} = 50\%$  and equivalence ratio  $\phi_q = 0.8$ , which is the unique point shared by the two burners in regime II. In this case,  $T_{w,fb}$  is equal to 872 K for burner *B*1, while it increases to 1068 K for burner *B*2.

Despite results highlight the crucial role of the wall temperature  $T_w$  and the gas temperature  $T_u$ , they are not sufficient to shed light on the fundamental mechanisms that drive this process. To elucidate this point, additional work is performed showing that H2-enriched flames could autoignite near the hot walls of the burner, triggering flashback via spontaneous ignition.

# **3.5. Investigation of flashback mechanisms in the regime II**

This section focuses on the phenomenological aspects that characterize the initial phase of the flashback regime II presented in Section [3.4.4](#page-52-0) and it aims at unveiling the mechanisms leading to flashback. This part is a common work made with Hugo Pers at IMFT and recently published [\[66\]](#page-157-0). For technical reasons only the burner *B*2 is investigated but, considering the similarities with *B*1 illustrated above, the following observations are reasonably valuable for other burners of similar geometry. The burner *B*2 is modified to ensure full optical access to its internal side and the Nikon camera is replaced by a high-speed Phantom V1612 camera equipped with a UV light intensifier to collect time-resolved images of the flashback process.

#### **3.5.1. Setup and diagnostics**

<span id="page-56-0"></span>Figure [3.15](#page-56-1) sketches the new configuration of the experimental setup. The whole bench presented in Sections [3.3](#page-40-0) is positioned horizontally (i.e. along the *x* axis) to ease flame imaging. The combustion chamber is not used. To secure the optical access to the internal side of the multiperforated surface, the metallic top part of the burner is removed and replaced by a quartz disk with a thickness of 8 mm. This transparent window is kept in the correct position by 4 tie-rods screwed into the upper part of the convergent element as illustrated in Fig. [3.15.](#page-56-1) These four

<span id="page-57-0"></span>

**Figure 3.15.** – Top view of the experimental setup. The curved double arrow illustrates the displacement of the imaging setup when switching from an internal side view to a front view. The y-axis corresponds to the vertical direction.

elements feature springs that provide a homogeneous compression of the quartz window against the top side of the burner. In this way, the stresses generated by the different thermal expansions between the metallic components of the burner and the quartz windows are accommodated without compromising their integrity. Leaks are prevented by using a layer of fiberglass placed between the top side of the burner and the quartz disk.

A Phantom V1612 camera is used to gather flame images with acquisition frequency of 16 kHz to track the position of the flame front during flashback.

The symmetry axes of the burner and of the camera are both coincident with the  $x - y$  plane in Fig. [3.15](#page-56-1) and only the angle  $\alpha$  between the axis of the camera and the axis of the burner is modified. To this respect, two different positions are considered:

- $-\alpha = 0$ . The central axis of the burner and the axis of the camera coincide. The flame images are the result of the line of sight integration of the  $OH^*$ emission signal over the entire length of the burner. This field of view enables a qualitative analysis of the flame propagation over the cross section of the burner.
- $-\alpha = 35^{\circ}$ . The camera is positioned off the axis in order to visualize a selected region of the surface of the burner. These images are used to identify the locations where flashback is initiated and how the flashback process begins.

#### **3.5.2. Flame front evolution over the burner cross section during flashback**

This section analyzes flashback with the high-speed camera aligned with the axis of the burner  $(\alpha = 0)$ . Two operating conditions are considered. The first, case A,



<span id="page-58-0"></span> $\phi = 0.75$ <br>PH<sub>2</sub> = 67%  $0.9$ weld Normalized image  $0.8$  $10 \text{ mm}$  $0.7$  $0.6$  $= 0.062 \text{ m}$  $t = 0.5$ ms  $t = 1.0$  ms 1053 K  $0.5$  $0.4$ mtensity  $0.3$  $0.2$  $0.1$  $\Omega$ 

**(b)** case B:  $\phi = 0.75$ ,  $P_{H_2} = 67\%$ ,  $P \approx 3$  kW

**Figure 3.16. –** Comparison of the flame front propagation during flashback for (a) a relatively low wall temperature  $T_{w,f} = 953$  K and (b) a relatively high wall temperature  $T_{w,f} = 1053$  K. Weld position is indicated by the white arrow. The burner surface is depicted by the dashed circle.

is characterized by a global equivalence ratio  $\phi_g = 0.60$  and a hydrogen substitution  $P_{H_2} = 100\%$ . The second, case B, features  $\phi_q = 0.75$  and  $P_{H_2} = 67\%$ . These cases were selected because the wall temperatures at which flashback occurs  $T_{w,fb}$  differ by more than 100 K, so that they are representative of extreme operating conditions observed in the regime II of Fig. [3.13](#page-54-0) for both burners. The power is fixed to P*th*  $\approx$  3 kW and the ratio between the mean bulk flow velocity and laminar burning velocity evaluated at the gas temperature  $(U_b/S_L)_{T_u}$  remains almost the same in both cases, being respectively 0*.*64 and 0*.*62.

The propagation of the flame front during flashback for cases A and B is presented in Figs.  $3.16(a-b)$  $3.16(a-b)$  with 6 snapshots over a time frame of 10 ms. The position of the weld is indicated by the white arrows, and the location of the burner wall is indicated with a white dashed circle. The colormap indicates the normalized light intensity. Overall, the dynamics of the flame propagation in Figs. [3.16](#page-57-0) (a-b) appears to be very similar for cases A and B. Initially  $(t = 0.062 \text{ ms})$  a single flame spot appears in the neighborhood of the weld. This is a preferential location where the flame starts propagating inside the burner, and it was verified to be so irrespective of the weld angular position [\[66\]](#page-157-0). As the flame propagates inside the burner, the expansion of the <span id="page-59-0"></span>hot gases pushes the fresh reactants on the opposite side through the burner outlets. This transient phenomenon generates an instantaneous and localized acceleration of the fresh gases, which leads to flames that are longer and more intense ( 3.0 ms  $< t < 10.0$  ms). Simultaneously, the flame propagation inside the burner volume is characterized by two different phases. Till  $t = 1.0$  ms the flame evolves as a hemispherical flame front centered around the location of the initial spot. Between *t*  $= 1.0$  ms and  $t = 10.0$  ms, instead, the flame front propagates more rapidly along the burner wall than along the central part of the burner. This feature was investigated considering the same experiments for operating conditions belonging to the flashback regime III, for which flashback occurs during ignition and so preventing the burner walls to heat up (see Section [3.4.4\)](#page-52-0). In this last case, the flame front does not accelerate along the burner walls but a large flame bulge propagates from the initial flame spot along the diametral direction (see [\[66\]](#page-157-0) for further details). Hence, it is demonstrated that the thermal state of the burner is not only determinant to trigger flashback, but it also influences substantially the flame dynamics inside the burner. Furthermore, it is interesting to note that for both cases investigated, A and B, the flashback begins near the weld and at relatively high temperature. In view of that, the mechanisms triggering the flashback phenomena are investigated by zooming with the high-speed camera over the weld region.

#### **3.5.3. Flashback mechanisms: autoignition vs flame propagation**

This section analyzes the flashback process with the high-speed camera positioned off axis  $(\alpha = 35^{\circ})$ , with a field of view that focuses on the weld location.

Figures [3.17\(](#page-59-0)a-b) display the flashback evolution for case A, in the left column, and case B, in the right column. The sampling rate of the images is 16 kHz, which allows to identify the exact location where the flashback process begins and track the flame front propagation afterwards. The first row of images shows the initial condition  $t = 0.0$  s, where flames are safely stabilized on the external side of the burner for both cases and they are not visible from the presented field of view. The flashback initiation is put in evidence in the second row of Fig.  $3.17(a-b)$  $3.17(a-b)$ , where a zooming view of the ignition point highlights two different mechanisms. In case A, the first flame spot occurs in correspondence of a *round hole* (see Fig. [2.3\)](#page-35-0). Presumably, the flame is able to propagate from the external to the internal side of the burner without quenching when it passes through the hole and then propagates freely in the fresh mixture of reactants. This mechanism is defined as *hole initiation*. In case B, instead, the first flame spot appears at the weld location and the initial flame kernel is far from the burner holes behind which the flames are normally stabilized. This case suggests that flashback originates from a spontaneous ignition of the combustible mixture in contact with the hot walls and, in virtue of that, is defined as *wall initiation*. Experiments were repeated 10 times for each operating condition giving consistent outcomes.

To investigate the origin of these two scenarios, one should recall that the only substantial difference between the two operating conditions is the temperature of the burner walls when flashback occurs. In case A,  $T_{w,fb}^A = 953$  K and, in case B, the temperature  $T_{w,fb}^B = 1053$  K is higher. The first one is close to the cross over temperature discussed in Section [1.2.5,](#page-24-0) while the latter  $T_{w,fb}^B$  is higher. The hypothesis is that this temperature difference results in a large variation of the mixture reactivity, that eventually governs the type of flashback observed. Hence, it is necessary to evaluate the temperature of the fresh gases when flashback occurs

<span id="page-60-0"></span>

a) case A:  $\phi_g = 0.60$ ;  $P_{H_2} = 100\%$  b) case B:  $\phi_g = 0.75$ ;  $P_{H_2} = 67\%$ 

**Figure 3.17.** – Five chronologically-ordered images (top-bottom) track the flame front dynamics illustrating the onset of flashback and the flame propagation inside the cylindrical burner with the camera positioned at  $\alpha = 35^{\circ}$ . The left column (a) shows the flashback evolution for the operating condition A:  $\phi_g$  $= 0.60$ ;  $P_{H_2} = 100\%$ . The right column (b) shows the flashback evolution for the operating condition B:  $\phi_g = 0.75$ ;  $P_{H_2} = 67\%$  (b). The top images report the location of the weld, indicated by a white arrow, and the local temperature near the weld, indicated as *Twd*.

<span id="page-61-1"></span>CHAPTER  $3: H_2$  substitution of natural-gas in multiperforated burners and implications for blow-off and flashback limits



**Figure 3.18.** – Evolution of ignition delay time for  $CH_4 - H_2/air$  mixtures at  $\phi = 0.6$ , as a function of inlet gas temperature  $T_u$  and  $H_2$ -hybridization power rate *PH*2. Studied cases A and B are represented by the filled disks.

and their propensity to autoignite for the different operating conditions. As a first approximation, the temperature of the fresh gases in contact with the internal walls of the burner surface can be approximated with the measured external wall temperature  $T_{w,fb}$ . In fact, since the thickness 0.6 mm of the burner wall is very small and the conductivity of the stainless steel relatively high  $\lambda \approx 15$  W m<sup>-1</sup> K<sup>-1</sup>, the characteristic Biot number is small and the wall temperature can be considered uniform over the wall thickness. Moreover, Fig. [3.18](#page-60-0) shows the characteristic autoignition time delay  $\tau_i$  with respect to the mixture temperature  $T_u = T_{w,f}$  for an equivalence ratio  $\phi_g = 0.6$  and for different mixture compositions, from pure methane  $P_{H_2}$  = 0% to pure hydrogen  $P_{H_2} = 100\%$ . Data are obtained from CANTERA 0D simulations performed with GRI-MECH 3.0 chemical mechanism. The points associated to the operating conditions A and B are reported in blue and red respectively in Fig. [3.18,](#page-60-0) showing that the difference between the autoignition time delay is almost two order of magnitudes:  $\tau_i^A \approx 1$  ms and  $\tau_i^B \approx 0.05$  ms. This suggests that when the temperature is above 1000 K the autoignition process is likely to happen and the *wall initiation* mechanism dominates. When the temperature is below the cross over temperature of 950 K, instead, the rate of reactions slows down. In this last case the autoignition time is too large and the preferential mechanism leading to flashback is the *hole initiation*.

<span id="page-61-0"></span>To check the consistency of these results and to analyze the cause-effect relation between the type of flashback mechanism and the burner wall temperature, 9 additional operating conditions listed in Table [3.5](#page-61-1) are considered. They share the same input thermal power  $P_{th} = 3$  kW while all the other main parameters considered in this study such as the global equivalence ratio  $\phi_g$ , hydrogen substitution  $P_{H_2}$  and the ratio of bulk velocity over laminar burning velocity evaluated at the preheated reactants temperature  $(U_b / S_L)_{T_u}$ , are varied. Data in Table [3.5](#page-61-1) shows that  $\tau_i$  is the only parameter well correlated with the type of flashback mechanism observed experimentally. There is a net distinction between the *hole initiation* cases with wall temperature at flashback  $T_{w,f}$  around 950 K and the *wall initiation* cases for which the temperature of the wall at flashback  $T_{w,f}$  is above 1000 K. This confirms that,

	$\phi_q$ - $P_{H_2}$	$(U_b/S_L)_{T_u}$ $T_{w,f}$		ms $\tau_i$	flashback mecha-
					nism
1.	$0.60 - 100\%$	0.64	953	5.43	hole initiation
2.	$0.61 - 100\%$	0.63	940	23.00	hole initiation
3.	$0.67 - 88\%$	0.61	953	5.65	hole initiation
4.	$0.70 - 85\%$	0.59	950	7.86	hole initiation
5.	$0.72 - 85\%$	0.57	937	25.00	hole initiation
6.	$0.71 - 72\%$	0.59	1050	0.28	wall initiation
7.	$0.73 - 68\%$	0.59	1055	0.26	wall initiation
8.	$0.75 - 67\%$	0.57	1058	0.30	wall initiation
9.	$0.78 - 65\%$	0.55	1067	0.29	wall initiation

**Table 3.5.** – Example of operating conditions that result in different flashback mechanisms. The thermal power is fixed to 3 kW. For each case, the global equivalence ratio  $\phi_g$ , the *H*<sub>2</sub> substitution in the fuel  $P_{H_2}$ , the velocity ratio  $U_b/S_L$  at  $T_{u,f}$ , wall temperature at flashback  $T_{w,f}$ , the characteristic autoignition time delay  $\tau_i$ and the flashback mechanism are indicated.

in case of hydrogen substitution, autoignition can be a potential cause of flashback in real applications that is never observed for  $CH<sub>4</sub>$ -air mixtures.

To sum up, two mechanisms have been identified for operating conditions pertaining to the flashback regime II. When the reactivity of the mixture is high enough, the flame gets closer to the burner wall and the temperature of the burner surface increases up to a point where it acts as source of ignition for the reactants that are flowing against the hot wall. Flashback is then dominated by autoignition. When the reactivity of the mixture remains moderate, instead, the burner wall temperature does not overcome the cross-over temperature [\[14\]](#page-154-0) (see chapter [1\)](#page-13-0). The reaction rate remains low and autoignition is inhibited. In this case, though, the temperature of the wall is sufficiently high to inhibit thermal quenching and the flame front is able to propagate upstream the hole.

# **3.6. Conclusions**

Hydrogen hybridization of two commercial premixed burners, used in condensing boiler applications and designed to operate with natural gas - air mixtures, has been investigated. The burners have been tested in the low-power range, analyzing blow-off and flashback limits over a wide range of equivalence ratio for methane, hydrogen and air mixtures. Stability maps demonstrate that  $H_2$  addition improves the blow-off resistance, but it also limits the maximum achievable equivalence ratio due to overheating or flashback, leaving the range of stable operating conditions roughly unchanged but shifted towards lower equivalence ratios as the hydrogen concentration in the fuel blend increased. Because of these constraints, pure hydrogen combustion is possible only at ultra-lean conditions, while the maximum hydrogen concentration for a given thermal power and equivalence ratio is found to be variable with the burner design.

The study also underlines the impact of hydrogen preferential diffusion associated to a lewis number *Le* lower than unity on lean flame stabilization. To this regard, it has been highlighted a specific mechanism that contributes to blow-off resistance related to the high diffusivity of hydrogen, through which flames stabilize in the wake flow between holes rather than in the shear layer of the jet through the holes.

For a fixed equivalence ratio, the increment of  $H_2$  enrichment above a certain threshold leads to flashback. It has been shown that this limit is governed by the burner wall temperature  $T_w$ . To this respect, three regimes have been identified depending on the mixture composition and on the burner design. The first regime (I) is characterized by stable flames, without risk of flashback. In regime II, flashback is piloted by the thermal state of the burner after ignition and occurs at a specific temperature  $T_w = T_{w,fb}$  reached by the wall. This threshold temperature  $T_{w,fb}$ decreases with increasing the reactivity of the mixture. In regime III, flashback occurs during the ignition process, irrespective of the burner wall temperature *Tw*. This regime is characterized by very high hydrogen content and equivalence ratio close to stoichiometry.

In order to shed light on the physical phenomena that govern the regime II, a modified version of the burner *B*2 with optical access has been tested. High-speed images of the flame dynamics focused on the location where flashback begins, put in evidence that two distinct mechanisms are possible depending on the temperature of the burner walls. When this temperature is below the cross over temperature of the reactive mixture (i.e. near 950 K), flashback takes place via a propagation of the flame through the burner holes. When the wall temperature is above 1000 K, instead, the autoignition delay time drops by two order of magnitude for large hydrogen enrichments and the flashback is dominated by the autoignition of the reactants flowing against the internal side of the burner surface. This double scenario only exists for H2-enriched mixtures and raises important safety issues that must be considered to design and optimize future technologies.

The results presented in this Chapter have been published in two peer reviewed articles in the International Journal of Hydrogen Energy [\[66,](#page-157-0) [104\]](#page-160-4).

# **Part II.**

**Numerical analysis of turbulent premixed CH**4**/H**2 **swirling flames: the MIRADAS burner case.**

# <span id="page-66-1"></span> $CHAPTER$ <sub>-</sub> $4$

# **Methodologies for high-fidelity LES in advanced combustion systems**

This chapter presents the system of equations used to model compressible and multi-component gaseous reactive flows underlining the main physical and numerical assumptions generally enforced for their implementation. The objective is to discuss the limitations of these hypothesis for  $H_2$ -enriched mixtures and consider how the specificity of the AVBP flow solver may be adapted to it. An exhaustive description of the topic is out of the scope of the present work, since all the details can be found in specialized literature, like for example in [\[105,](#page-160-5) [106,](#page-160-6) [107\]](#page-160-7).

#### **Overview**

<span id="page-66-2"></span>

# **4.1. Conservation equations**

<span id="page-66-0"></span>All the flow problems considered in this work can be well reproduced within the framework of continuous mechanics. The set of equations to be integrated in order to describe compressible viscous reactive flows read:

$$
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \quad i = 1, \dots, N_{dim} \tag{4.1}
$$

$$
\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i} \left( \rho \left( u_i + V_{k,j} \right) Y_k \right) = \dot{\omega}_k \quad k = 1, \dots, N_s \tag{4.2}
$$

$$
\frac{\partial}{\partial t}\rho u_j + \frac{\partial}{\partial x_i}\rho u_i u_j = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} + \rho \sum_{k=1}^N Y_k f_{k,j} \quad i, j = 1, ..., N_{dim} \tag{4.3}
$$

<span id="page-67-0"></span>
$$
\rho \frac{Dh_s}{Dt} = \dot{\omega}_T + \frac{Dp}{Dt} + \frac{\partial}{\partial x_i} \left( \lambda \frac{\partial T}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left( \rho \sum_{k=1}^N h_{s,k} Y_k V_{k,i} \right) + + \tau_{ij} \frac{\partial u_i}{\partial x_j} + \dot{\mathcal{Q}} + \rho \sum_{k=1}^N Y_k f_{k,i} V_{k,i}
$$
(4.4)

The first equation imposes the mass conservation where  $\rho$ ,  $t$  and  $u_i$  are the density, the time and the velocity component along the i-th direction, respectively. Here,  $x_i$ refers to the  $j^{th}$  spatial direction following the Einstein's notation.

Equation (4.2) describes the evolution of the  $N_s$  species mass fraction  $Y_k$  in time and space. The quantities  $V_{k,j}$  are the diffusion velocities of the species *k* in the  $j<sup>th</sup>$ direction. The source term  $\dot{\omega}_k$  on the RHS of [Eq. \(4.2\)](#page-65-1) represents the volumetric mass generation/consumption of species *k* due to chemical reactions.

Equation  $(4.3)$  corresponds to the momentum conservation. Here,  $p$  is the static pressure and  $\tau_{ij}$  is the second order symmetric viscous stress tensor, while  $f_{k,i}$  is the resulting volume force acting on the species *k* along the direction *i*. The latter is neglected in this work because it is negligible in the deflagration problems [\[105\]](#page-160-5) considered.

Finally, [Eq. \(4.4\)](#page-66-1) expresses the energy conservation and it is written considering the sensible enthalpy  $h_s$  per unit mass of the mixture:

$$
h_s = \sum_{k=1}^{N} Y_k h_{s,k}
$$
\n(4.5)

corresponding to the mass fraction weighted averaged of the sensible enthalpy *hs,k* of each of the *k* species. The term  $\dot{\omega}_T$  is the heat release rate due to the ensemble of the chemical reactions:

$$
\dot{\omega}_T = \sum_{k=1}^N \Delta h_{f,k}^0 \dot{\omega}_k \tag{4.6}
$$

where  $\Delta h_{f,k}^0$  is the formation enthalpy of the species *k*. This is a challenging term from modeling point of view and it will be briefly discussed in Section [4.1.4.](#page-69-0) The additional terms in Eq.  $(4.4)$  are the heat diffusion where T denotes the temperature and  $\lambda$  denotes the fluid conductivity of the mixture, the enthalpy variation created by species diffusion, the heat flux due to viscous dissipation, all external volumetric heat sources (i.e. a spark) and the power associated to the work of body forces.

#### **4.1.1. Ideal gas assumption**

Considering the ambient thermodynamic conditions investigated in this work, mixtures are rarefied enough to be modeled using the state equation of the ideal gas:

$$
\rho = p \frac{R}{W} T \tag{4.7}
$$

where  $W$  is the mean molecular weight of the gaseous mixture and  $R$  the universal constant  $R = 8.34$  J/mol/K

#### **4.1.2. Hypothesis of newtonian fluid**

<span id="page-68-0"></span>The constitutive Newton law is adopted to enforce a direct proportionality between the viscous stress tensor  $\tau_{i,j}$  and the velocity gradients. This relation reads:

$$
\tau_{i,j} = \left[ \left( -\frac{2}{3}\mu \right) \frac{\partial u_k}{\partial x_k} \delta_{ij} + \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right]
$$
(4.8)

where  $\delta_{ij}$  is the Kronecker operator and the molecular dynamic viscosity  $\mu$  is the constant of proportionality, that must be properly evaluated. Throughout the manuscript the strong assumption is that the dynamic viscosity depends only on temperature and not on the local mixture composition. Specific laws permit to evaluate its variation knowing a reference value  $\mu_{ref}$  for a defined temperature  $T_{ref}$ . This approach is reasonable in case of fully premixed combustion because the molar fraction of fuel is negligible with respect to the air molar fraction and the dynamic viscosity of the mixture can be approximated imposing  $\mu = \mu_{air}$ . Nevertheless, errors may arise when simulating non-premixed combustion, like in real systems in which the high reactivity of  $H_2$  (see Sec[.1.2\)](#page-18-0) requires to have separated injections. It is important to predict the correct mixing among reactants and, at least in case of *low Reynolds number flows*<sup>[1](#page-3-0)</sup>, requires a good evaluation of the molecular transport properties. This is important because in the AVBP solver the local evaluation of the molecular diffusion coefficients  $D_k$  for species k and  $D_{th}$  for heat depends on the dynamic viscosity following the sketch below:

$$
\mu \longrightarrow \lambda \longrightarrow_{Sc_k} D_{th} \longrightarrow D_k
$$

The Prandtl number *Pr*, the Schmidt number *Sc<sup>k</sup>* of the species *k* and the Lewis number  $Le_k$  of species  $k$  are inputs of the simulation that will be defined in the next Section. If  $\mu = \mu_{air}$  and it differs substantially from the fuel viscosity, the evaluation of the diffusion properties in fuel rich regions (i.e. where the majority of the mass fraction is fuel) may not be representative of the real physical problem. In other words, in case of non-premixed flames, the dynamic viscosity  $\mu$  should depend also on the local composition. The easiest alternative approach is to calculate the dynamic viscosity  $\mu_w$  by considering a fictitious mixture made of only two species (i.e.  $H_2$  and  $air$ ) and applying the Wilke law:

$$
\mu_w = \sum_{i=1}^{N} \frac{X_i \mu_{ref,i}}{\sum_{j=1}^{N} X_j \phi_{ij}} \tag{4.9}
$$

$$
\phi_{ij} = \frac{\left[1 + \left(\frac{\mu_{ref,i}}{\mu_{ref,j}}\right)^{1/2} \left(\frac{W_j}{W_i}\right)^{1/4}\right]^2}{2\sqrt{2}\left(1 + \frac{W_i}{W_j}\right)^{1/2}}
$$
(4.10)

where  $X_i$  is the molar fraction of species *i*,  $\mu_{ref,i}$  is the reference dynamic viscosity for the i<sup>th</sup> species, W<sub>i</sub> its molecular weight and  $\phi_{i,j}$  is given by [Eq. \(4.2\)](#page-65-1) and equal to unity in case of  $i = j$ .

For hydrogen-air mixtures the value of the actual molecular dynamic viscosity adopted in the computation varies between  $\mu_{air}$  and  $\mu_{H_2}$  depending only on the H<sub>2</sub> molar fraction. In AVBP this type of modeling has been introduced only recently and it is not used in the present manuscript. Nevertheless, the non-premixed  $H_2$ -air

<sup>1.</sup> What is low and what is high is always a tricky question to answer.

swirled flame computed in Part 3 of this manuscript will be used a-posteriori to test the impact of this approach on the final results.

#### <span id="page-69-0"></span>**4.1.3. Simplified molecular transport properties**

The transport of the species in the flow is regulated by Eq.  $(4.2)$ . In this expression, a proper evaluation of the diffusion velocities  $V_{k,i}$  would require to solve  $N_s^2$  $s^2$  equations for each position, time-step and direction [\[40,](#page-155-2) [105\]](#page-160-5). The cost of this computation increases with the squared number of species considered and, since numerical reactive simulations may require the adoption of complex chemistry, the computational cost becomes prohibitive. In the numerical flow model, this problem is overcome by using a non-binary equivalent diffusion coefficient  $D_k$  for each species *k* according to *Hirschfelder and Curtis* approximation [\[105\]](#page-160-5) and by prescribing a correction of the diffusion velocity to guarantee mass conservation.

<span id="page-69-1"></span>The molecular transport properties of each gaseous species are defined by the mean diffusion coefficient of the species  $D_k$  with respect to the mixture, the thermal conductivity  $\lambda$ , the kinematic viscosity  $\nu$  and the specific constant pressure heat capacity  $C_p$  of the mixture. This can be resumed considering the following nondimensional parameters:

$$
Sc_k = \frac{\nu}{D_k} \tag{4.11}
$$

$$
Le_k = \frac{\lambda}{\rho C_p D_k} = \frac{D_{th}}{D_k} \tag{4.12}
$$

$$
\Pr = \frac{\mu C_p}{\lambda} = \frac{\nu}{D_{th}} = \frac{Sc_k}{Le_k} \tag{4.13}
$$

In AVBP the standard approach considers a variable Schmidt number *Sc<sup>k</sup>* for the species *k* with respect to the rest of the mixture, and a constant *Pr* specified by the user. This approach defines univocally the Lewis number *Le<sup>k</sup>* of each species *k*. This simplified approach is reasonable in many problems where the variations of temperature and mixture composition across a flame do not affect the Prandtl number  $Pr$  consistently, like for instance in premixed  $CH<sub>4</sub>$ -air flames.

Nevertheless, there are cases in which the variation of the *Pr* becomes important and can affect the final result [\[108\]](#page-160-8). In non-premixed  $H_2$  flames the non-homogeneity of the mixture may cause a large variation of the local species and heat transport properties. Figure [4.1](#page-69-1) can be find in [\[108\]](#page-160-8) and shows the results of CANTERA calculations for a  $H_2$  diffusion flame computed with different transport models. The multicomponent transport highlights a large variation of the Schmidt number  $Sc_k$ of the species, which puts in evidence the limits of the constant Prandtl number assumption.

In particular, Fig  $4.1(d)$  $4.1(d)$  shows a contour map of the Schmidt number  $Sc_{N_2}$  of  $N_2$  and isolines of the Prandtl number *Pr* in a ternary mixture of  $H_2/CH_4$  and air. When the molar fraction of  $H_2$  tends to zero, the variations of  $Sc_{N_2}$  and  $Pr$ are negligible irrespective of the local composition, meaning that the assumption of simplified transport properties continues to hold. When the molar fraction of  $H_2$ increases in a ternary mixture, instead,  $Sc_{N_2}$  may change by a factor 5 and the  $Pr$ number reduces up to 35%. In this respect, it might be necessary to account for a variable  $Pr$ . This strategy is used in Part 2 for  $CH<sub>4</sub>/H<sub>2</sub>/air$  turbulent swirled flames. In practice, the Prandlt number *Pr* is tabulated as function of the local molar fractions of reactants and  $N_2$ , like in Fig. [4.1.](#page-69-1) The latter approach is then used to evaluate the local diffusion coefficients in time and space.

#### **4.1.4. The Arrhenius law formalism**

The energy equation [Eq. \(4.4\)](#page-66-1) for reactive flows includes the heat release rate per unit volume  $\dot{\omega}_T$ . To evaluate this term is necessary to know the sum of mass reaction rates  $\dot{\omega}_k$  of each species *k* through all the reactions *j* appearing in [Eq. \(4.6\).](#page-66-2) In a chemical system of *N<sup>s</sup>* species and *M* reactions, this term reads:

$$
\dot{\omega}_k = \sum_{j=1}^{M} \dot{\omega}_{kj} = W_k \sum_{j=1}^{M} \nu_{kj} \Omega_j,
$$
\n(4.14)

where  $\Omega_j$  is the rate of progress of the reaction *j* and  $\nu_{kj}$  derives from the difference between the molar stoichiometric coefficient of the species  $k$  in the reaction  $j$  [\[105,](#page-160-5) [106\]](#page-160-6). The unknown here is  $\Omega_i$ , which can be written for each reaction *j* as:

<span id="page-70-0"></span>

<span id="page-70-1"></span>**Figure 4.1.** – Figure adapted from [\[108\]](#page-160-8). (a-b) Comparison between flame structures computed with Cantera using GRI-3.0 including multicomponent transport and Soret effect (dashed lines), the ARC scheme with a mixture transport model (dark line) and simplified transport model (light line), for a  $H_2$  / burnt gases counterflow diffusion flame. Normalized profiles of (a) mass fraction of selected species; (b) temperature and heat release rate. (c) Profiles of the transport properties. Computation inputs are:  $p = 1$  bar, injection temperature of  $T_{i,H_2} = 570$  K and exhaust gas temperature  $T_{i,g} = 1800$  K. (d) Isolines of the Prandtl number and contour map of  $N_2$  Schmidt number in ternary mixture of  $H_2$ , CH<sub>4</sub> and  $N_2$  as a function of composition

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$$
\Omega_j = K_{fj} \prod_{k=1}^N \left[ X_k \right]^{\nu'_{kj}} - K_{rj} \prod_{k=1}^N \left[ X_k \right]^{\nu''_{kj}} \tag{4.15}
$$

where  $\nu'_{kj}$  and  $\nu''_{kj}$  are the molar stoichiometric coefficients of species *k* in reaction *j*,  $K_{fj}$  and  $K_{rj}$  are the forward and backward reaction rates of the reaction *j* and  $X_k$  the molar fraction of species  $k$ . These reaction rates must be known for each reaction and are indeed modeled with an Arrhenius law:

$$
K_{fj} = A_{fj} T^{\beta_j} \exp\left(-\frac{E_j}{RT}\right) = A_{fj} T^{\beta_j} \exp\left(-\frac{T_{aj}}{T}\right)
$$
(4.16)

where  $A_{fj}$ ,  $\beta$  and  $E_j$  are the pre-exponential factor, the exponent of the temperature and the activation energy for the  $j<sup>th</sup>$  reaction. Thanks to the Arrhenius assumption,  $\dot{\omega}_T$  is evaluated specifying three parameters for each reaction that can describe with accuracy the chemical kinetics of the system.

# **4.2. LES filtering and numerical modeling**

<span id="page-71-1"></span>The previous set of equations is not solved directly as in Direct Numerical Simulations. A Large Eddy Simulation (LES) framework is used instead. LES formalism is based on the Favre spatial filtering of the fully compressible Navier-Stokes equations presented in Section [4.1.](#page-65-0) The filtered equations are composed by (1) spatially filtered flow quantities and (2) *sub-grid* quantities. The first are resolved and correspond to the largest turbulent scales, while the second are not captured by the spatial filter and require a proper closure. LES filtered equations appear as follow:

$$
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho}\tilde{u}_i) = 0 \tag{4.17}
$$

$$
\frac{\partial \left(\bar{\rho}\tilde{Y}_k\right)}{\partial t} + \frac{\partial}{\partial x_i} \left(\bar{\rho}\tilde{u}_i \tilde{Y}_k\right) = \frac{\partial}{\partial x_i} \left[\overline{V_{k,i}Y_k} - \bar{\rho}\left(\widetilde{u_i Y_k} - \tilde{u}_i \tilde{Y}_k\right)\right] + \overline{\dot{\omega}}_k \quad k = 1, N \quad (4.18)
$$

$$
\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i \tilde{u}_j) + \frac{\partial \bar{\rho}}{\partial x_j} = \frac{\partial}{\partial x_i} [\bar{\tau}_{ij} - \bar{\rho} (\tilde{u}_i u_j - \tilde{u}_i \tilde{u}_j)] \tag{4.19}
$$

<span id="page-71-2"></span>
$$
\frac{\partial \bar{\rho} \tilde{h}_s}{\partial t} + \frac{\partial}{\partial x_i} \left( \bar{\rho} \tilde{u}_i \tilde{h}_s \right) = \frac{\overline{Dp}}{Dt} + \frac{\partial}{\partial x_i} \left[ \lambda \frac{\overline{\partial T}}{\partial x_i} - \bar{\rho} \left( \widetilde{u_i h_s} - \tilde{u}_i \tilde{h}_s \right) \right] + \frac{\overline{\partial u_i}}{\overline{\partial x_j}} - \frac{\partial}{\partial x_i} \left( \rho \sum_{k=1}^N V_{k,i} Y_k h_{s,k} \right) + \overline{\tilde{\omega}}_T \tag{4.20}
$$

where  $\overline{(.)}$  is the Reynolds averaged operator and  $\widetilde{(.)}$  represent the mass-weighted Favre average operator<sup>[2](#page-3-0)</sup>. In Eq.  $(4.20)$  body forces have been neglected and is also assumed that there is no external volumetric heat sources. The main terms to be modeled are described below.

<sup>2.</sup> The mass-weighted Favre average of a variable f,  $\widetilde{(f)}$  is defined such as:  $\widetilde{(\rho)(f)} = \widetilde{(\rho f)}$
# **4.2.1. Unresolved Reynolds stresses**  $\overline{\tau_{ij}}^t = (\widetilde{u}_i u_j - \widetilde{u}_i \widetilde{u}_j)$

Unresolved Reynolds stresses are generally modeled following the Boussinesq approximation which, under the hypothesis that turbulent fluxes follow similar functions and form as molecular diffusion, expresses the Sub-Grid Scale (SGS) stress tensor as function of a turbulent viscosity  $\nu_t = \mu_t / \overline{\rho}$ :

$$
\overline{\tau_{ij}}^t \approx 2\bar{\rho}\nu_t \left( \tilde{S}_{ij} - \frac{1}{3} \delta_{ij} \tilde{S}_{ll} \right) \tag{4.21}
$$

<span id="page-72-0"></span>where:

$$
\widetilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \widetilde{u}_j}{\partial x_i} + \frac{\partial \widetilde{u}_i}{\partial x_j} \right) \tag{4.22}
$$

Following this approach, the problem consists in finding a proper model for  $\nu_t$  that is suitable for the specific application. Several approaches are possible. For instance, algebraic static models rely on fixed constants that are highly dependent on the configuration investigated and are then limited to canonical cases for which exists enough experimental data for the calibration. Dynamic approaches, instead, exploit a double spatial filter to deduce the SGS dissipation in order to provide a turbulent kinematic viscosity  $\nu_t$  that adapts in time and space [\[109\]](#page-160-0). Those are more accurate and also more expensive. In the present work the SIGMA model [\[110\]](#page-160-1) is adopted.

### **4.2.2. Unresolved species**  $(\widetilde{u_iY_k}-\widetilde{u}_i\widetilde{Y}_k)$  and enthalpy  $(\widetilde{u_ih_s}-\widetilde{u}_i\widetilde{h}_s)$ **transport**

These unresolved scalar transport can be approximated adopting the gradient assumption. The following equation shows the approximation for the species diffusion flux:

$$
\widetilde{u_i Y_k} - \widetilde{u}_i \widetilde{Y}_k \approx \frac{\nu_t}{S c_k^t} \frac{\partial \widetilde{Y}_k}{\partial x_i} \tag{4.23}
$$

where the turbulent kinematic viscosity  $\nu_t$  is obtained from the  $\overline{\tau_{ij}}^t$  modeling described above, and the turbulent Schmidt number  $Sc<sup>t</sup><sub>k</sub>$  is specified by the user. A dual problem arises to model the SGS enthalpy flux, which requires the user to also specify a turbulent Prandtl number  $Pr_k^t$ .

#### **4.2.3. Chemical reaction rate**  $\dot{\omega}_T$

The simplest approach to evaluate the chemical reaction rate  $\dot{\omega}_T$  is to consider only the filtered quantities, neglecting the subgrid scale fluctuations. It supposes a perfect mixing at the subgrid scale level and it is not valid, for instance, when the turbulent mixing time scale  $\tau_t$  is much smaller than the characteristic chemical time scale *τchem* (i.e. low limit of the Damkholer number *Da*), which is the case in most LES. The limitations of this assumption can be relaxed by considering turbulent dynamic combustion models that exploit the resolved quantities to derive information at subgrid scale level to adapt the model locally, like for example in [\[111,](#page-160-2) [112\]](#page-160-3).

#### **4.2.3.1. Dynamic Thickened Flame Model (DTFLES)**

This study uses the dynamic thickened flame model DTFLES approach [\[113,](#page-160-4) [114,](#page-160-5) 115. In principle, this modeling method increases the molecular thermal diffusion  $D_{th}$  by a thickening factor  $F$  and simultaneously divides the pre-exponential factor shown in [Eq. \(4.16\)](#page-70-0)  $A_{fj}$  by the same amount *F*. For the seek of simplicity,  $A_{fj}$  is replaced by *A* in this paragraph. As a result the thickened flame propagates at the same flame speed  $S_L^0$  of the original one, but with a characteristic flame thickness  $F\delta_0$ , where  $\delta_0$  is the original thermal flame thickness. Since the resulting flame is *thicker*, it can be resolved on a coarser mesh with a reasonable and adjustable computational cost. Figures  $4.2(a-b)$  $4.2(a-b)$  sketch the differences between a fully resolved flame (a) and a thickened flame by a factor  $F$  (b). It can be qualitatively seen that,

<span id="page-73-0"></span>

**Figure 4.2.** – Figure taken from [\[105\]](#page-160-7). DNS of flame turbulence interactions. Reaction rate and vorticity fields are superimposed. (a) reference flame; (b) flame artificially thickened by a factor  $F = 5$ . Because of the change in the length scale ratio  $l_t/\delta_L^0$  , combustion/turbulence interaction is changed and the thickened flame is less wrinkled by turbulence motions. This effect can be parametrized using a subgrid scale model.

under turbulent conditions, the thickening factor reduces the wrinkling of the flame front and the flame-turbulence interaction is underestimated due to an artificial variation of the Damkhöler number . In fact, the flame surface of the computed flame reduces and this has a direct penalty on the turbulent flame speed S*<sup>T</sup>* [\[114,](#page-160-5) [115\]](#page-160-6). To overcome this problem is necessary to retrieve numerically the impact of turbulence on the thickened flame and inject it in the model formulation. This is done by introducing an efficiency function  $\Theta$ , which constitutes a model on itself, based on physical and geometrical aspects of premixed flames [\[116\]](#page-161-0). In principle, Θ multiplies the flame speed to retrieve the correct turbulent flame velocity  $S_T = S_L^0 \Theta$ .

In practice, the implementation of the combustion model is obtained modifying [Eq. \(4.2\)](#page-65-0) as follow:

$$
\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}(\rho (u_i + V_i^c) Y_k) = \frac{\partial}{\partial x_i} \left(\rho \Theta F D_k \frac{W_k}{W} \frac{\partial X_k}{\partial x_i}\right) + \frac{\Theta \dot{\omega}_k}{F}
$$

where the original molecular diffusion,  $D_k$ , becomes  $\Theta FD_k$  and the original preexponential constant, *A*, becomes Θ*A/F*. Phenomenologically speaking, the term *F* provides the thickening and the term  $\Theta$  compensate for the deficiency of wrinkling intrinsically induced by *F*. These two parameters do not account for the potential coupling between turbulence and thermal-diffusional effects that have been briefly introduced in Section [1.2](#page-18-0) for lean premixed  $H_2$ -air mixtures, which may increase the flame consumption speed irrespective of the turbulent-induced flame wrinkling. A preliminary approach to include thermo-diffusive instabilities effects in the DT- FLES model was developed during the 2022 Center for Turbulent Research summer program at Stanford University and is proposed in Appendix [A.](#page-125-0) In the latter, the main hypothesis is that the wrinkling induced by Lewis number effects acts only at subgrid-scale level, without interacting with the wrinkling induced by turbulence, that is supposed to take place at larger scales.

#### **4.2.3.2. Modeling approach for non-premixed H**2 **flames**

In Part 3 of the manuscript we consider non-premixed  $H_2$ -air turbulent swirling flames with separated injection of reactants. In these conditions, it is desirable to have a combustion modeling approach that captures both premixed and nonpremixed combustion regimes. In this manuscript, the following approach is proposed. The premixed parts of the flame are modeled via the DTFLES approach [\[117\]](#page-161-1) which has been used successfully for many hydrocarbon and hydrogen-blended flames in previous studies, like for instance in [\[108,](#page-160-8) [118\]](#page-161-2). However, this model is calibrated on the physical properties of premixed flames and it is inappropriate for non-premixed flamelets modeling. Therefore, in these zones, the mesh must be fine enough to have a proper resolution of the flame structure and avoid flame thickening. The parameter used to distinguish between the premixed and the diffusion regimes is the normalized Takeno index [\[119\]](#page-161-3), which is locally updated at each simulation time-step. This is based on the scalar product between the mass fraction gradients of  $H_2$  and  $O_2$ . A positive value enables the DTFLES, while a negative one identifies the regions where DTFLES is not suitable for a proper combustion modeling. It is worth underlining that the aforementioned switch does not impact the momentum equation, which is computed in the entire domain using the SIGMA turbulent closure for the subgrid Reynolds stresses [\[120\]](#page-161-4). Moreover, the thickening of the flame associated to the DTFLES is modulated by a filter that provides its fast and smooth relaxation outside the premixed zone. This avoids numerical discontinuity at the interface between the two regimes and ensures that the DTFLES does not influence artificially the species diffusion in the resolved regions.

The advantage of this strategy is the possibility to resolve different combustion regimes adopting the same numerical setup and exploiting already established approaches. Its main drawback is the "DNS-like" grid requirement in the zone of nonpremixed flamelets to resolve the flame front. However, this further computational cost can be limited knowing in advance the regions where non-premixed fronts are expected, when experimental data are available as in the laboratory-scale swirling flames studied in this work, or making use of mesh refinement techniques [\[121,](#page-161-5) [122\]](#page-161-6). This approach is used both in Part 2 and 3 of the manuscript, where it will be further discussed.

# <span id="page-76-0"></span>CHAPTER  $5$

# Influence of pilot  $H_2$  injection **on methane-air swirled flame acoustic response**

Large-Eddy Simulations are used to investigate the effect of a localized pilot  $H_2$ injection on the Flame Transfer Function (*FTF*) of a perfectly premixed CH4-air swirled flame. Simulations are validated against experiments in terms of global *FTF* values at selected forcing frequencies, acoustic pressure and velocity signals,  $CH^*$  flame images and flame root position dynamics. The unforced cases are first considered showing that the  $H_2$  pilot injection leads to a global redistribution of the heat release towards the flame root. Then, the flame acoustic responses for the two injection strategies are scrutinized at two distinct forcing frequencies: 240 Hz where the  $FTF$  gain difference is maximum, and 590 Hz where the  $FTF$  phase shift is maximum. LES reveal that, despite  $H_2$  pilot injection does not modify the evolution of the velocity field over the forcing cycle, the redistribution of the heat release towards the flame base weakens the extent of the interaction between the large vortical structures and the flame tip. In addition to that, at 240 Hz is observed a marked axial movement of the internal recirculation zone along the forcing cycle. For the pilot injection it leads to an oscillation of the lifted flame root while, for the  $CH<sub>4</sub>$ -air case, the flame anchoring point is not affected. This additional oscillation leads to heat release rate fluctuations acting in phase opposition with respect to those observed at the flame tip, generating a further drop of the *FTF* gain at this specific frequency for the piloted case. The increased burning rate at the flame root and the flame length reduction of the pilot hydrogen flame also affect the characteristic time lag of the flame response. These simulations confirm that pilot hydrogen injection is an efficient way to reduce the acoustic response of swirled flames over a large frequency bandwidth.

#### **Overview**



### **5.1. Motivations of the study**

This Chapter focuses on the Flame Transfer Function  $(FTF)$  of  $CH<sub>4</sub>/H<sub>2</sub>$  flames, considering that  $H_2$  addition to hydrocarbon-air mixtures opens new challenges in the context of thermoacoustic instabilities [\[30,](#page-155-0) [32,](#page-155-1) [123\]](#page-161-7). As anticipated un Sec-tion [1.2,](#page-18-0) the peculiar chemical properties of  $H_2$  molecule [\[14\]](#page-154-0) may translate in different flame responses. The higher consumption speed [\[16,](#page-154-1) [17,](#page-154-2) [22\]](#page-154-3) and the greater resistance to strain [\[43,](#page-156-0) [124\]](#page-161-8) of  $H_2$ -enriched blends reduce the flame length [\[28\]](#page-155-2) and also promote the transition from V- to M-shape stabilization [\[125,](#page-161-9) [126,](#page-161-10) [127,](#page-161-11) [128\]](#page-161-12). Since thermoacoustic instabilities originate from a constructive coupling between acoustic oscillations and heat release rate fluctuations, these changes affect directly the stability of the combustor [\[129,](#page-161-13) [130,](#page-162-0) [131,](#page-162-1) [132\]](#page-162-2).

<span id="page-77-0"></span>A recent work [\[133\]](#page-162-3) proposed a comprehensive review on the effect of hydrogen addition on flame dynamics. Experimental investigations on the modifications on the *FTF* of a non-swirling premixed jet methane-air flame stabilized on a bluff body when hydrogen is added into the fuel mixture have been reported in [\[131,](#page-162-1) [134\]](#page-162-4). They show that, at constant total thermal power, hydrogen addition decreases (respectively increases) *FTF* gain at low (respectively high) frequencies while increasing the cut-off frequency. Moreover, thanks to the larger flame speed, the  $FTF$  phase reduces almost linearly with the  $H_2$  concentration in the fuel blend. Similar results have also been found in recent simulations [\[135,](#page-162-5) [136\]](#page-162-6). Hydrogen enrichment also modifies the flame acoustic response of hydrocarbon swirl-stabilized flames  $[137, 138]$  $[137, 138]$ . In such a configuration, however, the effects of hydrogen addition combine with other mechanisms controlling the *FTF* of a swirled flame (e.g. [\[139\]](#page-162-9)) making the interpretation of results less straightforward. A recent study conducted on an annular combustion chamber [\[140\]](#page-162-10) demonstrated that  $H_2$  enrichment had nonlinear influence on the development of azimuthal self-sustained instabilities, which were maximized for a certain hydrogen content and decreased for further  $H_2$  addition. In the same study it was shown that pressure variation could produce a stabilizing or destabilizing effect depending on the hydrogen content. The acoustic response of  $H_2$ -enriched flame up to  $40\%$ vol was also investigated in a dual-nozzle swirl stabilized combustor [\[141\]](#page-162-11), showing a gain reduction and phase shift with increasing hydrogen content due to a dierent flame roll-up. A modification of the flame-vortex interaction due to hydrogen addition was also highlighted in [\[142\]](#page-162-12), where either transient and steady variations of  $H_2$  content in NG-air mixture were used to control thermoacoustic instabilities in a technically premixed model gas turbine combustor. Instability onset processes were highly repeatable irrespective of the duration of  $H_2$  injection, while the transitions from unstable to stable operation were not always consistent. This variance was justified with the increasing temperature of the centerbody favored by hydrogen injection, which was ultimately affecting the flame response.

In all aforementioned cases, when blended with another fuel, hydrogen is always injected fully premixed. Nevertheless, the adoption of radially-stratified mixtures was also proposed as a technical solution to improve the combustion stability of swirling flames powered by different fuel blends, like for instance in [\[143,](#page-163-0) [144,](#page-163-1) [145\]](#page-163-2). Furthermore, the addition of a central piloting injection has been also proposed as a technical solution to stabilize swirling natural-gas flames [\[146,](#page-163-3) [147\]](#page-163-4). Recent experimental results on a swirled coaxial injector have shown that a small central H2 injection can also modify the stability maps of a swirled combustor operated with premixed methane-air mixtures [\[148\]](#page-163-5). Interestingly, this outcome was found neither by premixing  $H_2$  with the CH<sub>4</sub>-air mixture in the main annular channel, nor via the pilot injection of pure-CH4 in the central tube, suggesting that it is the combined result of both  $H_2$  addition and pilot injection strategy. The fundamental mechanisms driving the change of flame dynamics were, however, not clarified.

Flame Describing Function (*FDF*) of this configuration were also measured [\[149\]](#page-163-6) showing that the change of the flame acoustic response in case of pilot  $H_2$  is due to the redistribution of heat release provided by this injection strategy towards the flame root. However, the influence of pilot injection on the velocity field and on the flame root stabilization were not investigated. This specific configuration was also studied in a stable operating condition via LES [\[108\]](#page-160-8) and demonstrated the importance of accounting for complex transport properties, described in Section [4.1.3,](#page-68-0) to predict the correct flame stabilization. Nevertheless, in this previous numerical study, only a low hydrogen content case was considered (2% by power) and the acoustic response of the burner was not analyzed. The present work aims at elucidating the fundamental mechanisms that control the pilot- $H_2$  injection flame response to acoustic perturbations with respect to a perfectly premixed methane-air case at specific forcing frequencies.

The experimental and numerical setups are described in Sections [5.2](#page-77-0) and [5.3.](#page-79-0) Validation and analysis of the two injection strategies for the unforced cases are provided in Section [5.4](#page-81-0) by comparing simulations with experimental results. Forced flow conditions for a perfectly premixed methane-air mixture and with the addition of pilot hydrogen injection are validated and analyzed in Section [5.5,](#page-83-0) where the impact of the pilot  $H_2$  is presented and its implication on the flame response discussed.

#### <span id="page-78-0"></span>**5.2. Experimental setup and diagnostic**

The experimental setup investigated corresponds to the MIRADAS burner built at IMFT by Dr. Gorkem Oztarlik and it is an evolution of a swirled combustor originally developed at EM2C laboratory [\[139,](#page-162-9) [150,](#page-163-7) [151,](#page-163-8) [152\]](#page-163-9). Sylvain Marragou also contributed to this joint work, gathering experimental results on this bench to make this numerical study possible. The objective of the MIRADAS configuration is to test the influence of  $H_2$  addition on the flame dynamics of perfectly premixed  $CH<sub>4</sub>$ -air swirled flames. To do so, the system exploits an annular swirled injector with a central tube that is coaxial with the burner axis.

A sketch of the burner configuration is presented in Fig  $5.1(a)$  $5.1(a)$  and additional details can be find in [\[108,](#page-160-8) [148,](#page-163-5) [149\]](#page-163-6). A loudspeaker is mounted at the bottom of the bench to impose the targeted acoustic forcing and perform *FTF* and *FDF* measurements for a fixed power and velocity modulation. The fully premixed  $CH<sub>4</sub>$ air mixture is injected at the bottom of the combustor via a cylindrical plenum of diameter  $D = 65$  mm and length  $L = 146$  mm. The mixture passes through honeycombs that break the larger vortical structures resulting from the injection. Above the plenum there is a convergent section to produce a top-hat laminar velocity profile and is followed by a cylindrical element of  $D = 22$  mm diameter suitable to locate probes. This flow feeds the annular duct of the coaxial injector with external and internal diameters equal to 12 mm and 6 mm, as shown in Fig. [5.1\(](#page-78-0)b). This annular duct is equipped with a radial swirler to confer a rotational motion to the flow and generate a vortex breakdown in the combustion chamber. The swirler is made of 8 radial tangential inlets of 4.5 mm diameter each, which are  $15^{\circ}$  off the injector axis. Figure  $5.1(a-b)$  $5.1(a-b)$  shows also the central tube used to supply hydrogen <span id="page-79-1"></span>via a central pilot injection. This tube has an internal diameter of 4 mm and protrudes through the injector inside the combustion chamber by 1.25 mm. The burner backplane is water-cooled and kept to atmospheric temperature. The flame is confined in a quartz tube of 46 mm diameter and 100 mm length allowing for a full optical access.

The design of the injector offers the possibility to analyze different injection strategies. In this study, the two of them are illustrated in Fig. [5.1\(](#page-78-0)c) and consider:

- **–** A fully-premixed CH4-air mixture is injected only in the annular channel of the injector. Hydrogen is not used and this case is named *REF*.
- **–** The methane mass flow rate in the annular channel is reduced and a complementary  $H_2$  mass flow rate is added via the pilot tube in order to guarantee the original overall thermal power  $P_{th} = 4$  kW In this study hydrogen supplies 10% of the total *Pth* and this injection strategy is denoted as *PH*10 in the rest of this chapter.

For the *PH*10 case the variation of the bulk velocity  $U_b$  in the annular duct is negligible and the equivalence ratio varies by less than 2%. The operating conditions of *REF* and *PH*10 cases are summarized in Tab. [5.1.](#page-79-1)

H2, CH4 and air mass flow rates are controlled via three Bronkhorst controllers in order to varies the thermal power  $P_{th}$ , the hydrogen substitution in the fuel blend  $P_{H_2}$  and the global equivalence ratio  $\phi_g$ , independently. A PIMAX-4 intensified CCD camera equipped with a 105 mm Nikon Rayfact PF10545MF-UV lens shown

<span id="page-79-0"></span>

**Figure 5.1.** – Figures taken from [\[148,](#page-163-5) [149\]](#page-163-6). Schematic of the MIRADAS setup (a). The zoom on the upper part of the injector (b) shows the cooling channel of the injector rim, the dimensions of the combustion chamber and of both central and annular nozzles. The two injection strategies *REF* and *PH*10 are illustrated in (c). Dimensions are in millimeters.

<span id="page-80-0"></span>

Case		Annular	Pilot	Global	
	$\dot{m}_{Air}$ (g/s)	$\dot{m}_{\text{CH}_4}$ (mg/s)	$\dot{m}_{\text{H}_2}$ (mg/s)		
REF	$1.69\,$	79.1		0.800	
PH10	$1.69\,$	71.2	3.30	0.787	

**Table 5.1. –** Mass flow rates of air, methane and hydrogen with respective global equivalence ratios adopted for the two operating conditions.

in Fig. [5.1\(](#page-78-0)a) is used to record long exposure time flame images and phase conditional averages with respect to the acoustic forcing signal provided by the loudspeaker at the bottom of the burner. The camera is equipped with a narrow band interferometric filter centered at  $\lambda = 430$ nm to isolate the emission intensity of the CH<sup>\*</sup> radicals, which is a marker of the heat release rate distribution. A photomultiplier equipped with the same  $CH^*$  filter is also used to infer the global heat release rate fluctuations. As shown in Fig. [5.1\(](#page-78-0)a), a hot wire and a microphone are installed downstream of the convergent to measure the velocity *u* and the acoustic pressure fluctuations  $p'$ , respectively. These probes not only allow to control the amplitude of the acoustic forcing, but they are also used to validate the accuracy of the LES acoustic boundary conditions described in Section [5.5.](#page-83-0) Eventually one must note that the acoustic velocity oscillation must be known at the flame base to compute the FTF. This is achieved by reconstructing it at the injector lip using the low order model described in [\[148\]](#page-163-5).

#### **5.3. Description of the numerical setup**

LES are performed using the AVBP solver with modified transport properties as described in Section [4.1.3.](#page-68-0) In particular, the variable Prandtl number *Pr* and the variable nitrogen Schmidt number  $Sc_{N_2}$  depend on the local molar fraction of  $H_2$ , CH<sub>4</sub> and N<sub>2</sub>, as described in [\[108\]](#page-160-8). The SIGMA model is used as closure for the subgrid scale Reynolds stresses and the governing equations are integrated using a Taylor Galerkin finite-element convection scheme that is third order in space and time [\[153\]](#page-163-10). The turbulent combustion modeling is performed by adopting the Dynamic Thickened Flame Model DTFLES [\[117\]](#page-161-1) with Charlette efficiency function [\[116\]](#page-161-0). However, since the *PH*10 strategy generates a non-premixed combustion region at the flame base due to the local hydrogen injection, the DTFLES is only triggered in case of premixed combustion, while the diffusion flame front generated from H2 laminar pilot injection is fully resolved prescribing a proper grid resolution. Premixed and diffusion flamelets are identified by using the Takeno index [\[119\]](#page-161-3) as described in Section [4.2.3.2.](#page-73-0)

The computational domain is illustrated in Fig. [5.2](#page-80-0) and consists mainly of the cylindrical combustion chamber (a) and the swirled coaxial injector (b). The inlet of the CH4-air mixture coincides with the outlet section of the convergent element of the MIRADAS setup, where the velocity profile is known to be flat from experiments. In addition to that, the surrounding atmosphere around the chamber outlet is also simulated (see Fig.  $5.2(c)$  $5.2(c)$ ). This approach has a negligible computational cost and it allows to avoid the specification of any numerical impedance at the combustion chamber outlet. As illustrated in Fig. [5.2\(](#page-80-0)e), a small co-flow is imposed at the inlet of the hemispherical dome, prescribing a homogeneous inlet velocity *Uatm*  $\approx 0.2$  m/s. Inlet and outlet boundary conditions are modeled using the NSCBC formalism. Figure [5.2\(](#page-80-0)f) shows an axial plane of the computational domain. The

<span id="page-81-0"></span>

Constant mass flow rate  $\dot{m}_{H_2}$ 

 $+++$ 

 $\epsilon$ ) Co-flow  $U_{atm}$ 

 $+++$ 

f)

 $\mathbf{L}$ 

 $10 \text{ mm}$ 

Cell size (µm)

Oscillating mass flow rate  $\overline{\dot{m}}_{CH_4,air}$ 

c) CFD domain

d) Swirler

<span id="page-81-1"></span>b) Injector

**Figure 5.2.** – Representation of the computational domain made of the combustion chamber (a), the injector (b) and the hemispherical dome to simulate the surrounding atmosphere (c). A detail of the annular swirler is also illustrated (d). The axial section of the computational domain is used to present the grid size adopted for the surrounding atmosphere (e) and the burner (f) with the associated inlet conditions.

amplitude of the velocity fluctuation imposed in the external duct is tuned by an iterative procedure to match the experimental velocity *u* measured by the hot-wire in Fig. [5.2\(](#page-80-0)a). The relax of the NSBC is also tuned to match the acoustic pressure  $p'$  measured by the microphone in front of the hot wire. The boundary condition for the bottom patch of the hydrogen nozzle depends on the injection strategy simulated. In the case of pilot  $H_2$  injection  $(PH10)$  the bottom patch is an inlet with constant mass flow rate  $\dot{m}_{H_2}$  and a Poiseuille velocity profile while, for the *REF* strategy, the bottom patch is considered as a wall since hydrogen is not injected.

The inlet temperature is 298 K for both  $H_2$  and the CH<sub>4</sub>-air streams. Figures [5.2\(](#page-80-0)e-f) display a contour map of the cell size. The global mesh contains roughly 30 M elements and the initial grid is obtained from cold flow simulations using adaptive mesh refinement methods [\[121\]](#page-161-5). Then the grid is refined by hand in the combustion zones. In the swirler the average cell size is roughly  $200 \mu m$ , sufficiently small to retrieve the correct rotative motion [\[154\]](#page-163-11) at this operating conditions. The upper part of the annular injector and the central nozzle that supplies  $H_2$  are discretized using a cell size of roughly 100  $\mu$ m, while in the region occupied by the flame root the spatial discretization goes down to 50  $\mu$ m. The grid size is increased from the bottom to the top of the combustion chamber reaching several millimeters in the atmosphere (see Fig. [5.2\(](#page-80-0)e))

Wall heat losses are accounted for by imposing a thermal resistance and the experimental wall temperature profiles  $T_c$  that were measured along the axial direction of the cylindrical combustion chamber, the temperature of the burner lips  $T_l$  and the combustor backplane  $T_b$ . An analytically-reduced chemical scheme (ARC) for CH4-H2-air combustion based on 20 species and 166 reactions provided by the CFD team at CERFACS is used.

#### <span id="page-82-0"></span>**5.4. Unforced flames stabilization and structure**

This section presents the analysis of the *REF* and *PH*10 flames without acoustic forcing to focus on the impact of the central  $H_2$  injection on the flame shape and its structure. Figures [5.3\(](#page-81-1)a-b) compare the experimental Abel-deconvoluted normalized CH<sup>\*</sup> chemiluminescence line-of-sight integrated signal taken with the camera against the angle averaged normalized heat release rate (*HRRnorm*) from the LES for *REF* and *PH*10 cases, respectively.



Figure 5.3. – Comparison between experimental Abel deconvoluted mean CH<sup>\*</sup> intensity against the angle-averaged and normalized heat release rate *HRRnorm* for *REF* (a) and *PH*10 (b) unforced flames.

Figure [5.3](#page-81-1) shows that LES correctly retrieve the differences between the two injection strategies both in terms of flame angle and flame length reduction. In the presence of hydrogen pilot injection, the flame is approximately 10 mm shorter than the pure methane case and this is expected considering the higher reactivity of  $H_2$ . Moreover, Fig. [5.3](#page-81-1) illustrates a global redistribution of the heat release rate between the two injection strategies. In the *REF* case, *HRRnorm* is more homogeneously distributed along the entire flame brush, while in the *PH*10 flame, a maximum is observed at the flame root. In Fig. [5.3\(](#page-81-1)b) LES also reproduce the correct *PH*10 flame lift-off height of approximately 3 mm above the backplane, showing a different flame base stabilization with respect to the *REF* case.

Figure [5.4\(](#page-82-0)a) shows the comparison of the axial velocity field given by mean LES data between the *REF* and *PH*10 cases and put in evidence that this flame lifting is due to the presence of the laminar hydrogen jet exiting the central lance which, as shown below, modifies both the mean axial velocity field and mixture characteristics close to the injector lip. Furthermore, the pilot injection reduces the intensity of the Inner Recirculation Zone  $(IRZ)$  without affecting significantly the methane-air swirling jet flow. Figure [5.4\(](#page-82-0)b) shows the mean temperature fields over an axial plane. The isoline at 1300 K indicates roughly the separation between fresh and hot gases for both injection strategies. The main difference between *REF* and  $PH10$  cases occurs downstream the  $H_2$  jet, where the pocket of high temperature

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<span id="page-83-1"></span>

<span id="page-83-0"></span>**Figure 5.4. –** Comparison of time-averaged numerical results for *REF* and *PH*10 in terms of axial velocity (a) and mean temperature (b) for unforced conditions.

above 2000 K is the result of the central hydrogen injection. In fact, this flame zone is characterized by a non-premixed reaction that involves simultaneously  $H_2$ , the premixed CH4-air mixture and the recirculation zone. To shed light on the flame structure of the  $PH10$  flame base, Figs.  $5.5(a-b)$  $5.5(a-b)$  are considered. These figures display a close up of the injector outlet over an axial section for an instantaneous solution. The background of these images highlights the jet of the premixed  $CH<sub>4</sub>$ -air and the pure- $H_2$  streams. To isolate the effect of  $H_2$  addition, either the normalized fuel source terms or the flame indeces for both methane  $FI_{CH_4}$  and hydrogen  $FI_{H_2}$ are conditioned by the heat release rate and superimposed to the velocity fields. The flame index of the fuel  $F$  is based on the Takeno index [\[119\]](#page-161-3) and is defined as:

<span id="page-83-2"></span>
$$
FI_{\mathcal{F}} = \frac{\nabla_{\mathcal{O}_2} \cdot \nabla_{\mathcal{F}}}{\|\nabla_{\mathcal{O}_2} \cdot \nabla_{\mathcal{F}}\|}\tag{5.1}
$$

It results in positive or negative values to indicate premixed and diffusion combus-tion, respectively. Figure [5.5\(](#page-83-1)a) shows the normalized source term of  $CH_4$  (left) and the associated flame index (right), both conditioned by the heat release rate to ease the visualization. As expected, the positive value of the flame index confirms that methane consumption occurs in premixed mode along the main flame wings. Figure [5.5\(](#page-83-1)b), instead, evidences that  $H_2$  consumption takes place both along the flame wing and immediately downstream of the hydrogen injection. Nevertheless, the first is due to intermediate reactions of  $CH<sub>4</sub>$  oxidation, the latter is due to the combustion of  $H_2$  pilot injection. The associated flame index demonstrates that the pilot  $H_2$  creates a diffusion branch located at the flame base, contributing to the redistribution of the heat release rate towards the flame root observed in Fig. [5.3\(](#page-81-1)b) and it justifies the temperature peak seen in Fig. [5.4\(](#page-82-0)b).

<span id="page-84-1"></span>

**Figure 5.5. –** Instantaneous axial cut of the *PH*10 case showing on the left the source term of  $CH_4$  (a) and  $H_2$  (b) conditioned by the heat release rate and on the right the associated Takeno index. The background of the images evidences the premixed  $CH_4$ -air mixture and the  $H_2$  stream exiting the coaxial injector.

# **5.5. Acoustically forced flames: flow dynamics and global flame response**

The global *FTF* and the flame response to imposed acoustic perturbations of both cases, *REF* and *PH*10, are now discussed by forcing the air-CH4 stream with acoustic waves. The flame transfer function is defined as:

$$
\frac{\tilde{Q}}{\overline{Q}} = G \exp(i\varphi) \frac{\tilde{u}_0}{\overline{u_0}} \tag{5.2}
$$

<span id="page-84-0"></span>where  $\dot{Q}$  and  $u_0$  are the heat release rate and the velocity in the annular channel at the burner outlet cross section. The operator ˜*.* represents the Fourier component of the signal at the forcing frequency *f* and the operator *.* stands for its time averaged value.

Figure [5.6](#page-84-1) shows the experimental *FTF* in terms of gain *G* and phase lag  $\varphi$ collected over a span of forcing frequencies between 10 and 600 Hz. More details on the determination of this *FTF* are given in [\[149\]](#page-163-6). For these tests, the modulation level of the flow rate in the annular channel is set to 30% of the mean bulk velocity  $U_b \simeq 18 \text{ m/s}$  that is measured in the annular cross section of the injector. Numerical results obtained for both injection strategies at four characteristic frequencies of 100 Hz, 240 Hz, 400 Hz and 590 Hz are superposed on the experimental data, showing that the simulations accurately reproduce the *FTF* over the entire range of frequencies. For each forcing condition, at least 10 forcing cycles are simulated to compute the gain *G* and phase  $\varphi$  in [Eq. \(5.2\).](#page-83-2)

The flow and flame response at 240 Hz and 590 Hz are now considered. The first frequency is chosen because it corresponds to the drop of the *FTF* gain for the pilot- $H<sub>2</sub>$  case, while the second one coincides with the maximum phase lag between the two injection strategies. Figure [5.7](#page-85-0) shows the comparison between the experimental and numerical cycle-averaged signals of acoustic pressure  $p'$  at  $L1$ , acoustic velocity oscillation  $u'$  at  $L2$  (see Fig. [5.2\(](#page-80-0)f)) and the resulting normalized heat release rate fluctuations  $\dot{Q}'$  for *REF* and *PH*10 at  $f = 240$  Hz and  $f = 590$  Hz. In Figs. [5.7\(](#page-85-0)a-

<span id="page-85-0"></span>

**Figure 5.6. –** Comparison between experimental and numerical *FTF* for the perfectly premixed methane-air mixture *REF* and with H<sub>2</sub> pilot injection *PH*10. Data are gathered for a constant thermal power  $P_{th} = 4$  kW and a forcing level  $u'/U_{\rm b} = 0.3$ .

d) numerical and experimental signals of the acoustic pressure are synchronized defining the beginning of the forcing cycle, showing that the computed acoustic velocity, acoustic pressure and heat release rate oscillations are in good agreement with experiments both in terms of amplitude and relative phases.

#### **5.5.1. Flame dynamics over a forcing cycle**

LES are first validated against experiments and then used to analyze the flame acoustic response for the two injection strategies.

Phase conditioned images of the flame front dynamics for *REF* and *PH*10 are compared in Fig. [5.8\(](#page-86-0)a-b) when forced at 240 Hz and in Fig. [5.9\(](#page-86-1)a-b) when forced at 590 Hz. Experimental images are obtained via an inverse Abel transform of the normalized phase-conditioned cycle-averaged line-of-sight CH<sup>\*</sup> signal collected by a camera equipped with  $CH^*$  filter as described in [\[149\]](#page-163-6). LES images show the angle-average phase-conditioned images of two fields: the normalized heat release rate *HRRnorm* and the Q-criterion *Qcrit*. The first is meant to be compared to the  $\epsilon$  experimental CH<sup>\*</sup> chemiluminescence images, while the second highlights intensity and position of the coherent vortical structures shedded within the flow over the acoustic cycle. This set of figures is used to interpret the interaction between the vortices shed at the injector rim and the flame front. The label on top of each image of Figs. [5.8](#page-86-0) and [5.9](#page-86-1) corresponds to the phase lag with respect to the harmonic pressure oscillation  $p'$  shown in Fig. [5.7.](#page-85-0)

Numerical simulations capture accurately the flame motion, irrespective of the frequency imposed and the injection strategy adopted. For instance, Fig. [5.8\(](#page-86-0)a) shows that between  $\varphi = 0^{\circ}$  and  $90^{\circ}$ , the *REF* flame root changes its concavity and,

<span id="page-86-1"></span><span id="page-86-0"></span>

**Figure 5.7.** – Comparison between experimental and numerical cycle-averaged signals of acoustic pressure  $p'$  (*L*1), acoustic velocity  $u'$  (*L*2) and heat release rate fluctuation  $\dot{Q}'$  for  $\overline{REF}$  at 240 Hz (a),  $\overline{REF}$  at 590 Hz (b),  $PH10$  at 240 Hz (c) and *PH*10 at 590 Hz (d).

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<span id="page-87-0"></span>

**Figure 5.8. –** Forcing frequency 240 Hz: Comparison between experimental and numerical phase averaged conditioned images of *HRR* for *REF* (a) and *PH*10 (b). Experiments (left) consider the Abel deconvoluted  $CH^*$  signal. LES results (right) present the angle-averaged fields of *HRR* and *Qcrit*.



**Figure 5.9.** – Forcing frequency 590 Hz: Comparison between experimental and numerical phase averaged conditioned images of *HRR* for *REF* (a) and *PH*10 (b). Experiments (left) consider the Abel deconvoluted  $CH^*$  signal. LES results (right) present the angle-averaged fields of *HRR* and *Qcrit*.

simultaneously, the global flame length is reduced. Later in the forcing cycle the flame lengthens along the axial direction of the burner and, at  $\varphi = 270^{\circ}$ , it shows a pronounced roll-up of the flame tip. In case of *PH*10 and for a forcing frequency of 240 Hz in Fig. [5.8\(](#page-86-0)b), the LES is in good agreement with experiments over the entire forcing cycle.

The flame roll-up due to the vortical structures seen for the *REF* case in Fig. [5.8\(](#page-86-0)a) and in Fig.  $5.9(a)$  $5.9(a)$  is substantially attenuated in case of  $H<sub>2</sub>$  pilot injection, as shown in Figs.  $5.8(a-b)$  $5.8(a-b)$ .

Moreover, at 590 Hz in Fig.  $5.9(a-b)$  $5.9(a-b)$ , simulations capture a marked wrinkling of the flame front, which is stronger than the one observed at 240 Hz for both *REF* and *PH*10 cases. This is in agreement with the greater values of the vorticity *Qcrit* observed at  $f = 590$  Hz, which shows the intensity of the vortical structures predicted by LES. At this frequency the characteristic Strouhal number of the flow through

<span id="page-88-0"></span>

**Figure 5.10. –** *REF* vs *PH*10: numerical phase averaged conditioned images of axial velocity for a forcing frequency of 240 Hz (a) and 590 Hz (b). The white line defines axial velocity  $w = 0$  m/s.

the injector  $St = f D_H / U_b$  is 0.32, where  $D_H = 10$  mm is the injector hydraulic diameter and  $U_b = 18$  m/s is the bulk velocity in the annular injector channel. This value is close to the natural shedding frequency  $St \simeq 0.2$ -0.3 of unswirled jets, which only weakly depends on Reynolds number [\[155\]](#page-163-12). The Strouhal number decreases to  $St = 0.13$  at 240 Hz, which is consistent with the lower intensity of vortices seen in the LES. Finally, as in the unforced case shown in Fig. [5.3,](#page-81-1) two additional features related to hydrogen pilot injection are well retrieved by the LES also under acoustically forced conditions: (1) the substantial increase in the burning rate at the flame base and (2) the reduction of the flame length.

Furthermore, the evolution of the axial velocity field over the acoustic cycle for the two injection strategies at 240 Hz and 590 Hz is reported in Fig. [5.10.](#page-87-0) The images show the white isoline defining zero axial velocity  $w = 0$  m/s and a black contour of the *HRRnorm* already displayed in Figs. [5.8](#page-86-0) and [5.9.](#page-86-1) Overall, the figures show that the variation of the phase-averaged axial velocity field mainly depends on the forcing frequency and it is only marginally influenced by the injection strategy adopted. At 240 Hz, for instance, the two injection strategies show similar penetration of the outer swirling jet, which protrudes inside the combustion chamber with comparable angles for all phases. In Fig. [5.11\(](#page-88-0)a), at 240 Hz, both *REF* and *PH*10 exhibit a pronounced oscillation of the IRZ along the axial direction as result of the periodic velocity modulation. Between  $\varphi = 0^{\circ}$  and  $90^{\circ}$  the axial velocity in the annular duct increases and the IRZ is pushed downstream, whereas it moves towards the injector rim as consequence of the axial velocity deceleration. Moreover, Fig. [5.11\(](#page-88-0)a) shows that the width of the IRZ changes along the forcing cycle, experiencing a more intense negative axial velocity at phases  $\varphi = 270^{\circ}$  and 0° for both *REF* and *PH*10. Despite the marginal variations of the axial velocity field, the mutual interaction between the flame and the flow differs substantially between *REF* and *PH*10. First of all, Fig. [5.10\(](#page-87-0)a) shows the flame length variation between phase  $\varphi = 90^{\circ}$  and 270<sup>°</sup> is more pronounced for the *REF* case. Secondly, while the root of the *REF* flame remains anchored to the injector lip, the flame base of the pilot  $H_2$  case oscillates

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<span id="page-89-0"></span>

**Figure 5.11. –** Detailed view of the numerical phase averaged flame root position for *REF* and  $PH10$  at forcing frequencies of 240 Hz (a) and 590 Hz (b). The flames are identified by the threshold HRR*norm >* 0*.*1 , the IRZ and the isocontour of the H<sup>2</sup> molar fraction superposed.

under the periodic velocity oscillation caused by the acoustic forcing.

The dynamics of the flame root is further scrutinized in Fig.  $5.11(a)$  $5.11(a)$ , which highlights the position of the flame root for both injection strategies over the forcing cycle at 240 Hz. The negative axial velocity contour (*w <* -6 m/s) shown in Fig. [5.11](#page-88-0) marks the inner recirculation zone and the isoline of the molar fraction of  $H_2$ , displayed for the  $PH10$  case, indicates the penetration of the central  $H_2$  stream. The flame root of the fully premixed *REF* case stabilizes in the low velocity region above the injector lip and does not move. In constrast, the stabilization of the lifted flame *PH*10 is much more sensitive to the variation of the local velocity field. The isolines of H<sup>2</sup> molar fraction, *XH*<sup>2</sup> , show a variation of the local hydrogen concentration due to the interaction between the central jet and the local velocity field. When the size and the intensity of the IRZ decrease ( $\varphi = 90^{\circ}$ ), the isocontour of  $X_{H_2}$  moves downstream indicating a deeper penetration of the hydrogen jet. When the size and intensity of the IRZ increase during the cycle phases  $\varphi = 180^{\circ}$  and 270°, instead, the isolines of  $X_{H_2}$  are pushed towards the injector.

Figure [5.10\(](#page-87-0)b) shows the phase averaged axial velocity field for a forcing frequency of 590 Hz. As demonstrated for 240 Hz, the impact of the injection strategy on the axial velocity field is marginal but the flow distribution shows multiple zones of high axial velocity coexisting at the same phase (e.g., see phase  $\varphi = 90^{\circ}$ ). This marks a substantial change with respect to the case at 240 Hz, and can be explained by comparing the period of the forcing cycle at 590 Hz ( $T_{590} = 1.7$  ms) with the characteristic convective time needed by the velocity disturbances to travel from the bottom to the top of the flame. This time delay can be for example estimated by calculating the ratio between the mean *REF* flame length  $h \approx 40$  mm (see Fig. [5.3\)](#page-81-1) and the time-averaged bulk flow velocity in the annular injector  $18 \text{ m/s}$ , which results in a characteristic convective time for the vortices to travel across the flame of 2.2 ms. The latter being greater than the acoustic forcing period, the second perturbation hits the flame base before the previous velocity disturbance reaches the flame tip. These zones of greater axial velocity coincide with the position of the vortices shedded at the burner rim highlighted in Fig. [5.8](#page-86-0) by the *Qcrit* contour and are further investigated below. Moreover Fig. [5.11\(](#page-88-0)b) shows that, in contrast

<span id="page-90-0"></span>

**Figure 5.12.** – Experimental and numerical flame root axial displacement with respect to the injector lip over the forcing cycle for *REF* and *PH*10 at 240 Hz (a) and 590 Hz (b).

with the case at 240 Hz, the results for the forcing frequency  $f = 590$  Hz do not show any relevant axial oscillations of the IRZ for any of the two injection strategies. Figure [5.11\(](#page-88-0)b) shows that, as a consequence of that, the central H2 jet in *PH*10 case remains undisturbed during the whole forcing cycle at 590 Hz: the IRZ does not oscillate and the isocontours of  $X_{H_2}$  do not indicate any relevant movement and the flame root position, which remains roughly unchanged for both *REF* and *PH*10 cases.

To quantify this phenomenon, Fig. [5.12](#page-89-0) shows the axial position of the flame anchoring point *zroot* with respect to the injector lip over the acoustic cycle for *REF* and *PH*10 at both 240 Hz and 590 Hz. The flame root is numerically defined as the lowest point occupied by the white contour  $HRR_{norm} = 0.1$  in Figs. [5.8](#page-86-0) and [5.9.](#page-86-1) These numerical data are superimposed to experimental measurements where the flame root is defined as the minimum axial coordinate at which 10% intensity of the Abel-deconvoluted CH<sup>\*</sup> emission signal is detected in the image. There is a good qualitative agreement between LES and experiments in Fig. [5.12\(](#page-89-0)a). In the *REF* case the flame root remains attached to the lip, for both forcing frequencies. With hydrogen injection, instead, both experiments and LES reveal a flame root cyclic axial displacement of about 2*.*5 mm at 240 Hz, which corresponds roughly to 10% of the total flame length. At the higher forcing frequency of 590 Hz, instead, the fluctuations are less pronounced. Since these oscillations interfere with the disturbances of the flame front produced by the incoming vortices, they affect to different extents the *REF* and *PH*10 flame acoustic responses at different forcing frequencies.

To sum up, as observed for the 240 Hz case, the phase-averaged shape of the flame over the 590 Hz cycle confirms that the dynamics of the *REF* flame differs from the *PH*10 both in terms of interactions with large vortical structures synchronized by the acoustic forcing and altering the flame length variation and the flame <span id="page-91-0"></span>root movements. The impact of these aspects on the *FTF* gain and phase is now discussed.

#### **5.5.2.** *FTF* **gain analysis**

It is worth recalling that during *FTF* measurements only the methane-air fuel line is acoustically modulated in both cases. Since the bulk velocity modulation level is kept constant through the entire study, at a given forcing frequency, no differences in the swirl number fluctuations between the two injection strategies are expected. Hence, the impact of this mechanism on the flame response [\[139\]](#page-162-9) is neglected in the following.

For a given harmonic velocity modulation, the gain of the *FTF* depends on the magnitude of the global heat release rate fluctuation  $\dot{Q}'$  during the forcing cycle. This depends on the evolution of the flame surface area and the burning rate distribution along the flame brush itself [\[29\]](#page-155-3). Hence, the main mechanism altering flame surface wrinkling concerns the flame interaction with the large vortical structures shed at the injector rim. Changes in the burning rate along the flame determines the extent of the heat release rate variation associated to the local change of flame surface area.

Flame surface area variation resulting from interaction with hydrodynamic eddies is first considered. Figure [5.10](#page-87-0) showed that *REF* and *PH*10 flames are subjected to the same velocity field with vortical structures of comparable intensity when forced at the same modulation frequency. Hence, the change of flame shape due to hydrogen injection does not affect the vortex shedding associated with Kelvin-Helmholtz instabilities. This is confirmed by the similarities of the isocontours of the *Qcrit* field in Fig. [5.8\(](#page-86-0)a-b). At 240 Hz, eddies are released at the injector lip at phase  $\varphi = 0^{\circ}$  and dissipated along the flame brush before being completely consumed at the end of the forcing cycle (phase  $\varphi = 270^{\circ}$ ) for both *REF* and *PH*10. Remarkably, despite these similarities, the flame interaction with the vortical structures differs for the two cases. To highlight this aspect, the white iso-contour corresponding to 10% of the maximum normalized heat release rate  $HRR_{norm} =$ 0.1 in Fig. [5.8](#page-86-0) can be considered as a qualitative marker of the flame surface area evolution through the oscillating cycle. It shows that the relative flame surface variation differs substantially between the two cases. In Fig.  $5.8(a)$  $5.8(a)$ , the *REF* flame surface area changes from a minimum around phase  $\varphi = 90^{\circ}$  to a maximum at roughly  $270^{\circ}$  when forced at 240 Hz. This increase is driven by a vortical structure that generates a large roll up of the flame tip in Fig. [5.8.](#page-86-0) However, the *PH*10 flame does not undergo the same roll up. In this second case, the flame tip roll up is strongly attenuated due to the reduction of the flame length caused by the H2 addition. Figure [5.9](#page-86-1) shows results at 590 Hz with similar outcomes: the *REF* flame undergoes a larger surface area variation with respect to the *PH*10 flame. Furthermore, despite the intensity of the eddies at 590 Hz is greater than the ones shed at 240 Hz, the tip roll up is less pronounced for the higher frequency, which is in agreement with the low *FTF* gain observed in this case.

The effect of  $H_2$  pilot injection on the distribution of the heat release rate is now investigated. Figure [5.13](#page-91-0) shows the axial evolution of the radially-integrated heat release rate for a given axial coordinate,  $HRR_z$ , for both  $REF$  (a) and  $PH10$  (b) at four phases of the forcing cycle for a frequency of 240 Hz. This allows to put in evidence the contribution of the different flame zones to the global heat release rate for each phase of the forcing cycle. For the *REF* case in Fig. [5.13\(](#page-91-0)a), the flame response is dominated by the flame tip dynamics  $(z \approx 25 \text{ mm})$ , where the

<span id="page-92-0"></span>

**Figure 5.13.** – Numerical distribution of the maximum heat release rate at a given axial coordinate  $HRR_z$  for four phases:  $0^\circ$ ,  $90^\circ$ ,  $180^\circ$ ,  $270^\circ$  at  $f = 240$  Hz. (a) *REF* and (b) *PH*10.

extent of the  $HRR_z$  reaches consistently its maximum. At  $\varphi = 90^\circ$  the flame tip is not perturbed by any vortical structure (see Fig.  $5.8(a)$  $5.8(a)$ ) and its contribution to the global heat release rate is low. Conversely, the flame tip roll-up reaches its maximum at  $\varphi = 270^{\circ}$  ((see Fig. [5.8\(](#page-86-0)a)) and the  $HRR_z$  in this region increases in Fig. [5.13\(](#page-91-0)a). The contribution of the flame root remains negligible along the entire forcing cycle for the *REF* case in Fig.  $5.13(a)$  $5.13(a)$ .

The response differs for *PH*10. Figure [5.13\(](#page-91-0)b) shows that for the case *PH*10, the flame base ( $z \approx 5$  mm) and the flame tip ( $z \approx 25$  mm) contribute to similar extent to the overall heat release oscillation and they both influence the global flame response. This is a consequence of the redistribution of the heat release rate due to H2 pilot injection towards the flame root and corroborate the observations and analysis made in [\[149\]](#page-163-6). At  $\varphi = 0^{\circ}$  and 90°, the vortical structures are absent and the largest budget of the heat release is localized near the flame root. Between  $\varphi$  $= 180^{\circ}$  and  $\varphi = 270^{\circ}$  the vortices interfere with the flame tip (see Fig. [5.8\(](#page-86-0)b)) and the profile of  $HRR_z$  exhibits a plateau between  $z = 5$  mm and  $z = 25$  mm. At these phases the contribution of the flame tip increases due to its interaction with the vortices, such as it reaches the same extent of the one at the flame base.

The global flame responses can be also analyzed by means of a Dynamic Mode Decomposition (DMD) [\[156\]](#page-163-13) to reconstruct the spatial structure of the fluctuating component of the heat release rate at the corresponding forcing frequency and to highlight flame regions that contribute with a certain phase to the global heat release fluctuation  $\dot{Q}'$  during the cycle. The DMD algorithm uses more than 200 3D-solutions for each condition. Since the flame is compact with respect to the acoustic wavelength, the acoustic pressure is considered constant over the entire computational domain and used as reference to compare simultaneously different flame regions. Figures  $5.14(a)$  $5.14(a)$  and (c) show DMD results at 240 Hz and 590 Hz for both injection strategies, while Figs. [5.14\(](#page-92-0)b) and (d) show  $\dot{Q}'_r$ , the normalized

<span id="page-93-0"></span>

<span id="page-93-1"></span>**Figure 5.14. –** Spatial distribution of heat release rate at 240 Hz (a) and 590 Hz (c) for *REF* (left) and *PH*10 (right) injection strategies. The axial evolution of the radial integration of these signals (right image) highlights the relative contribution of the several flame regions to the global *FTF* gain for 240 Hz (b) and 590 Hz (d).

<span id="page-93-2"></span>radial integration of  $\dot{Q}'$  along the axial coordinate, to elucidate the contribution of several parts of the flame along the burner axis. Figure [5.14\(](#page-92-0)a) shows the importance of the flame roll up between  $z = 20$  mm and  $z = 30$  mm, near the chamber walls for the *REF* case (left). This is corroborated in Fig. [5.14\(](#page-92-0)b), which shows the dominant contribution of the flame tip with respect to other flame regions. Since the *REF* flame is V-shaped, its acoustic response is mainly driven by the flame tip dynamics. Perturbations of the flame tip accounts for most of the flame surface area variation with respect to the flame base contribution, that is closer to the burner axis. Figure [5.14\(](#page-92-0)a) shows that for the *PH*10 case (right) the relative intensity of the heat release rate oscillation at the flame tip is reduced with respect to the *REF* case. Figure [5.14\(](#page-92-0)b) highlights that the global heat release rate oscillation of *PH*10 is the result of an out-of-phase contribution among different parts of the flame. The impact of the redistribution of the burning rate for *PH*10 can be seen in Fig. [5.13.](#page-91-0) This generates an interference among several flame regions that partially compensate each other, leading to an overall reduction of the global heat release rate oscillation associated to a drop of the  $FTF$  gain in Fig. [5.6](#page-84-1) at 240 Hz. Moreover, Fig. [5.14\(](#page-92-0)b) underlines that *PH*10 at 240 Hz, is the only operating condition showing an impact of the flame root  $(z < 8$  mm) to  $\dot{Q}'_r$ . This is associated to the flame root axial motion observed in Figs. [5.11](#page-88-0) and [5.12,](#page-89-0) which makes the lower part of the flame to contribute with a certain phase lag to the global *FTF* gain, while, in the other conditions this effect is inhibited. According to the low-pass filter behavior of V-shaped swirl stabilized flames [\[150,](#page-163-7) [152\]](#page-163-9), DMD results at 590Hz in Fig. [5.14](#page-92-0) show that, both the *REF* and *PH*10 flame exhibit several positive and negative contributions to the global heat release rate perturbation over the extent of the flame brush. This is mostly related to the simultaneous interference of several eddies with the flame brush during a forcing cycle, which drives down the global heat release fluctuations (see Fig. [5.14\)](#page-92-0) and *FTF* gain in Fig. [5.6](#page-84-1) at 590 Hz.

#### **5.5.3.** *FTF* **phase analysis**

The experimental  $FTF$  phase lag  $\varphi$  in Fig. [5.6](#page-84-1) shows that, without considering the local plateau observed for *PH*10 at 240 Hz, the slope of the two curves remains roughly constant. Hence the characteristic time delay of the two flame responses does not depend on the forcing frequency. Moreover, it was shown in the previous section that the *REF* flame acoustic response is dominated by the dynamics at the flame tip, while *PH*10 flame exhibits an out-of-phase contribution of disturbances at the flame tip with those at the flame root. Therefore, in both cases, the entire flame length must be considered to interpret the global flame response and the *FTF* phase lag associated to the time lag between velocity perturbations at the burner outlet and the global heat release rate oscillation. One may interpret the variation of the *FTF* phase lag shift in light of the different flame lengths. To this purpose, the mean axial convective velocity of the vortical disturbances is retrieved as the ratio between the

<span id="page-94-0"></span>

**Figure 5.15.** – Evolution of the flame height  $h_{fl}$  over the forcing cycle for *REF* and *PH*10 at 240 Hz and 590 Hz.

**Table 5.2.** – Numerical flame time lag difference  $\Delta \tau$  and *FTF* phase shift  $\Delta \varphi$  between *REF* and *PH*10 calculated considering the mean bulk velocity  $U_b$  and the flame height differences  $\Delta h$  at both 240 Hz and 590 Hz.

$\frac{1}{2}$							
				$h_{REF}$ $h_{PH10}$ $\Delta h$ $\Delta \tau = \Delta h / U_b$ $\Delta \varphi = \omega \Delta h$			
Hz	mm	mm	mm	$\rm ms$	rad		
240	36	28		0.44	$0.21\pi$		
590	-36	25		0.61	$0.72\pi$		

mean flame length *h* and the time needed by these structures to reach the flame tip. This convective velocity is evaluated by tracking the axial position of the vortices released at the injector rim and results approximately to  $U_b = 18$  m/s, irrespective of the injection strategy adopted. Figure [5.15](#page-93-1) shows the instantaneous flame height over the acoustic cycle for *REF* and *PH*10 at 240 Hz and 590 Hz, which is obtained numerically by considering the highest point occupied by the isocontour *HRRnorm*  $= 0.1$  in Figs. [5.8](#page-86-0) and [5.9.](#page-86-1) The mean flame height differences between  $REF$  and *PH*10 at 240 Hz and 590 Hz are  $\Delta h_{240}$ =8 mm and  $\Delta h_{590}$ =11 mm, respectively. The associated differential time lag between the two injection strategies is calculated as  $\Delta \tau = \Delta h / U_b$ , which leads to  $\Delta \tau_{240} = 0.44$  ms at 240 Hz and  $\Delta \tau_{590} = 0.61$  ms at 590 Hz. This translates into a phase shift  $\Delta \varphi = \omega \Delta \tau$  between the *REF* and *PH*10 flames which is equal to  $\Delta\varphi_{240}=0.21$   $\pi$  and  $\Delta\varphi_{590}=0.72$   $\pi$  (Tab. [5.2\)](#page-93-2). These results are in good agreement with the *FTF* measurements in Fig. [5.6:](#page-84-1)  $\Delta \varphi = 0.25\pi$  at 240 Hz and  $0.73\pi$  at 590 Hz. The *FTF* phase reduction due to hydrogen pilot injection can be relatively well predicted by considering the reduction of the flame size due to hydrogen injection, but it is not excluded that additional effects due to the axial redistribution of the burning rate need to be taken into account while  $H_2$  pilot injection might become more significant under different operating conditions.

### **5.6. Conclusions**

Numerical simulations of the MIRADAS bench have been used to elucidate the impact of a small central  $H_2$  injection ( $PH10$ ) on the acoustic response of a  $CH_4$ air swirling premixed flame (*REF*). First, LES have been used to analyze the stabilization and the flame structure associated to the two injection strategies for the unforced configurations. In the  $PH10$  case the  $H_2$  central injection reduces the global flame length, induces flame lift-off and generates an increased reactivity at the flame base that contributes to a spatial redistribution of the heat release towards the flame base.

These features are also found when the flames are subjected to acoustic forcing. Two forcing frequencies have been investigated: 240 Hz and 590 Hz. The first corresponding to the minimum of the *FTF* gain for the *PH*10 case, the latter being representative of the maximum phase lag between the two injection strategies. LES demonstrate that the addition of  $H_2$  injection has a negligible impact on the phase-averaged velocity field distribution, which is instead strongly dependent on the forcing frequency investigated. At 240 Hz, phase-averaged velocity fields put in evidence a significant axial oscillation of the IRZ for both injection strategies, which is instead absent at 590 Hz. Moreover, in the *PH*10 case, the movement of the IRZ affects the hydrogen jet penetration inside the combustion chamber, contributing to an oscillation of the flame root.

Considering these results, the heat release rate distribution at different phases of the forcing cycle for the two injection strategies has been analyzed: at 240 Hz the acoustic response of the *REF* flame is entirely dominated by the flame tip dynamics, while the *PH*10 flame shows an out-of-phase contribution of several flame regions that reduce the overall *FTF* gain. First, a marked redistribution of the heat release rate towards the flame base caused by pilot  $H_2$  injection led to a higher contribution of this region to the global heat release rate oscillation, which is not found in the *REF* case. Second, it has been shown that the reduction of the flame length observed for the *PH*10 case weakens the impact of vortical structures produced by the acoustic forcing at the burner rim on the flame tip roll-up, resulting in a smaller periodic variation of the flame front surface area at both 240 Hz and 590 Hz. A DMD analysis performed at 240 Hz and 590 Hz confirms the aforementioned results and reveals that the axial displacement of the flame root, driven by the acoustic velocity modulation, can interfere with the perturbation generated by the hydrodynamic eddies affecting the resulting *FTF* gain. The *FTF* phase shift between the injection strategies, can also be predicted by considering the changes of flame length. However, this does not exclude that the impact of the  $HRR$  redistribution due to  $H_2$  pilot injection that could become more relevant at different operating conditions.

More generally, this study confirms that even small  $H_2$  pilot injections near the flame base may change significantly the response of swirled flames to incident acoustic perturbations, thereby opening new possibilities to use  $H_2$  in the future to control flame dynamics.

# **Part III.**

# **Numerical analysis of pure H**2**-air turbulent swirling flames: HYLON burner**

CHAPTER<sub>1</sub>

# <span id="page-100-0"></span>**Investigation of two flames stabilization regimes observed in a dual swirl H**2**-air injector**

This chapter presents an investigation of pure  $H_2$ -air flames for a laboratory scale coaxial dual-swirl injector in which fuel and oxidizer are injected separately. Two flame archetypes are observed experimentally for the same global equivalence ratio  $\phi_g \approx 0.45$  and different thermal powers: a flame anchored to the injector ( $\approx 4$  kW) and an aerodynamically stabilized flame exhibiting a characteristic V-shape ( $\approx 10$ ) kW). LES is used to investigate these datasets and analyze the two stabilization modes. The numerical setup is first validated against Particle Image Velocimetry measurements gathered in isothermal and reactive conditions and  $OH^*$  chemiluminescence images. The mean velocity field of both operating conditions reveals the existence of a strong inner recirculation zone (IRZ) that, penetrating inside the injector nozzles, leads to a radial divergence of the central hydrogen jet, which ultimately favors one stabilization regime over the other. The first flame anchors on the hydrogen injector lip and it develops along the mixing layer between  $H_2$ and air swirling jets. The lifted flame, instead, stabilizes in the inner shear layer between the IRZ and the exiting swirling jet of reactants, burning over a wide range of equivalence ratios. LES also unveils the flame structures typical of each flame: the anchored one is entirely controlled by diffusion, while the lifted flame is characterized by a partially premixed branch and a second diffusion front. Finally, high-speed OH<sup> $*$ </sup> images and LES are used to analyze the unsteady transition from lifted to anchored flames.

#### **Overview**



**[6.5. Conclusions](#page-119-0)** .......................... **107**

### **6.1. Motivations of the study**

As already discussed in the introduction of the manuscript, the use of hydrogen in energy applications is limited due to its atypical combustion properties [\[5,](#page-153-0) [15,](#page-154-4) [23\]](#page-154-5). In gas turbine applications, one of the possibilities to achieve a gradual decarbonization is to keep exploiting perfectly premixed systems already optimized for methane-air combustion, and substitute hydrogen in the fueling system. Moreover,  $H_2$  reactivity increases the risk of spontaneous ignition [\[157,](#page-164-0) [158\]](#page-164-1) and flashback [\[57,](#page-157-0) [159\]](#page-164-2) raising safety concerns. To avoid these problems, in industrial applications the separated injection of reactants is generally preferred and recent years have revealed various alternative injector designs, like for instance Micro-mix injectors [\[7\]](#page-153-1). Nevertheless, separated fuel and air injection devices lead to non-premixed or partially-premixed flames, whose stabilization represents a classical problem for the combustion community  $[160, 161]$  $[160, 161]$  and substantially affect the burner performances as well as the pollutant emissions [\[31\]](#page-155-4).

Pioneering works conducted on academic turbulent jet diffusion flames, for instance, assumed that the flame leading point burns in perfectly premixed mode at stoichiometric conditions [\[162\]](#page-164-5), while subsequent studies generalized these findings demonstrating that the leading point is located preferentially along the mixture fraction corresponding to the maximum laminar burning velocity [\[163\]](#page-164-6). Other works justify instead the transition from anchored to lifted jet flame by local flame extinction [\[164,](#page-164-7) [165\]](#page-164-8). A more recent work on  $\text{CH}_4$ -air jet diffusion flames exploits cinema-PIV for Reynolds numbers up to  $Re = 8500$  to analyze the dynamics of the flame leading edge considering both the local turbulent intensity and the passage of large vortical structures through the flame zone [\[166\]](#page-164-9). This study does not show a strict correlation between the flame position and the turbulent vortices that are expected to boost the flame displacement speed, but it reveals a divergence of the flow streamlines upstream of the flame that is compatible with the concept of triple flame [\[167,](#page-164-10) [168\]](#page-164-11). The deceleration of the flow in front of the triple flame leading edge is due to the gas expansion over the non-flat flame surface and facilitates flame stabilization in high velocity flows, as demonstrated by theory [\[169\]](#page-164-12). This result corroborates previous studies on  $CH<sub>4</sub>$ -air mixtures [\[170,](#page-164-13) [171\]](#page-164-14), which identify triple flame propagation as the main mechanism for turbulent jet diffusion flame stabilization. The impact of the degree of mixing on the lift-off height in jet diffusion flames was also investigated [\[172,](#page-164-15) [173\]](#page-165-0).

<span id="page-101-1"></span><span id="page-101-0"></span>When swirling flows are considered, additional phenomena must be taken into account [\[174\]](#page-165-1). First, an Inner Recirculation Zone (IRZ) of hot gases enhances flame stabilization, which serves as a source of energy for the incoming reactants. The interaction between the flame and IRZ may also lead to bifurcations between anchored and lifted regimes [\[175\]](#page-165-2). Secondly, irrespective of the injection strategy, swirling flames can exhibit hydrodynamic instabilities such as Precessing Vortex Core that perturb the flow near the injector outlet modifying the flame dynamics [\[128,](#page-161-12) [176,](#page-165-3) [177,](#page-165-4) [178\]](#page-165-5). Moreover, experimental studies show that the transition from V-shape to M-shape for  $\text{CH}_4/\text{H}_2$ /air premixed swirling flames can be driven by increased strain resistance due to hydrogen addition [\[44\]](#page-156-1), confirming results found in [\[179\]](#page-165-6). Experimental and numerical works also indicate that flame shape transition can be triggered by heat losses when flames interact with the chamber walls [\[127,](#page-161-11) [180\]](#page-165-7).

<span id="page-102-0"></span>Both separated injection and swirling motion can be created in coaxial dual-swirl injectors. They represent a potential concept for future  $H_2$ -propulsion devices because they guarantee simultaneously flashback resistance and fast mixing to mitigate  $NO<sub>x</sub>$  [\[181,](#page-165-8) [182\]](#page-165-9). Experimental parametric studies on CH<sub>4</sub> oxy-flames demonstrated, for example, that the transition between lifted and attached flames in this kind of systems is piloted by the position of the IRZ with respect to the injector outlet and the lift-off height of the flame depends on the level of internal and external swirl [\[183\]](#page-165-10). A similar configuration was recently tested with  $H_2$ -enriched mixtures [\[184\]](#page-165-11) showing that the level of the internal swirl is a key parameter to control the flame shape, confirming the results provided in [\[185\]](#page-165-12) for unconfined flames.

From a numerical perspective, the separated injection strategy leads to flames exhibiting multiple combustion regimes for which the choice of the proper turbulent combustion modelling becomes critical. In this context, a general flamelet transformation was proposed in Flamelet Progress Variable (FPV) models to retrieve the local budget of heat source associated with premixed/diffusion combustion [\[186\]](#page-165-13). A different method relies on the use of a flame index  $[119]$  to discriminate between combustion regimes and apply the corresponding premix/diffusion turbulent combustion model as illustrated in Section [4.2.3.2.](#page-73-0) In this study, this second approach is followed. The modelling relies on the dynamic thickened flame model DTFLES [\[117\]](#page-161-1) for addressing turbulent/flame interactions in premixed regions, while the resolution of the flame front is ensured for the diffusion zone. This hybrid approach was largely used to describe multi-regime combustion in various spray [\[187,](#page-166-0) [188\]](#page-166-1) or gaseous [\[108\]](#page-160-8) flames and is used here for pure  $H_2$ -air gaseous mixtures.

This chapter deals with LES challenges of such flames. The novelty consists in the fact that only few simulations of hydrogen swirling flames exist in literature and mostly for technically premixed combustion, like in [\[189,](#page-166-2) [190\]](#page-166-3). The first objective is to validate the numerical setup used to investigate  $H_2$ -air swirled non-premixed flames [\[184\]](#page-165-11) obtained with the HYdrogen LOw NOx injector (HYLON) developed at IMFT [\[65\]](#page-157-1). Second, the flame structure and the flame stabilization mechanisms associated to anchored and lifted  $H_2$ -air swirled flames observed experimentally are analyzed. Third, the governing the unsteady transition from lifted to attached flame are investigated experimentally and numerically.

The rig and the diagnostics are presented in Section [6.2.](#page-101-0) Section [6.3](#page-105-0) describes the numerical setup. In Section [6.4,](#page-108-0) LES results are validated against experimental measurements. The main characteristics of anchored and lifted flames are examined in the rest of the study. The unsteady transition with lip reattachment of a lifted flame is finally discussed.

#### **6.2. Experimental setup and operating conditions**

#### **6.2.1. Burner geometry**

The experimental setup has been developed by Sylvain Marragou at IMFT during his PhD  $[184, 191]$  $[184, 191]$ . Figure [6.1\(](#page-102-0)a) shows a schematic description of the MIRADAS setup investigated in Chapter 5 and equipped with the HYLON injector. The bottom side of the bench shown in Fig.  $6.1(a)$  $6.1(a)$  corresponds to the one described in Section [5.2:](#page-77-0) air is injected at the bottom of the main plenum and goes through a honeycomb in order to break the turbulent structures generated with the injection, while a convergent section mounted on top of it is used to generate a top-hat velocity profile at the inlet of the injector. A close up of the HYdrogen LOw NOx injector (HYLON)

<span id="page-103-0"></span>

(d) External swirler for air

Figure 6.1. – Sketch of the cross section of the entire MIRADAS setup with the HYLON injector showing the global geometry of the burner and the separated air and  $H_2$  injection lines (a). The close up of the HYLON injection system with the main characteristic dimensions (b). The axial swirler of the hydrogen nozzle (c) and the radial swirler in the air annular tube (d).

<span id="page-104-1"></span>is presented in Fig. [6.1\(](#page-102-0)b). This system was developed with the objective to stabilize pure H2-air swirled flames and contains two swirling coaxial ducts to inject fuel and oxidizer separately [\[65\]](#page-157-1). The annular channel supplies the air mass flow rate with an external diameter  $d_e = 18$  mm. A swirler made of eight cylindrical vanes of diameter  $d_h = 4$  mm, oriented at  $42^{\circ}$  with respect to the burner radial direction, is embedded in the external passage as shown in Fig.  $6.1(c)$  $6.1(c)$ . The inner injector supplies hydrogen through a  $d_i = 6$  mm diameter tube with 2 mm radial thickness, which contains an axial swirler of helicoidal shape shown in Fig.  $6.1(d)$  $6.1(d)$ . According to [\[184\]](#page-165-11), the external and the internal swirlers generate a flow with swirl number  $S_e = 0.65$  and  $S_i = 0.60$ , respectively. The coaxial injector also features a recess  $z_i = 4$  mm between the lip of the hydrogen injector and the burner backplane that favors mixing of the reactants before burning. The injector feeds a square combustion chamber made of four quartz windows to ensure optical access to the flame region. The chamber is 78 mm wide, 180 mm long and ends with a nozzle that provides a section reduction to avoid reverse flow at the combustor outlet. More details can be found in [\[184\]](#page-165-11).

#### **6.2.2. Diagnostic and measurements**

Mean flame images are recorded with a PIMAX-4 intensified CCD camera equipped with a 105 mm f/4.5 Nikon Rayfact UV-105 Multispectral lens. This camera with an appropriate  $308\pm10$  nm narrow band filter ASAHI XHQA310 centered on the OH<sup>\*</sup> peak emission gives indication on both the shape and heat release rate distribution of the flame.

<span id="page-104-2"></span><span id="page-104-0"></span>Particle Image Velocimetry (PIV) is performed to characterize the velocity field over a vertical plane in the proximity of the injector outlet either in isothermal  $(T =$  $300 \text{ K}$ ) or reactive conditions. Image pairs are recorded by a  $1024\times1028$  pixels PCO SensiCam CCD Imaging, while in reactive conditions a  $2560\times2160$  pixels LaVision CMOS CLHS camera is employed. In both cases, the cameras are equipped with a Nikkor 105 mm f/2.8G. The laser system consists of a Quantel Big Sky Laser CFR200 with 200 mJ maximum energy per shot at 4/15 Hz repetition rate for cold/hot conditions. The laser passes through a LaVision sheet generator resulting in a relatively thick light sheet of 1.5 mm thickness in the center of the combustion chamber. More than 1000 instantaneous fields are recorded with a LaVision Davis acquisition system to get statistically converged measurements for the mean and rms velocity fluctuations. For safety reasons, in cold flow conditions, the hydrogen stream is replaced by air and its mass flow rate in the pilot line is imposed to conserve the original momentum flux ratio between the internal and external ducts:  $J = \rho_e u_e^2 / (\rho_i u_i^2)$ <sup>2</sup><sub>*i*</sub></sub>), where  $\rho_e$  ( $\rho_i$ ) and  $u_e$  ( $u_i$ ) are the density and the bulk flow velocity in the external (internal) duct [\[183\]](#page-165-10). Non-reactive and reactive PIV measurements are performed with different seeding particles. For cold flow, oil droplets with a Sauter mean diameter  $D_{32} = 2 \mu m$  are injected both in the external and internal nozzles. In reactive conditions, air and  $H_2$  flows are seeded with Alumina particles AlO<sub>3</sub> of Sauter mean diameter  $D_{32}$  < 1.0  $\mu$ m. Measurements are taken on the *zy* axial plane illustrated in Fig. [6.3\(](#page-105-2)d) over an interrogation window defined by 2 mm  $\le z \le 32$  mm and  $-25$  mm  $\le y \le 25$  mm. It was also verified that the azimuthal position of the internal and external swirlers in the computational domain matches the experimental setup in order to maximize the reliability of the comparison between the two.

A thermal characterization of the burner components is also performed for the different operating conditions investigated. For the metallic components a bichro-

<span id="page-105-1"></span>

are reactive adopted for the two operating conditions reading to attached (11)								
			and lifted $(L)$ flames.					
Case				$\dot{m}_{air}$ [g/s] $\dot{m}_{\text{H}_2}$ [g/s] $U_b^{air}$ [m/s] $U_b^{H2}$ [m/s] $P_{th}$ [kW]				
	2.41		0.032	11.4	13.6	$3.89\,$	0.45	
	6.03		0.080	28.5	34.0	9.73	0.45	

<span id="page-105-0"></span>**Table 6.1. –** Mass flow rates of air and hydrogen, nominal thermal power and global equivalence ratio adopted for the two operating conditions leading to attached (*A*)

matic infrared FLUKE Endurance series pyrometer is used with spectral response between 1.5  $\mu$ m and 1.6  $\mu$ m. It operates between 250°C and 1200°C, with a relative error equal to  $\pm$  0.3% of the measurement. The combustion chamber axial temperature profile is also measured along the centerline of the quartz window with pasted thermocouples. Localized temperature data are also collected on the exhaust nozzle and over the burner backplane. Furthermore, a system made of two R-type thermocouples is used to estimate the hot gas temperature at the outlet of the combustion chamber via the reduced radiation error method [\[192\]](#page-166-5). Probes are inserted a few millimeters below the combustion chamber outlet cross section to estimate the radial temperature profile of the burned gases.

In addition, pressure losses between the injector inlets and ambient are measured for both fuel and oxidizer lines using a differential pressure gauge. Brooks SLA 585x series mass flow controllers are used to regulate hydrogen and air mass flow rates. Fuel and oxidizer are injected at  $T_u = 298$  K.

#### **6.2.3. Operating conditions**

Two H2-air flames, one anchored at the H2 injector lip (flame *A*) and the other aerodynamically stabilized downstream of the injector (flame *L*), are investigated. They correspond to the operating conditions indicated in Table [6.1.](#page-104-1) The global equivalence ratio is kept constant to  $\phi_q = 0.45$ , while the total thermal power varies from  $P_{th} = 3.89$  kW for flame *A* to  $P_{th} = 9.73$  kW for flame *L*. The Reynolds number based on the air bulk velocity and on the equivalent hydraulic diameter of the injector annular cross section are 11000 and 28000 for conditions *A* and *L*, respectively. Figure [6.2](#page-104-2) shows direct visualizations of the flames corresponding to the two operating conditions that will be scrutinized in the following sections.

<span id="page-105-2"></span>

**Figure 6.2.** – Direct flame images corresponding to (a) attached flame and (b) lifted flame stabilizations.

## <span id="page-106-1"></span>**6.3. LES methodology**

#### **6.3.1. Numerical setup**

The fluid computational domain is illustrated in Fig. [6.3](#page-105-2) and consists of the injector system shown in Fig.  $6.3(a)$  $6.3(a)$  and the combustion chamber. It is delimited at the bottom by the injector inlet and contains both the outer swirler shown in Fig.  $6.3(b)$  $6.3(b)$  and the inner swirler in Fig.  $6.3(c)$ . The spatial discretization is identical for the two operating conditions investigated and exploits different levels of refinement as illustrated in Fig.  $6.3(e)$  $6.3(e)$ . Overall, the grid counts 58 M tetrahedral cells with a minimum characteristic size of 100  $\mu$ m near the H<sub>2</sub>-injector lip and inside the envelope of the regions occupied by non-premixed flame fronts. The  $H_2$  duct spatial discretization is progressively refined approaching the injector lip. The mesh size distribution in the narrow channels of the helicoidal hydrogen swirler is chosen to capture the strong radial velocity gradients of the hydrogen flow and retrieve the correct velocity field at the injector outlet. A cell size  $\Delta x = 200 \ \mu m$  is prescribed for the outer swirler. The heat losses through the walls are modeled for the two flames by imposing the experimental axial temperature profile measured along the external side of the combustion chamber for operating conditions *A* and *L* shown in Fig. [6.4.](#page-106-1) For the combustion chamber, a constant global heat transfer coefficient per unit surface  $U = 0.004 \text{ W/m}^2\text{K}$  is imposed considering the thickness of the quartz windows  $l_q = 8$  mm and a thermal conductivity  $\lambda_q = 2.07$  W/mK. Thermal radiation through the quartz windows is neglected [\[193\]](#page-166-6). Inlet mass flow rates and outlet pressure are imposed using the NSCBC formalism [\[194\]](#page-166-7). The numerical setup relies on a semi-detailed SanDiego chemical mechanism [\[195\]](#page-166-8) that comprises 9 transported species and 21 reactions.

<span id="page-106-0"></span>The simulation strategy adopted was already discussed in Section [4.2](#page-70-1) and aims at capturing both premixed and non-premixed combustion regimes expected for conditions *A* and *L*: perfectly premixed flames are modeled via the DTFLES approach [\[117\]](#page-161-1) and in case of non-premixed flamelets the grid ensures a proper resolu-



**Figure 6.3.** – Main components of HYLON injector (a) with the air swirler (b) and the hydrogen swirler (c). Computational domain with the cartesian system of reference (d). Characteristic cell size distribution adopted for spatial discretization (e).



**Figure 6.4.** – Experimental temperature profiles along the axial direction  $z$  of the quartz windows for attached  $T_w^A$  and lifted  $T_w^L$  operating conditions.

tion of the flame structure. The Takeno index [\[119\]](#page-161-3) is used to distinguish between the two regimes.

#### **6.3.2. Mesh independence of numerical results**

<span id="page-107-0"></span>To prove that results are mesh-independent and that the diffusion-controlled flame region is indeed well resolved, a comparison between two grids is proposed in Fig. [6.5.](#page-107-0) A reference mesh (Ref) of 58 M tetrahedral elements and a more refined grid (Finer) of roughly 215 M elements are considered. Figure [6.5\(](#page-107-0)a) shows the cell size  $(\Delta x)$ distribution for the two grids. The flame is visualized by the black contour, which shows the normalized time averaged heat release rate *HRRnorm* = *HRR/HRRmax*  $= 0.5$  where the  $HRR_{max}$  is the maximum mean heat release rate. The Ref and the Finer meshes prescribe in this area a cell size  $\Delta x = 100 \ \mu \text{m}$  and 75  $\mu \text{m}$ , respectively. Overall,  $\Delta x$  in the flame region is reduced by roughly 30% in the second case. In the reference mesh, the grid for the fuel and oxidizer nozzles shows a mesh size between 200  $\mu$ m and 300  $\mu$ m, while for the Finer mesh  $\Delta x$  varies between 100  $\mu$ m and 200  $\mu$ m. Local refinements are imposed at the injector walls to limit the  $y^+$ , which largest values are recorded along the annular external wall of the oxidizer ducts:  $y^+$ is below 15 for the Ref mesh and less than 8 for the Finer mesh. The quality of these grids is compared by computing the anchored flame *A* which, considering the alignment between isoline of the stoichiometric mixture fraction *zst* and the heat release rate *HRRnorm* distribution shown in Fig. [6.5\(](#page-107-0)b), is mainly controlled by diffusion. Data are time-averaged over 30 ms and then spatially averaged along the azimuthal direction before being compared. Figure [6.5\(](#page-107-0)b) shows the contour map of *HRRnorm* over an axial cut for the Ref mesh (left) and the Finer mesh (right). The isolines of axial velocity  $U_z = 0$  and stoichiometric mixture fraction  $z_{st}$  are reported in blue and white, respectively. Overall, the flame size and the global stabilization mechanism are the same irrespective of the grid adopted. The width and the position of the IRZ, which plays a key role in swirling flows, is also unchanged. In addition to that, Figs.  $6.6(a-f)$  $6.6(a-f)$  display the time-averaged fields of heat release rate (a), gas temperature (b), mixture fraction (c), mean axial velocity (d) and two minor species distributions (e-f) along the radial direction of the burner for three axial coordinates:  $z = 5$  mm, 10 mm and 15 mm. The local heat release rate of the reaction and the distribution of the gas temperature for the two meshes are in good agreement. The spatial distribution of the mixture fraction is also consistent in the two cases, while the good agreements for  $Y_H$  and  $Y_{HO_2}$  show that the structure of the mean flame is equally captured, independently of the grid. Hence, the resolution of the original
<span id="page-108-0"></span>mesh is sufficient to produce mesh-independent results for both velocity fields and the mixing process, which are the main parameters driving flame stabilization of diffusion flames.

To check the turbulent flow resolution, the Kolmogorov turbulent scale *η<sup>k</sup>* is presented in Fig.  $6.7(a)$  $6.7(a)$  together with the white line indicating the flame location and  $U_z = 0$  isoline in blue delineating the IRZ. The Kolmogorov length scale is evaluated under the simplified hypothesis of isotropic turbulence  $\eta_k = L/Re_t^{3/4}$ , where *L* is the diameter of the exit cross section of the injector and the turbulent Reynolds number  $Re_t = u'L/\nu$  is computed knowing the local time-averaged rms velocity *u*' and the local kinematic viscosity  $\nu^1$  $\nu^1$ . Figure [6.7\(](#page-109-0)a) illustrates that the smallest turbulent structures in the region of interest range roughly between 50  $\mu$ m and 75  $\mu$ m, which are of the order of magnitude of the local cell size and guarantee a reasonable resolution of the flow. Moreover, Fig. [6.7\(](#page-109-0)b) shows that, because of the penetration of the IRZ inside the injector outlet, the  $H_2$  flow is rapidly heated. As result, the viscosity increases and the kinetic energy dissipation limits the energy cascade to eddies that are bigger than  $\eta_k$ . Since a very little activity is expected at the Kolmogorov scale (see Fig. [6.6\)](#page-108-0), the resolution of the grid can be considered appropriate.

<sup>1.</sup> Considering the good agreement with experimental data shown in Figs. [6.10](#page-111-0) and [6.11,](#page-111-0) only the resolved part of  $u'$  is retained for the calculation of  $Re_t$ 



**Figure 6.5.** – (a) Comparison between the reference (Ref) and the refined (Finer) mesh. The cell size  $\Delta x$  distribution highlights the different grid refinements with superposition of normalized heat release rate isocontour. (b) The time averaged normalized heat release rate *HRRnorm* field for the two grids is displayed with the isolines of axial velocity  $U_z = 0$  and the isolines of the stoichiometric mixture fraction *zst*.

<span id="page-109-0"></span>

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**Figure 6.6.** – Comparison for the reference (solid) and the finer (dashed) grid in terms of (a)  $HRR$ , (b) temperature *T*, (c) mixture fraction  $z_{st}$ , (d) mean axial velocity  $U_z$ , and mass fractions of  $Y_H$  (e) and  $Y_{HO_2}$  (f). The variable distributions are presented over the radial direction  $(y)$  for three different axial coordinates:  $z = 5$  mm, 10 mm and 15 mm.

## **6.4. Results and discussion**

### **6.4.1. Velocity fields and pressure losses validation**

First, velocity fields obtained with LES are compared to measurements made in isothermal and reactive conditions for the two investigated operating points. LES results and PIV data are gathered on the axial *zy* plane. Time-averaged solutions are obtained performing LES for an entire flow-through time of the combustion chamber corresponding roughly to 55 ms for the operating condition *A* and 25 ms for *L*. The physical time simulated before collecting statistics corresponds to roughly 150 ms to ensure statistically converged solutions in both conditions.

Figures [6.8](#page-110-0) and [6.9](#page-110-0) show the comparison between experimental and LES data for non-reacting flows extracted at  $z = 5$  mm and  $z = 15$  mm, respectively. Note that these two heights correspond roughly to the middle and upper parts of the flame. The top graphs in each figure consider the operating condition *A*, while the bottom

<span id="page-110-0"></span>

**Figure 6.7.** – Contour map of the estimated local Kolmogorov scale (a) and the temperature (b) for the anchored flame *A*. The white and the blue iso-lines define the flame location and the limit  $U_z$  of the IRZ, respectively.

ones refer to condition *L*. LES are in good agreement with experimental data for both cases. The accurate prediction of the mean axial velocity  $U_z$  profile proves that simulations correctly capture the size and the intensity of the IRZ. Moreover, the agreement between experimental and numerical mean radial velocity *U<sup>r</sup>* profiles at both heights indicates that LES accurately predicts the swirling jet opening angle at both operating conditions, thus being representative of the aerodynamics of the injector. In addition to that, the good agreement in terms of rms for both axial  $U_z$ and radial  $U_r$  components shows that the turbulent velocity fluctuations are also well retrieved by the simulations.

Reactive flows are now considered. Figures [6.10](#page-111-0) and [6.11](#page-111-0) show the comparison between PIV and LES velocity profiles for the reactive flow at  $z = 5$  mm and  $z =$ 15 mm, respectively. Axial and radial velocities are in very good agreement with experiments, both in terms of mean and rms profiles. LES well captures the changes in the velocity field due to the presence of the flame. The peaks of the velocity profiles move outward because of thermal expansion, the width of the IRZ increases and the modulus of the axial velocity inside it reduces. The only marginal difference between experiments and LES is found in Fig. [6.10](#page-111-0) for the rms values of the axial  $U_z$  and radial  $U_r$  velocities near  $y = \pm 10$  mm. At  $z = 5$  mm this zone corresponds to the location of the outer shear layer which separates the exiting swirling jet from the outer recirculation zone. Figure  $6.5(a)$  $6.5(a)$  shows that the mesh refinement in this region slightly degrades, justifying this small gap.

Numerical results in terms of injector pressure losses and hot gases outlet temperatures are compared to experimental data in Table [6.2.](#page-112-0) The pressure drop  $\Delta P_{air}/\Delta P_{H_2}$  represents the differential pressure between the inlet of the air/H<sub>2</sub> injector and ambient. LES data show an overestimation of the absolute pressure losses for both operating conditions *A* and *L*. It must be underlined that, even considering the Finer mesh (see Section [6.3.2\)](#page-106-0) with better refinement of the injector walls, the calculated pressure losses reduce by only 20 Pa. This is because, in these

<span id="page-111-0"></span>

**Figure 6.8.** – Cold PIV data (symbols) at  $z = 5$  mm on the axial plane vs LES results for the mean (a) and rms (b) axial velocity  $U_z$  and the mean (c) and rms (d) radial velocity  $U_r$  for the operating conditions  $A$  (top) and  $L$  (bottom). Velocities are in [m*/*s].



**Figure 6.9.** – Cold PIV data (symbols) at  $z = 15$  mm on the axial plane vs LES results for the mean (a) and rms (b) axial velocity  $U_z$  and the mean (c) and rms (d) radial velocity  $U_r$  for the operating conditions  $A$  (top) and  $L$  (bottom). Velocities are in [m*/*s].



<span id="page-112-0"></span>**Figure 6.10.** – Hot PIV data at  $z = 5$  mm on the axial plane vs LES reactive results for the mean (a) and rms (b) axial velocity  $U_z$  and the mean (c) and rms (d) radial velocity *U<sup>r</sup>* for operating conditions *A* (top) and *L* (bottom). Velocities are in [m/s].



**Figure 6.11.** – Hot PIV data at  $z = 15$  mm on the axial plane vs LES reactive results for the mean (a) and rms (b) axial velocity  $U_z$  and the mean (c) and rms (d) radial velocity  $U_r$  for operating conditions  $A$  (top) and  $L$  (bottom). Velocities are in [m/s].

configurations, most of the pressure losses are due to the swirler [\[121,](#page-161-0) [154\]](#page-163-0), suggesting that a further mesh refinement in this zone is needed to improve the prediction of experimental pressure variations. However, considering the agreement between PIV and LES as well as the good qualitative trend of the pressure losses for the two operating conditions, results are considered adequate.

<span id="page-113-0"></span>Finally, the comparison between time-averaged outlet gas temperature *Tout* that differ by less than  $200 \text{ K}$  underlines a satisfactory agreement for both operating conditions, showing that the simulated heat losses are representative of the ones found in the real burner. The gap between measurements and simulations could be partly due to the assumptions made implementing the reduced radiation error method [\[192\]](#page-166-0) on experimental data and also the strong assumption made on the thermal resistance of the quartz wall with a temperature profile that only depends on the axial direction.

**Table 6.2. –** Measured (*EXP*) and calculated (*LES*) pressures losses for the air injector  $\Delta P_{air}$  and the  $H_2$  injector  $\Delta P_{H_2}$ . Mean outlet gas temperature  $T_{out}$  for conditions *A* and *L*.

	$\Delta P_{air}$ (Pa)	$\Delta P_{H_2}$ (Pa)	$T_{out}$ (K)
$A_{EXP}$	918	165	1138
$A_{LES}$	$1135 (+19\%)$	$215 (+23%)$	$1010(-11\%)$
$L_{EXP}$	5750	821	1280
$L_{LES}$	6820 $(+16\%)$	$925 (+11\%)$	$1100 (-16\%)$

## **6.4.2. Attached flame (***A***)**

Figure [6.12](#page-113-0) compares the experimental normalized Abel deconvoluted images of the  $OH^*$  chemiluminescence signal with the LES normalized azimuthal average of the heat release rate *HRRnorm*. Simulations allow to capture the *M*-shape of the attached flame, which can be divided into two main branches. The first one, defined I in Fig. [6.12,](#page-113-0) is a vigorous reactive front that develops in the mixing layer between hydrogen and air streams. The second one, named II, lies downstream of the first one inside the wake of the  $H_2$  injector. According to  $OH^*$  chemiluminescence measurements, the burning rate in branch II is much weaker than in branch I. For a recess of  $z_i = 4$  mm, the zone between the  $H_2$  injector lip and the chamber backplane is not optically accessible from the present field of view, but LES results in Fig. [6.12](#page-113-0) show that flame *A* is anchored to the injector lip via the branch I which, separating fuel and oxidizer, burns in diffusion-controlled mode. This is corroborated in Fig. [6.13,](#page-113-0) which shows the instantaneous fields of the Takeno index  $(Fig. 6.13(a))$  $(Fig. 6.13(a))$  $(Fig. 6.13(a))$ and the flame thickening distribution  $(Fig. 6.13(b))$  $(Fig. 6.13(b))$  $(Fig. 6.13(b))$ , both conditioned on the same *HRRnorm* threshold. The white contour indicates the instantaneous spatial location of the stoichiometric mixture fraction *zst*, while the red lines are isocontours of normalized heat release rate  $HRR_{norm} = 0.45, 0.65$  and 0.80. The Takeno index is negative over the entire flame front, meaning that both branches I and II burn in non-premixed mode. Figure [6.13\(](#page-113-0)b) shows that, as prescribed, flame thickening is not applied for this regime. The flame is entirely resolved by the computational grid and the model is capable of retrieving the global characteristics of the attached configuration.

<span id="page-114-0"></span>

**Figure 6.12. –** Comparison between experimental mean normalized Abel-deconvoluted OH<sup>\*</sup> chemiluminescence signal (left) and LES normalized time averaged heat release rate distribution *HRRnorm* (right) for flame *A*. The two main flame branches are labelled as I and II.



**Figure 6.13. –** Instantaneous flame structure for flame *A*. Isocontours of normalized heat release rate  $HRR_{norm} = 0.45, 0.65, 0.80$  (solid red) and spatial distribution of stoichiometric mixture fraction *zst* (solid white) superposed to the Takeno index (a) and thickening factor of the DTFLES model (b).



**Figure 6.14. –** Comparison between experimental mean normalized Abel-deconvoluted OH<sup>\*</sup> chemiluminescence signal (left) and LES normalized time averaged heat release rate distribution *HRRnorm* (right) for flame *L*. The two main flame branches are labelled as I and II.

<span id="page-115-0"></span>

**Figure 6.15. –** Instantaneous flame structure for flame *L*. Isocontours of normalized heat release rate  $HRR_{norm} = 0.45, 0.65, 0.80$  (solid red) and spatial distribution of stoichiometric mixture fraction *zst* (solid white) superposed to the Takeno index (a) and to thickening factor of the DTFLES model (b).

### <span id="page-116-0"></span>**6.4.3. Lifted flame (***L***)**

The lifted flame L is now discussed. Figure  $6.14$  compares the normalized  $OH^*$ chemiluminescience Abel-deconvoluted signal against the numerical normalized heat release rate *HRRnorm*. The flame stabilization mechanism changes abruptly with respect to the anchored flame. Both experiments and LES show that the location of the maximum mean burning intensity moves downstream and is lifted by roughly 8 mm above the chamber backplane. Remarkably, Fig. [6.14](#page-114-0) shows that LES also captures the presence of a second weak reaction front II at the flame base that crosses the burner axis. Unlike flame *A*, flame *L* is aerodynamically stabilized in the wake of the hydrogen injector and is not anchored to the burner. The axial distance between the hydrogen injector lip and the main flame front allows a certain degree of mixing between hydrogen and air before burning. The conditioned Takeno index for flame  $L$  in Fig.  $6.15(a)$  $6.15(a)$ , indicates that the main reactive front I is partially premixed, since positive and negative values alternate over time and space. On the other side, branch II burns constantly in a diffusion mode as confirmed by both the Takeno index and the alignment between the stoichiometric mixture fraction *zst* and the heat release rate field.

### **6.4.4. Flame structure comparison**

Figure [6.16](#page-115-0) presents the mean absolute velocity field associated to flame *A* (left) and *L* (right). Isolines of  $U_z = 0$  in white highlight the recirculation zones, while the black isocontours of *HRRnorm* = 0.15 enclose the region of the main flame branch I for both operating conditions. Both the attached and lifted flames exhibit a wide IRZ that, favored by the recess  $z_i = 4$  mm, protrudes inside the injector. Figure [6.16\(](#page-115-0)a) shows that the recirculating mass flow rate creates a blockage at the outlet section of the hydrogen injector, forcing the  $H_2$  stream to spread radially before reaching the chamber backplane  $(z = 0)$ . Figures [6.16\(](#page-115-0)b-c) show the evolution of axial and radial velocity profiles between the outlet section of the  $H_2$  injector and the backplane at  $z = -3$ ,  $-2$  and 0 mm. The  $U_z$  profiles show two distinct peaks for both operating conditions. The internal one is due to the  $H_2$  jet, while the outer one is associated to the lateral air stream. Between these two zones, the local minimum corresponds to



**Figure 6.16.** – Time averaged distribution of the absolute velocity for the attached (left) and lifted (right) flames (a). The isocontour of  $U_z = 0$  delineating recirculation zones is reported in white, while the isoline  $HRR_{norm} = 0.15$ defining the main flame branch is depicted in black. The radial and axial normalized velocities are reported in (b) and (c) respectively, showing the velocity distribution in the region of the recess at  $z = 0$  mm,  $z = -2$  mm and  $z = -3$  mm.

<span id="page-117-0"></span>

**Figure 6.17. –** Isocontour of *HRRnorm* defining the main flame branch superposed to the isolines of equivalence ratio to highlight the mixture distribution with respect to the flame location. The two flame branches I and II are highlighted for both types of stabilization.

the small recirculation zone highlighted in Fig. [6.16,](#page-115-0) while the negative  $U_z$  velocities near the axis are due to the IRZ that penetrates into the central injector outlet. The mean axial velocity of  $H_2$  reduces along the axial direction due to the radial deviation of the flow. The mean axial velocity of the external air stream, instead, slightly increases before reaching the chamber backplane because the recirculation zone near the lip and the hydrogen flow reduces the cross section available for the annular flow. Despite the larger flow velocities for the lifted flames (Tab. [A.2\)](#page-130-0), the overall flow structure is comparable. In both cases the flow squeezes between the IRZ and the recirculation zone above the injector lips, resulting in a peak of *U<sup>r</sup>* at roughly  $z = -2$  mm. Hence, the injector design creates a large recirculation zone that forces the fuel to accelerate radially against the incoming oxidizer. The fact that the velocity field is similar in the two flames, suggests that the stabilization must depend on the magnitude of the velocities.

Furthermore, flow separation develops at the top of the  $H_2$  injector lip creating a small recirculation zone that may affect the flame stabilization directly. For example, the left side of Fig. [6.16\(](#page-115-0)a) shows that the attached flame *A* anchors preferentially in this low velocity region. The right side of Fig. [6.16\(](#page-115-0)a) shows that flame *L* anchors near the inner shear layer between the hot IRZ and the swirling jet of fresh reactants. A comparison between the main flame branches I associated to attached and lifted stabilization mechanisms is now provided. Figure [6.17](#page-116-0) shows isocontours of equivalence ratio colored by the normalized heat release rate for flames *A* and *L*. The region corresponding to the main heat release rate  $HRR_{norm} = 0.15$  is highlighted in red for the two cases. The main branch of the attached flame *A* develops along the stoichiometric mixture fraction  $z_{st}$  (see also Fig. [6.13\)](#page-113-0). In case of flame  $L$ , instead, Fig. [6.17](#page-116-0) shows that the main flame branch I is characterized by a wide range of mixture compositions. The mean lifted flame is stratified with a local equivalence ratio that gradually decreases from  $\phi = 6.0$  at the bottom to roughly  $\phi = 0.5$  at



**Figure 6.18.** – Scatter plots of axial velocity  $U_z$  against the axial coordinate z conditioned by  $HRR_{norm} > 0.15$  and colored according to the local equivalence ratio *φ* for flame *A* (a) and flame *L* (b).

the top. This range is coherently within the flammable limits predicted for freely propagating H2 air mixtures.

Figure [6.18](#page-117-0) shows the scatter plots of the axial velocity  $U_z$  against the coordinate *z* conditioned by values of  $HRR_{nrom} > 0.15$  for flames *A* and *L*. Data are colored according to the local equivalence ratio  $\phi$ . Figure [6.18\(](#page-117-0)a) shows that the attached flame is characterized by a wide range of equivalence ratios along its entire length. The upper part of the flame  $(z > 0)$  is subjected to axial velocities  $U_z$  that are much higher than the laminar burning velocity  $(U_z \gg S_L)$ , which is generally not compatible with flame stabilization. However, in this case the flame anchors inside the recirculation zone above the  $H_2$  injector lip  $-4$  mm  $\lt z \lt 0$  mm remaining far from the low velocity region defined by the IRZ, as shown in Fig.  $6.16(a)$  $6.16(a)$ . Hence, the bottom part of the flame is able to sustain the combustion downstream, even though the flow conditions are less favorable. Figure  $6.18(b)$  $6.18(b)$  shows the same scatter plot for the lifted flame *L*. In this case, the low velocity region that serves as anchoring point around  $z = 5$  mm lies near the inner shear layer between the swirling jet and the IRZ. Here, reactants are ignited thanks to the recirculation of hot gases and the flame stabilizes between 5 and 10 mm above the backplane. Figure [6.18\(](#page-117-0)b) shows that the upper part of the flame is subjected to high velocity and that the flame root serves as ignition source for the rest of the flame front allowing for a stable combustion. These results suggest that eliminating the small reverse flow near the H2 lips would favor flame lifting. Furthermore, the fast mixing and the existence of a wide IRZ provided by the specific injector design leads to the presence of the lifted flame.

### **6.4.5. Transition dynamics**

Previous sections demonstrated that simulations predict correctly two stabilization regimes observed in the experiments for steady state conditions and they allow to investigate their flame structures. This section shows the overall transition from lifted to attached flame, from both experimental and numerical perspectives. Note <span id="page-119-0"></span>that, because of hysteresis [\[196\]](#page-166-1) and variations of the local flow field due to the specific flame position, the passage from lifted to attached flames must not be considered as a simple consequence of the two different steady stabilization modes. In fact, the same operating point may lead to different flame characteristics depending on the initial condition. In the laboratory, the change of stabilization from lifted flame (*L*) is forced by imposing the hydrogen and the air mass flow rates that correspond to the attached one  $(A)$ . The transition is captured with a Phantom V1612 high speed camera sensible to visible light with a frame rate of 10 kHz. Figure [6.19](#page-119-0) shows 4 instantaneous line of sight integrated images describing the passage from lifted to attached stabilization:

- <span id="page-119-1"></span>1. Figure [6.19\(](#page-119-0)a) shows the initial lifted flame. At this point the central part of the flame  $(II)$  is close to the injector exit and the main flame region  $(I)$  is located on the edge of the IRZ.
- 2. The second phase is shown in Figure [6.19\(](#page-119-0)b). The black arrow indicates that the flame re-attachment starts with the formation of a lateral reacting front that propagates upstream.
- 3. Fig. [6.19\(](#page-119-0)c) shows that this lateral branch propagates upstream towards the injector lip. This evolution is not expected to be axi-symmetric because of local mixture variations and flow inhomogeneities of the turbulent swirling flow. Note that during this phase, the branch II of the flame remains close to the injector outlet.
- 4. Eventually, when the flame is completely attached around the injector lip, the central diffusion flame II moves downstream along the axial direction recovering the shape of the attached configuration as indicated by the arrow in Fig.  $6.19(d)$  $6.19(d)$ .

Numerically, the procedure is mimicked starting from an instantaneous solution of the lifted flame *L*. The inlet mass flow rate boundary conditions for air and hydrogen are changed at the beginning of the simulation imposing the ones of flame *A* (see Table [6.1\)](#page-104-0). Four chronologically-ordered snapshots representative of the computed transition from *L* to *A* are illustrated in Fig. [6.20.](#page-119-1) The normalized heat release rate *HRRnorm* is displayed with the superposition of three isocontours corresponding to  $HRR_{norm} = 0.025$  in red,  $z_{st}$  in green and the isoline  $U_z = 0$  in blue. LES recovers the global mechanism described in Fig. [6.19.](#page-119-0) In addition to that, simulations allow to appreciate that between Figs. [6.20\(](#page-119-1)a) and (c) the flame moves preferentially along the stoichiometric line *zst*, which corresponds to the location of the most favorable mixture in non-premixed combustion. In these snapshots the position of the isoline  $U_z = 0$  is also close to the flame leading point during the entire process. This suggests that the flame propagates along a narrow flammable region under the effect of a low instantaneous axial velocity  $U_z$ . Note that, irrespective of the flame position, the stoichiometric line passes near or through the small recirculation zone above the  $H_2$ injector lip. As consequence, during its upstream propagation, the flame is trapped inside this zone, where it eventually stabilizes as in Fig. [6.20\(](#page-119-1)d). This corroborates the observations made for the steady state case *A*.

These results confirm that the numerical setup can capture the main features of the investigated flame stabilization both for steady injection and transient conditions. A detailed investigation of the transition mechanisms from lifted to attached flames and vice-versa will be the object of future investigations.



**Figure 6.19.** – Line of sight integrated images describing the transition to flame lip reattachment: (a) lifted flame, (b) the formation of a lateral branch, (c) propagation of this branch towards the lip and (d) anchored flame.



**Figure 6.20.** – Time evolution in the axial plane of the normalized heat release rate distribution  $HRR_{norm}$  with superposition of two isocontours:  $HRR_{norm} =$ 0.025 and  $z_{st}$  during the transition from lifted  $L$  (a) to attached  $A$  (d) flame stabilization as consequence of the change of inlet boundary conditions.

# **6.5. Conclusions**

LES has been used to investigate the stabilization mechanisms and the structure of two H2-air flames obtained experimentally with a dual-swirl coaxial injector (HYLON), in which fuel and air are supplied via a central and an annular duct, respectively. One flame is attached to the injector  $(A)$  and the other one is aerodynamically stabilized (*L*), hence multiple combustion regimes are involved. Flames feature the same equivalence ratio  $\phi_q = 0.45$  but different input thermal powers.

First, the numerical setup has been validated against a large set of experimental data including PIV in isothermal and reactive conditions and  $OH^*$  flame images, demonstrating that the proposed modeling approach is suitable to compute the non-premixed flames investigated.

The velocity fields for the two operating conditions show the presence of a large IRZ which, penetrating inside the injector, causes a strong radial expansion of the central H2 swirling jet. Despite the similar flow pattern for the two operating conditions, the flame stabilizations differ. Flame *A* anchors in a low velocity region above the hydrogen injector lip, serving as source of ignition for the rest of the flame branch. In this case the flame evolves in a high velocity region along the mixing layer that separates fuel and oxidizer. This part of the flame burns in diffusion mode along the stoichiometric mixture fraction. The main branch of the lifted flame *L*, instead, stabilizes in the inner shear layer between the IRZ and the exiting hydrogen swirling jet. The flame lift-off permits a degree of mixing that results in a main stratified reaction front characterized by a wide range of equivalence ratios  $0.5 < \phi < 6.0$ . Both experiments and simulations also show that a second reaction front is found at the interface between the hot recirculating gases and the central  $H_2$  stream. This part of the flame is controlled by diffusion and it only changes in its mean position when passing from lifted to attached stabilization.

Finally, the unsteady transition from lifted to anchored flame has been investigated experimentally and numerically. When the flame power is reduced, the lifted flame develops a lateral flame branch that starts propagating towards the injector. LES instantaneous snapshots demonstrate that the flame leading point travels upstream along a trajectory characterized by low axial velocities and near-stoichiometric mixture fractions. Eventually, this front is trapped in a small recirculation zone above the  $H_2$  injector lip and the anchored flame is then retrieved. These observations corroborate the scenario recently proposed in [\[191\]](#page-166-2) for conditions leading to flame reattachment.

The material presented in this chapter was published in the peer reviewed international journal Combustion and Flame [\[197\]](#page-166-3).

CHAPTER<sub>1</sub>

# **General conclusions**

The thesis investigates  $H_2$  combustion either when it is part of fuel blends or injected pure, with the objective to improve the comprehension of the fundamental mechanisms to pave the way to develop safe and reliable  $H_2$  combustion technologies.

Part I presents experiments conducted on two laminar premixed multi-perforated burners, originally designed for  $CH_4$ -air combustion. A new test bench, named CoMix, has been developed to test the risk associated to  $H_2$  combustion by increasing its substitution in the  $\text{CH}_4/\text{H}_2$  fuel blend over a wide range of equivalence ratios and two input thermal powers. Measurements at steady operation showed that  $H_2$ addition in the fuel blend improves the blow off resistance, not only because hydrogen extends the flammability limits of the combustible mixture, but also because of the high diffusivity of  $H_2$  molecules. Nevertheless, it was also shown that the thermal load on the burner increases with the  $H_2$  content and ultimately favors flashback. Hence, the achievable range of operating conditions when hydrogen is added remains roughly unchanged and the fuel flexibility of the system is compromised. Additional tests during transient operation put in evidence the existence of different flashback regimes. It was shown that for high equivalence ratios and large hydrogen substitutions, flashback is triggered immediately during ignition, when the burner walls are at ambient temperature. For moderate equivalence ratios and moderate hydrogen substitutions, instead, flashback occurs for a specific temperature of the hot metallic walls that only depends on the mixture composition. Considering this last flashback regime, high speed flame visualization demonstrated that two flashback mechanisms are possible when  $H_2$  is added to the fuel blend in this kind of systems. In one case the flame propagates through the burner holes, moving upstream in the injection system. In the second case, the temperature of the hot metallic walls is sufficiently high to act as a source of energy for the autoignition of the combustible mixture.

In Part II, high-fidelity Large-Eddy Simulations (LES) have been used to compare the acoustic response of a perfectly premixed CH4-air swirling flame (*REF*) with the one observed after the addition of a central pilot  $H_2$  injection that supplied 10% of the total thermal power (*PH*10). The first objective was to identify the mechanisms leading to reduced heat release rate oscillations at 240 Hz for the pilot flame compared to the fully premixed case which is observed in experiments. The second objective was to understand the modification of the phase lag between heat release rate disturbances with respect to incoming acoustic disturbances between the two cases. First, LES unveiled the formation of a diffusion flame downstream the hydrogen lance responsible for a redistribution of the global heat release rate towards the flame base with respect to the *REF* case as also observed in experiments. The numerical analysis of the forced flames also showed that the hydrogen pilot injection reduces the overall flame length, weakening the interactions between the flame and the vortical structures shed at the injector rim as consequence of the flow modulation. Phase averaged conditioned images gathered at both 240 Hz and 590 Hz showed that the CH4-air flame acoustic response was dominated by the rollup of the flame tip, while in case of  $H_2$  pilot addition this mechanism was strongly reduced. In addition to that, at 240 Hz, LES show that the phase-averaged velocity fields unveil a significant axial oscillation of the internal recirculation zone for both injection strategies. While this mouvement had no effect on the *REF* flame base that was solidly anchored to the injector lips, this second mechanism modulated the penetration of the hydrogen jet into the combustion chamber for the *PH*10 flame, favoring a consequent oscillation of the flame root. The reduced roll-up of the flame tip due to the shorter flames produced with the addition of  $H_2$  and the oscillation of the flame base due to the pilot injection interact with each other and generate destructive interferences of the acoustic response of the  $H_2$  piloted flame at 240 Hz, which is responsible for the deep of the flame transfer function gain observed at 240 Hz. These results demonstrated that both the pilot injection and H2 addition are necessary to produce this effect and corroborate experimental findings for which neither a pilot injection of  $\text{CH}_4$ , nor premixing  $\text{H}_2$  to the  $\text{CH}_4$ -air mixture, were able to produce the same alteration of the *FTF*. LES also showed that the phase shift between *REF* and *PH*10 can be predicted by considering the impact of the mean flame length reduction on the characteristic time lag of the flame response.

In Part III, high-fidelity LES are used to investigate the stabilization mechanisms of pure  $H_2$ -air non-premixed swirling flames. Simulations are validated with experiments also conducted at IMFT on an injector patented in partnership with SAFRAN SHE. It consists of a coaxial dual-swirl injector named HYLON, which geometry has been optimized with several test campaigns and apriori numerical simulations. A flame anchored to the injector lips and an aerodynamically stabilized flame, lifted above the combustion chamber backplane, have been scrutinized. First, a modeling approach intended to capture simultaneously multiple combustion regimes was validated against experimental data for the two cases analyzed. LES unveiled that the first flame anchors inside small recirculation zones formed in the wake of the internal lips of the hydrogen injector, where the low velocities favor the mixing between fuel and oxidizer. It has been demonstrated that this flame archetype is completely controlled by diffusion processes and is formed by two different reaction branches branches. The first one develops along the jet mixing layer between the reactants, far from the low velocity region induced by the IRZ. The second branch stabilizes at the center of the combustion chamber, right above injector outlet. It is formed between the exiting hydrogen jet and the excess of  $O_2$  in the recirculating burnt gases resulting from a globally lean combustion. This second flame branch appears also as part of the lifted flame but, because of higher recirculating velocities inside the IRZ, it is located closer to the injector outlet. LES shows that the lateral branch of the lifted flame, instead, is partially premixed and stabilizes in the shear layer between the IRZ and the exiting swirling jet. Eventually, the unsteady transition from lifted to anchored flame has also been investigated, mimicking the observations made in experiments with high-speed cameras. LES instantaneous results are exploited to show that the flame leading point moves along a region characterized by both low velocity and nearly-stoichiometric mixture. These evidences support a re-attachment mechanism, for which a triple flame exists in the shear mixing layer above the injector outlet and propagates upstream through low velocity regions.

**Appendices**



# **Introducing thermodiffusive effects in LES turbulent combustion for lean H<sub>2</sub>-air flames**

The material presented in this appendix was published in the Proceeding of the CTR Summer Program 2022 [\[198\]](#page-166-4).

# **A.1. Motivations and objectives**

Understanding and predicting hydrogen-air flame stabilization and structures is crucial to develop future engine applications. A classical problem in the combustion community [\[171,](#page-164-0) [199,](#page-166-5) [200,](#page-166-6) [201,](#page-167-0) [202\]](#page-167-1). From modelling perspective, hydrogen unique physical characteristics open new challenges in the context of high-fidelity simulations. For example, in many applications, the high hydrogen reactivity allows to assume that the characteristic chemical timescale is much smaller than the convective one so that simplified modeling approaches can be used, like for instance strained diffusion flamelets  $[105, 203, 204]$  $[105, 203, 204]$  $[105, 203, 204]$  $[105, 203, 204]$  or even infinitely fast chemistry assumption in the case of  $H_2/O_2$  flames [\[205\]](#page-167-4).

Moreover, it was discussed in Section. [1.2](#page-18-0) that one of the premixed  $H_2$  lean flame specificities is the capacity to develop thermodiffusive instabilities  $[201, 206]$  $[201, 206]$  due to the large disparity between molecular and thermal diffusions. When a propagating planar laminar flame is perturbed, the initial modification of the reaction layer is self-amplified leading to the formation of cellular structures that modify the local flame burning rate and induce additional wrinkling of the flame front. These in turn increase the global consumption speed by a factor between 2 and 4 [\[53,](#page-156-0) [55\]](#page-156-1).

These flames result shorter than normally expected for unity Lewis number and show local super-adiabaticity that may potentially lead to higher NOx emissions, which is another concern of  $H_2$  flames. Clearly, a turbulent combustion model for LES of hydrogen flames that aims at being representative of the flame shape and pollutant emissions must contain these effects. This is the main topic of this appendix.

An additional complexity of hydrogen flames is created by the effects due to the increase of pressure. While most laboratory experiments are performed at 1 bar, in fact, real gas turbine chambers operate from 15 to 50 bars. Under these conditions all molecular diffusivity coefficients decrease ( $\approx 1/P$ ), the Reynolds number increases and the characteristic flame thickness decreases. As consequence, a direct simulation of those operating conditions becomes prohibitive and reliable subgrid scale combustion models must be adopted for flame-turbulence interaction. Of course, similar issues arise for kerosene or methane flames too, but for hydrogen, <span id="page-127-0"></span>more complex dynamics is expected since pressure amplifies the impact of thermodiffusive instabilities: the stabilization mechanisms or thermo-acoustic responses of hydrogen flame at high pressure can be completely different than the ones at atmospheric conditions. Another important aspect specific of hydrogen flames is that the impact of thermodiffusive instabilities depends on the combustion regime: diffusion flames do not exhibit any intrinsic thermodiffusive instability, while lean premixed flames are highly susceptible to their effects. As consequence, a fair evaluation of thermodiffusive phenomena requires a proper prediction of the dominant combustion regimes in the specific applications. This is particularly important for *H*2 flames since, as shown in Part III, in order to avoid safety issues, the reactants are commonly injected separately leading to a variety of potential stabilization and combustion regimes. Such flames can be anchored near the lip of the injection devices. In this first case, as result of the long mechanical mixing times compared to chemical times associated to hydrogen chemistry, flames are mainly diffusioncontrolled and thermodiffusive effects are negligible. However, depending on the flow, and the mixing devices implemented inside a hydrogen injection device, flames can also be lifted from the injection lips, a property which is useful to limit the thermal load on walls and the NOx emissions. In this second case, depending on the distance between the flame and the injector lips, various degrees of mixing between reactants are possible and fronts propagating in lean zones may trigger thermodiffusive effects. Hence, LES combustion models for hydrogen must account not only for the thermodiffusive instabilities, but also modulate their influence depending on the combustion regime encountered. This aspect is specific of LES of real flames: most DNS of hydrogen flames have been limited to perfectly premixed cases so that new additional physics is expected when real hydrogen combustors are considered. The present study proposes a first and preliminary LES model, in the framework of the TFLES formulation  $[115]$ , taking into account hydrogen thermodiffusive effects by introducing DNS correlations obtained in  $[49, 50]$  $[49, 50]$  to account for thermodiffusive effects. The initial model is called TFLES while the new one is designated as TD-TFLES for "thermodiffusive"-TFLES. The implementation and the limits of the proposed model are described in the next section. The TD-TFLES is then tested against experimental data gathered at IMFT on a swirled hydrogen - air turbulent flame and compared to the results previously obtained with the standard TFLES approach.

# **A.2. A DNS-based TFLES model incorporating thermodiffusive effects for hydrogen flames (TD-TFLES)**

This study proposes to include the effect of thermodiffusive instabilities in LES combustion model based on the thickened flame formalism. Both flame / turbulence interaction and thermodiffusive instabilities generate flame surface wrinkling that can alter the local burning rate. Hence, these two mechanisms are expected to compete, or at least co-exist, in the same model.

At this point, it is useful to introduce notations: following [\[53\]](#page-156-0), *I<sup>o</sup>* is the ratio of the local consumption speed  $\langle s_c \rangle$  over the laminar burning velocity  $s_L^0$ . The flame wrinkling induced by thermodiffusive effects will be designated as  $\Theta_0$  and the wrinkling induced by turbulence Θ. As basic assumption for the first form of the TD-TFLES model, we loosely imply that the wrinkling induced by thermodiffusive

<span id="page-128-0"></span>

**Figure A.1. –** Scale separation principle of the TD-TFLES model for LES of turbulent hydrogen flames including thermodiffusive effects.  $\Theta$  is the wrinkling induced by turbulence.  $\Theta_0$  is the wrinkling induced by thermodiffusive effects at subgrid scale.  $I_0$  measures the changes of the local consumption speed induced by thermodiffusive phenomena.

effects  $(\Theta_0)$  and by turbulence  $(\Theta)$  are decoupled. Therefore, the starting point of the model consists in considering that the length scales of the cellular structures produced by thermodiffusive effects that scale with the laminar flame thickness  $\delta_I^0$ *L* are much smaller than the wrinkling scales induced by flame - turbulence interaction (Fig. [A.1\)](#page-127-0). These turbulent scales vary widely between the integral scale *L* of the turbulence and the Kolmogorov scale *η*. In spectral space, this model works under the assumption of scale separations (Fig. [A.2\)](#page-128-0): thermodiffusive instabilities act at small scales while turbulence scales are all larger.

Clearly, not all flames will satisfy the assumption used to build the TD-TFLES model. Consider a burner where typical integral scales, imposed by the geometry, are of order *L*. This size *L* for most burners of interest is much larger than the flame thickness  $\delta_L^0$  so that the TD-TFLES idea works for them. However, the question is to know whether all other turbulent scales also fulfill the scale separation assumption. The smallest one will be the Kolmogov scale. For the TD-TFLES to work at all scale, the Kolmogorov scale should also be larger than the characteristic flame length  $\delta_L^0$ . This is verified for low Reynolds numbers and in this case the Kolmogorov scale *η* will also be large compared to  $\delta_L^0$  so that the TD-TFLES model idea can be applied (the Karlovitz number  $K_a = (\delta_L^0/\eta)^2$  will be low). When the flow rates and the Reynolds number increase, however, the Kolmogorov scale  $\eta$  will decrease and eventually reach the same order of magnitude as  $\delta_L^0$  at which thermodiffusive instabilities occur. In this case, the TD-TFLES model should not be used: the small turbulence scales will interact with the thermodiffusive scales in a manner which is still open to speculations and these regimes are left for further research.

Under the TD-TFLES assumption, the turbulent flame speed  $s_T$  can then be expressed as

$$
s_T = s_L^0 I_o \Theta_0 \Theta. \tag{A.1}
$$

In this TD-TFLES approach, thermodiffusive effects are completely modeled as a subgrid scale phenomena, since the spatial discretization provided by the LES solver is supposed to be too coarse to capture the thermodiffusive scales. Hence,  $I<sub>o</sub>$  and Θ<sup>0</sup> are not resolved by the LES solver. The wrinkling Θ due to turbulence/flame interaction, instead, has a resolved part which is captured by the LES solver and a <span id="page-129-0"></span>subgrid part which is modeled through the efficiency function of the TFLES model as usually done [\[115\]](#page-160-1).



**Figure A.2.** – Representation of the scale separation assumption between thermodiffusiive wrinkling and turbulence wrinkling used in the TD-TFLES model .

<span id="page-129-1"></span>Furthermore, it must be underlined that the present model can be regarded as a pure extension of the classical TFLES: fuels which do not exhibit TD instabilities will simply work under the assumption  $I_0 = 1$  and  $\Theta_0 = 1$ , retrieving the standard modeling. In the general case, instead, the closure of the new LES approach requires models for the two terms  $I_0$  and  $\Theta_0$ . Here, this closure was obtained using the correlations of  $[49, 50]$  $[49, 50]$  extracted from DNS of lean  $H_2$ -air flames. In these DNS the overall speed of a laminar flame developing self-excited thermodiffusive instabilities was measured in a range of pressure P from 1 bar to 20 bar, fresh gas temperatures  $T_{\text{fresh}}$  ranging from 300 K to 700 K and a large range of equivalence ratios  $\phi$ . These thermodynamic conditions are representative of several combustion chambers targeted for real applications. A typical snapshot of such DNS throughout the non-linear regime is given in Figure [A.3](#page-129-0) left, which shows the temperature field of a premixed H<sub>2</sub> - air flame at  $\phi = 0.4$  subjected to thermodiffusive instabilities. The flame front, initially flat, increases its surface and produces a self sustained wrinkling due to low Lewis number effects as well as a non-uniform wake of burnt gas temperature behind the flame front. Figure [A.3](#page-129-0) right shows the resulting form for the correction  $I_o\Theta_0$  as a function of  $T_{fresh}$  and *P* and  $\phi$ :  $I_o\Theta_0$  tends to unity for near-stoichiometric or rich flames while, at atmospheric pressure, it can go up to 4 for very lean conditions ( $\phi$  < 0.4). These correlations for  $I_o\Theta_0$  are tabulated and implemented in the LES model.

In the specific case of the swirling flame tested here, *Tfresh* and *P* are fixed to the inlet temperature of reactants and to the operating pressure of the combustion chamber, respectively. Because of a potential separated injection (like in this study), only the equivalence ratio variation must be considered locally and at each timestep to retrieve the correct instantaneous efficiency value. The model can be extended to other systems characterized by temperature and pressure variations during the combustion processes (piston engines for example) informing the model for the thermodiffusive effects of the instantaneous and local thermodynamic conditions.

Once the increase of chemical reaction due to thermodiffusive effects  $I_o \Theta_0$  is known, it is implemented into the TD-TFLES model for combustion by multiplying both the diffusion term and the combustion term by  $I_o\Theta_0$ , exactly like for the efficiency function of the original TFLES model  $[105]$ . The influence of thermodiffusive instabilities must be eliminated for diffusion flame. This is done by evaluating the

<span id="page-130-1"></span>

**Figure A.3.** – Left: DNS of hydrogen-air laminar flames at equivalence ratio  $\phi = 0.4$  ex-hibiting thermodiffusive effects in hydrogen flames [\[50\]](#page-156-3). Right: extracted values for  $I_o\Theta_0$  depending on *P*, *T* and  $\phi$  used for the TD-TFLES implementation at 1 bar [\[50\]](#page-156-3).

Case			$\dot{m}_{air}$ [g/s] $\dot{m}_{H_2}$ [g/s] $U_b^{air}$ [m/s] $U_b^{H2}$ [m/s] $P_{th}$ [kW]			$\phi_a$
	2.41	0.032		13.6	3.89	0.45
	6.03	0.080	28.5	34.0	9.73	0.45

<span id="page-130-0"></span>**Table A.1.** – Mass flow rates of air and hydrogen, nominal thermal power  $P_{th}$  and global equivalence ratio  $\phi_g$  adopted for the two operating conditions *A* (attached flame) and *L* (lifted flame).

Takeno index  $[119]$  in space and time to distinguish between premixed or diffusion regimes and conditioning the application of the TD-TFLES accordingly.

# **A.3. Application of the TD-TFLES models to a swirled hydrogen - air non-premixed flame**

The TD-TFLES formulation was tested on the HYLON swirled hydrogen - air turbulent burner investigated in Section [6.](#page-99-0)

In the inlet section of the burner, turbulent mixing induced by the turbulent flow competes with the chemical times of hydrogen - air chemistry and the outcome of this competition leads to either an anchored flame or to a lifted one. It is shown in Chapter [6](#page-99-0) that flame stabilization is controlled by the aerodynamic field imposed at the injector outlet and by both hydrogen and air flow rates (Table [A.1\)](#page-129-1). The first are attached to the lips of the injection system and are completely diffusion-controlled. The latter has the potential of creating intense mixing before combustion and a large portion of the flame burns in premixed conditions (case L in Figure [A.4\)](#page-130-1).

The simulation tool is the compressible solver AVBP [\[30,](#page-155-0) [207\]](#page-167-6) in which flame / turbulence interactions are modeled using the TFLES model [\[112,](#page-160-2) [115,](#page-160-1) [208\]](#page-167-7). The numerical setup, including mesh and boundary conditions, is the same that has been described and validated in Chapter [6.](#page-99-0)

Hence, the effects of the model are assessed by comparing the standard TFLES and TD-TFLES for the lifted flame *L*, which corresponds to the case of practical interest. Both simulations using TFLES and TD-TFLES were run for 25 ms corresponding to two flow-through times at the bulk velocity which was found sufficient to reach steady state and gather statistics. For this flame, Table [A.2](#page-130-0) summarizes numerical CHAPTER A : Introducing thermodiffusive effects in LES turbulent combustion for lean  $H_2$ -air flames

<span id="page-131-0"></span>

<span id="page-131-1"></span>**Figure A.4.** – The HYLON dual-swirl burner for hydrogen - air combustion. Left: schematic of the injection system with annular injection of air and central injection of hydrogen stream.  $S_1$  and  $S_2$  denote the internal and external swirlers of the coaxial injectors. Right: line of sight integrated images for lifted (top) and attached (bottom) flames (Courtesy of H. Magnes, S. Marragou, T. Schuller, IMFT).

Total mesh cells	$\approx$ 51 M Unstructured
Convection Scheme	Lax Wendroff
CFL	0.7
time step [s]	$9.0e-9$
Chemical scheme	San Diego $(ARC 9s21r)$

**Table A.2. –** Numerical setup characteristics in terms of mesh size, convection and chemical schemes.

and physical parameters used in the LES.

Since the injection lines of hydrogen and air in HYLON are separated, a wide range of equivalence ratios is expected in the chamber zone where combustion takes place so that the  $I_0\Theta_0$  correction of Figure [A.3](#page-129-0) should be active on the premixed lean side of the flame in multiple places.

The first overall result is that the introduction of the TD model does not change the flame position or behavior radically with respect to the previous formulation. Figure [A.5](#page-131-0) shows the time averaged fields of the reaction rates for the standard TFLES (right) and the TD-TFLES (left) over an axial plane of the combustor. Even if the TD-TFLES increases the local mean combustion intensity, the flame remains constrained by the recirculation zone and does not change its position significantly, as shown by an instantaneous field of heat release rate in Figure [A.6,](#page-131-1) which also shows the lifted nature of the flame. First, the lower side of the flame wings is characterized by premixed combustion (*Takeno >* 0): hydrogen and air mix at the injector mouth before burning in premixed mode. Above the injector lips of the combustor (inside the line  $z = z_{st}$  line), the mixture is very rich  $(2 < \phi < 8)$  since the supply of reactants in this zone is mainly due to the central injection. Further downstream along the flame wings, the longer mixing time allowed between hydrogen

<span id="page-132-0"></span>

A.3 Application of the TD-TFLES models to a swirled hydrogen - air non-premixed flame

**Figure A.5.** – Cut in the central plane of the combustor for flame L. Mean fields of heat release rate for TD-TFLES (left) and TFLES (right).



**Figure A.6.** – Cut in the central plane of the combustor for flame L. Instantaneous field of heat release rate for TD-TFLES. Red line: stoechiometric line  $z=z_{st}$ computed using the definition of Bilger [\[209\]](#page-167-8). The heat release rate distribution is divided in two zones: the first one indicating premixed regions (*Takeno >* 0) and the second one, in transparence, where the flame is diffusion-controlled  $(Takeno < 0)$ .

and air leads to leaner flames ( $\phi < 0.5$ ). On the combustor axis, a diffusion flame  $(Takeno < 0)$  is formed between the hydrogen central stream and the equilibrium products (stilll rich in  $O_2$ ) recirculating in the inner recirculation zone.



**Figure A.7.** – Cut in the central plane of the combustor for flame L. Fields of the thermodiffusive efficiency  $I_0\Theta_0$  for TD-TFLES conditioned on the flame location. Line: stoechiometric line z*st*.

As expected, the  $I_o\Theta_0$  correction introduced in the TD-TFLES model does not modify the diffusion flame zones or the rich premixed flamelets: the field of  $I_0\Theta_0$ (Figure [A.7\)](#page-132-0) shows that the model leads to  $I_o\Theta_0$  values different from unity (unity corresponding to "no effect") only in the lean premixed flames at the flame tip, increasing the local reaction rate by factors up to 4 in the very lean zones. The model is also inactive in the zones where mixing takes place, close to the  $H_2$  injector.

# **A.4. Conclusions**

A model for thermodiffusive instabilities for lean hydrogen - air flames was added in the classical TFLES formalism, assuming scale separation between (small) thermodiffusive scales and (large) turbulent scales. This additional model requires closure laws for two effects: (1) subgrid scale wrinkling  $(\Theta_0)$  due to cell formations and (2) modification of the mean consumption rate  $(I_0)$ . Both were obtained from the DNS of self-excited atmospheric hydrogen - air flames by [\[50\]](#page-156-3).

The DNS correlations were introduced in the LES AVBP code as a tabulation and used as an additional efficiency function to increase the local reaction rates accordingly.

The LES solver was run for the swirler hydrogen-air injector developed by IMFT. Results show that thermodiffusive instabilities increase local reaction rates by a significant factor in the lean parts of the flame ( $\phi < 0.5$ ) but leaving the diffusion flame zones as well as the rich premixed flamelets unaffected.

In the case of the IMFT injector studied here, the modified TD-TFLES model leads to a negligible increase of local reaction rates but the flame position, which is fixed mainly by the flow, is marginally affected because the lean premixed regions are limited and the flame is dominated by a large diffusion zone as well as premixed rich zones.

Future work will be needed to test the model on other flames and improve it to relax the scale separation assumptions used to build it. The effects of the model on  $NO<sub>x</sub>$  emissions will also be evaluated.

# <span id="page-136-0"></span>APPENDIX .

# **Comparison among Lattice Boltzmann and finite volume solvers for swirled confined flows**

The material presented in this appendix was published in the peer reviewed international journal Computers and Fluids [\[154\]](#page-163-0).

# **B.1. Introduction**

The question of the efficiency of CFD solvers is an issue which has virtually disappeared for classical RANS (Reynolds Averaged Navier-Stokes) methods but remains essential when it comes to Large Eddy Simulation approaches [\[210,](#page-167-9) [211\]](#page-167-10) as pointed out recently by Löhner [\[212\]](#page-167-11). Arguing that a certain class of CFD methods is the fastest to solve LES critical problems is a game played by multiple teams worldwide: in most cases, these discussions focus on the theoretical reasons which should make such or such approach faster than others for LES. However, the actual speed of CFD solvers for LES does not depend only on the theoretical efficiency of the method: in most cases, the mesh management, the boundary conditions, the sub models, the parallel implementation of the method also play critical roles so that the determination of an exact CPU efficiency is difficult before running real simulations. Furthermore, when simulations are run, the comparison itself between methods becomes difficult: in many cases, each author runs his own code and does not try to compare fully with competing methods. Workshops are commonly organized to compare methods but their conclusions are rarely clear because the collaboration to ensure a proper comparison remains difficult to set up (see for example [\[213\]](#page-167-12) for such a workshop on compressible methods for LES of turbomachinery).

<span id="page-136-1"></span>This paper follows a different path as it compares three LES solvers (Table [B.1\)](#page-136-0) which were all run by the same group of people at IMFT and CERFACS: an incompressible finite volume solver: AVBP*pgs* and two Lattice Boltzmann (LB) codes: ProLB and WALBERLA. All computations were performed on the same machines, with the same number of processors and a systematic comparison was organized to ensure a fair evaluation of methods. The target configuration was the internal turbulent flow in a swirling burner but all cases correspond to a non reacting situation. Unlike many previous studies, the present one focuses on an internal flow, at moderate Reynolds numbers, as found in combustion chambers and not on external flows as found in aerodynamic and aeracoustic studies. Experiments were performed by the EM2C laboratory and include enough detailed data to evaluate the precision of the solvers in terms of pressure losses and full mean and RMS velocity fields.

Of course, the first difficulty in such an exercise is the definition of the rules of the

<span id="page-137-0"></span>

	swirled confined flows		
Code	Formulation	Method	
$\text{AVBP}_{\text{pqs}}$	Incompressible	Finite	volume
		(Galerkin)	
ProLB	Athermal	Lattice Boltzmann	
WALBERLA	Athermal	Lattice Boltzmann	

Chapter B : Comparison among Lattice Boltzmann and finite volume solvers for swirled confined flows

**Table B.1. –** Presentation of solvers used for LES simulations.

game. In the present case they can be explained as follows: "for each code, build a numerical setup which provides a minimal accuracy in terms of flow field resolution (pressure loss as well as mean and RMS velocity profiles within experimental accuracy levels) and compare the CPU efficiency". Since multiple solvers are used, with different meshes, different algorithms and different submodels, the notion of minimal accuracy remains arbitrary: here, long discussions between CFD and experimental teams members have lead to a minimum quality which was expected from the match between experimental and LES results in terms of average and RMS velocity fields for multiple locations. This was used for the three solvers to determine the minimum grid size required to reach this sufficient level of agreement. Once all solvers were found to provide comparable agreement with the experimental data (taking into account experimental uncertainties), CPU efficiencies were determined. This procedure still contains a clear level of arbitrariness that authors do not want to deny. The error bars expected on the results are certainly significant and of the order of tens of percents. However, the main issue here is not to determine if a method is 50 percent faster than another one: we are interested in orders of magnitudes as required for example for industry to move from one class of methods to another one.

The paper is organized as follows: the experimental configuration is described first in Section [B.2.](#page-136-1) The three solvers and the corresponding numerical setups are described next (Section [B.3\)](#page-139-0) before discussing results in Section [B.4](#page-144-0) in terms of velocity profiles (mean, RMS and spectra). Finally the computational efficiency of the three codes is discussed in Section [B.5.](#page-148-0)

# **B.2. Experimental setup**

The configuration (Fig. [B.1\)](#page-137-0) was designed to analyze the response of swirled flames to flow rate modulations in [\[152,](#page-163-1) [214\]](#page-167-13).

Dry air is injected from two diametrically opposed apertures at the bottom of a plenum. The flow crosses a grid and a honeycomb to break the largest turbulent scales. A convergent section produces a top-hat laminar velocity profile with a boundary layer of about 1 mm thickness that was characterized by a hot wire probe (Dantec Dynamics - Probe 55P16 with a mini-CTA 54T30). The diameter of this section is  $D = 22$  mm and the bulk flow velocity is fixed to  $u_b = 5.44 \pm 0.05 \text{ m s}^{-1}$ corresponding to a Reynolds number  $\text{Re}_D = 7620$  at room temperature  $T = 300$  K. The pressure drop with respect to ambient conditions is recorded in front of the hot wire probe with a differential pressure gauge and indicates  $\Delta p = 335 \pm 15$  Pa. The setup was originally designed to analyze effects of geometrical modifications of the injector on flame dynamics and the burner replaceable components are represented in Fig. [B.1.](#page-137-0) In the configuration explored, the radial swirling vane consists of  $n = 6$ cylindrical tangential inlets of diameter  $D_s = 6$  mm with an offset  $H = 6$  mm as indicated in Fig. [B.1c](#page-137-0). The flow leaves the swirler into a central injection tube. The

<span id="page-138-0"></span>

**Figure B.1.** – Experimental setup with detailed representation of the injector region and swirler geometry. All dimensions in mm.

diameter of this tube is  $D = 22$  mm, over a first section of length  $\delta_1 = 16$  mm, followed by a central insert of length  $\delta_2 = 34$  mm and diameter  $D_0 = 20$  mm. A central rod of diameter  $d = 6$  mm ending with a cone of diameter at the top  $C = 10$  mm is inserted in the injection tube. The distance between the swirler exit and the combustion chamber back plane is here fixed at  $\delta = \delta_1 + \delta_2 = 50$  mm. The central rod protrudes inside the combustion chamber and the distance between the top of the cone and the backplane is 1*.*5 mm. The combustion chamber, made of 4 transparent quartz windows, has a 82 mm squared cross-section and length 150 mm. It is extended by a nozzle with a square inlet section and a circular outlet section of diameter 70 mm. Transition between this square to circular sections is made over a 104 mm length. This device ensures that there is no reverse flow at the setup outlet. The cartesian system of reference used through the paper is presented in Fig. [B.2:](#page-138-0) *z* corresponds to the symmetry axis of the injector, while the plane defined by axes

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<span id="page-139-0"></span>

**Figure B.2.** – Presentation of cartesian system of reference (left). Identification of points *P* and *Q* used for modal analysis (center) and representation of PIV transverse and axial planes of investigation (right).

*x* and *y* corresponds to the backplane of the combustion chamber  $(z = 0 \text{ mm})$ .

Particle Image Velocimetry (PIV) is used to measure the cold flow velocity fields. For these measurements, the flow is seeded with small oil droplets of diameter 1-  $3 \mu$ m. PIV data are gathered on both axial and transverse planes within the combustion chamber. The first is identified by  $z$  and  $x$  directions  $(y = 0 \text{ mm})$ , while the second one is parallel to the burner backplane and located at  $z = 3.5$  mm. No PIV data is available at lower axial coordinates. The PIV system consists of  $2 \times 400$  mJ Nd:YAG laser doubled at 532 nm operated at 10 Hz and a  $2048 \times 2048$  pixels CCD camera (Dantec Dynamics, FlowSense EO 4M). Two different optical setups are used with a time interval between the two laser pulses  $\Delta t = 10 \mu s$  and a pixel pitch of 27.88 pixels mm<sup>-1</sup> for measurements in the axial plane and  $\Delta t = 25 \mu s$  and a pixel pitch of 40.14 pixels mm<sup>-1</sup> for measurements in a transverse plane. Eight hundred images are taken to assure the convergence of the mean and RMS values of the velocity field, which is computed from the cross-correlation of the PIV images by a three passes window deformation technique (from  $64 \times 64$  pixels to  $16 \times 16$  pixels interrogation areas), with an uncertainty of 0*.*1 pixels on the calculated displacement.

The measurements are completed by Laser Doppler Velocimetry (LDV) to capture the time resolved velocity profiles at  $z = 3$  mm above the top central insert (see Fig. [B.2\)](#page-138-0). The Power Spectral Density (PSD) of the axial velocity is calculated to detect the presence of potential hydrodynamic or acoustic modes. To ease optical access the combustion chamber is removed for those latter measurements and LDV data are collected in unconfined configurations. Two laser beams at  $\lambda = 514.5$  nm (green) allow to probe the axial velocity. Two other beams at  $\lambda = 488$  nm (blue) are used to measure the velocity component along *x* direction. The data collection rate is always greater than  $10000 \text{ s}^{-1}$  and for each measurement point at least 250000 particles are considered, in order to obtain fully converged mean and RMS values for all components of velocity. The statistical bias is corrected by the transit time of each particle. The analysis of time traces and PSD of these signals does not reveal any specific coherent structures associated to helical flow instabilities.

# **B.3. Presentation of solvers**

### **B.3.1. High-order finite volume solver**

AVBP is a multi-species LES explicit solver for Navier-Stokes compressible equations developed at CERFACS (www.cerfacs.fr/avbp7x). This Cell-Vertex (CV) highorder Finite Volume (FV) code [\[215,](#page-168-0) [216\]](#page-168-1) is able to handle structured, unstructured and hybrid grids in both two and three space dimensions. It is a world standard code to compute turbulent reacting flows in combustion chambers [**?** ] or explosions in confined domains [\[217\]](#page-168-2). A critical aspect of compressible codes is the treatment of numerical boundary conditions where acoustic reflections must be controlled to avoid spurious phenomena. In order to fulfill those requirements, AVBP exploits Navier-Stokes Characteristic Boundary Conditions (NSCBC) [\[218,](#page-168-3) [219,](#page-168-4) [220](#page-168-5)**?** ].

<span id="page-140-1"></span>Like any explicit compressible code, AVBP tends to be less efficient for low Mach number simulations. The problem arises from the large disparity between time scales associated to sound waves propagation and convection: the CFL stability condition imposed by the sound speed is uselessly severe with respect to the limit established by convection alone, resulting in an unnecessarily small time step. In order to overcome this limitation and to be representative of another class of FV solvers, which use incompressible or low-Mach number formulations, a modified version of AVBP, called here AVBP*pgs* is used to remove the acoustic time step limitation: the governing equations solved are manipulated according to the Pressure Gradient Scaling (PGS) technique [\[221\]](#page-168-6). PGS rescales the pressure gradient in the momentum equations to reduce the computational sound speed, so that the time step is not limited by the true sound speed which is irrelevant. The PGS methodology is limited to low-speed incompressible flows like the present configuration. Overall, the procedure is equivalent to the  $\alpha$ -transformation developed in [\[222\]](#page-168-7), but with the advantage of both easier implementation and wider applicability. Since the Lattice Boltzmann solvers are used here in their athermal weakly compressible form, it seems reasonable to utilise AVBP*pgs* which uses similar assumptions.

## **B.3.2. Lattice-Boltzmann solvers**

### **B.3.2.1. General description of the method**

The LBM considers the dynamic evolution of a mass distribution function of particles  $f(t, \mathbf{x}, \xi)$  that collide and propagate at time t, position **x** on a discrete velocity stencil called Lattice, commonly noted D*d*Q*q* (*d* for spatial dimension and *q* for velocities). In this study, two solvers were compared, ProLB and WALBERLA. Both employ a D3Q19 lattice given by:

<span id="page-140-0"></span>
$$
\xi_i = \begin{cases}\n(0,0,0), & i = 0 \\
(\pm 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1), & i = 1 - 6 \\
(\pm 1, \pm 1, 0), (\pm 1, 0, \pm 1), (0, \pm 1, \pm 1), & i = 7 - 18.\n\end{cases}
$$
\n(B.1)

At a mesoscopic scale, each function  $f_i = f(t, \mathbf{x}, \xi_i)$  is governed by the Lattice-Boltzmann scheme with the time step  $\Delta t$  and space step  $\Delta \mathbf{x} = \xi_i \Delta t$ :

$$
f_i(\mathbf{x} + \xi_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t) = \Delta t \Omega_i(\mathbf{x}, t),
$$
\n(B.2)

where  $\Omega_i$  is the collision operator. Modeling the collision component circumvents considering its non-linear behavior and therefore, makes this approach particularly well suited for parallel simulations of athermal weakly-compressible flows. The purpose is to preserve the main characteristics of the collision operator  $\Omega_i$  such as the convergence through a local thermodynamic equilibrium during a relaxation time *τ* and the conservation of mass and momentum.

While the macroscopic quantities (density  $\rho$  and momentum  $\rho$ **u**) are retrieved from the velocity moments of the distribution function given by:

$$
\rho = \sum_{i=0}^{q} f_i, \quad \rho \mathbf{u} = \sum_{i=0}^{q} f_i \xi_i,
$$
\n(B.3)

the pressure *p* is computed from the barotropic equation of state,  $p = \rho RT_0$  where  $R$  is the gas constant and  $T_0$  is a characteristic temperature, instead of the Poisson equation involved in most Navier-Stokes solvers allowing to considerably reduce the computational costs.

Finally, the Lattice-Boltzmann equation is discretized on cartesian cubic grids automatically generated in most solvers which alleviates cumbersome and timedemanding meshing. Both solvers are based on this description but use different numerical implementations.

Code	ProLB	WALBERLA
Number of nodes [M]	26.3	39.3
Number of fluid nodes [M]	26.3	30.2
Octree level distribution fluid nodes $[\%]$	[67, 25, 5, 3, 0, 0]	[59, 24, 13, 1.9, 1.5]
Equivalent Fine Nodes [M]	21.4	29.8
Equivalent Fluid Fine Nodes [M]	21.4	22.6

**Table B.2. –** Level distribution of fluid nodes in LBM solvers

A key difference between FV and LBM algorithms is that the FV solver uses the same time step in the whole computational domain, whereas in LBM the time step depends on the level of refinement. A cell on the coarser grid level has twice the size but also the time step is two times bigger compared to the finer level. To take this effect into account we generally use the term Equivalent Fine Nodes (EFN) which counts cells on coarser levels *L* as a fraction of the finest level (Eq[.Eq. \(B.4\)\)](#page-140-0). This quantity reflects the workload equivalent of a mesh using only the minimal mesh size min( $\Delta x$ ) and is therefore more suitable for comparison between the codes.

$$
EFN = \sum_{L} N_{\text{nodes on L}} \left(\frac{1}{2}\right)^{L-1} \tag{B.4}
$$

Another consequence is that the main part of the workload is generated by the finest level in the domain. In order to do a fast computation it is essential to minimize the regions with minimal cell size. The differences between the two LBM meshes are summarized in table [B.2.](#page-140-1) The ProLB algorithm typically needs fewer EFN to accurately resolve a given problem, whereas the approach of WALBERLA generates a non negligible amount of excess cells, that are not part of the fluid domain but have to be computed anyway.

### **B.3.2.2. ProLB**

ProLB is a commercial suite of tools which emerged from LaBS and CLIMB [\[223\]](#page-168-8) French research projects carried out by a consortium of industrial companies, universities, research laboratories and institutes. Its inherent massively-parallel solver includes an octree mesher which efficiently handles both complex geometries [\[224\]](#page-168-9) and multi-resolution refinement layers [\[225\]](#page-168-10).

For the present study, a modified version of the commercially available ProLB software is used. The numerical resolution of the Lattice-Boltzmann equation is performed through the D3Q19 lattice with a hybrid version [\[226\]](#page-168-11) of the recursive regularized collision operator [\[227\]](#page-168-12) (H-RR). It shows superior stability properties than the classical Bhatnager-Gross-Krook (BGK) [\[228\]](#page-169-0) for high-turbulent flows [\[229\]](#page-169-1) by filtering out the spurious and non-hydrodynamic modes that could be amplified at grid transitions [\[230\]](#page-169-2).

To handle mesh refinement, a Direct-Coupling (DC) algorithm is employed [\[231\]](#page-169-3). By ensuring mass and momentum conservation at the transition nodes, a singular equilibrium distribution function is computed to recover the missing distributions at both coarse and fine sides. This combination of the H-RR collision model and the DC algorithm offers better accuracy and locality in complex configurations than the classical overlapping method [\[232\]](#page-169-4).

The boundary nodes need a specific treatment in LBM approaches: since the mesh is completely cartesian, an immersed boundary condition is implemented to handle the solid walls [\[233\]](#page-169-5) [\[234\]](#page-169-6) allowing first the automatic generation of the mesh and second to flag the interface nodes. It is then supplemented by a Grad's moment approximation of the missing populations to recover macroscopic quantities at the interface. This yields a more stable and accurate approach than the well-known interpolated bounce-back [\[235\]](#page-169-7).

Thanks to the octree multi-resolution mesher, the ultimate grid is built upon a static adaptive refinement strategy [\[236\]](#page-169-8) where the considered sensor is the dissipation of kinetic energy [\[237\]](#page-169-9). From an initial coarse simulation, the time-averaged field of this sensor is computed. Therefore, a smoothed iso-volume based on a lower case-dependent threshold of the sensor yields a finer resolution domain which is directly reintroduced in the octree mesher. Thereby, this process is repeated twice in order to predict pressure losses and optimize the number of fluid nodes by refining only the relevant areas and minimizing computational costs.

#### <span id="page-142-0"></span>**B.3.2.3. waLBerla**

WALBERLA  $[238]$  is an extreme scale, open-source,  $C++$  multiphysics software framework. It can be used as a tool box for designing various types of applications such as the LBM computation performed here [\[239\]](#page-169-11).

waLBerla was designed from the ground up for high-performance computing (HPC) on massively parallel clusters [\[240,](#page-169-12) [241\]](#page-170-0) and GPU-based systems [\[242\]](#page-170-1), so that it is used as a reference implementation for LBM performance studies [\[243\]](#page-170-2).

waLBerla uses automatic code generation [\[244\]](#page-170-3) to ensure excellent execution performance on a wide range of different architectures. This meta-programming paradigm allows to start the application development from a high-level description of the LBM method. All steps to derive the LBM kernel codes can be performed automatically: the code is not only optimized for specific architectures, but also becomes easier to change to test variants of the LBM methods.

The framework is based on a block-structured domain partitioning in order to achieve extreme scalability and node level performance [\[245,](#page-170-4) [246\]](#page-170-5). The full domain is divided into equally sized cuboids that can only be refined as a whole at desired zones and at a size ratio of 2:1 with direct neighbors. These subdomains are called blocks and all hold the same number of grid cells. The computational domain <span id="page-143-0"></span>partitioning is partitioned in such blocks that can be assigned to processes. Load balancing is achieved on the level of blocks, not individual cells.

Every process can hold several blocks, but a block can only be assigned to one single process. Data from blocks is only available to the block that it has been assigned to. This structure allows code parallelization by the Message Passing Interface (MPI) or using hybrid MPI/OpenMPI to guarantee optimal scalability on a wide range of different supercomputer architectures. In complex geometries, the meshing algorithm will loop over all blocks and all cells to determine if they are inside or outside the surface mesh and accordingly set them as fluid or empty cells. Blocks that hold no fluid cells can be discarded, but blocks that hold one or more fluid cells will be kept and stocked with the same set of data. This is necessary because the LBM kernels iterate over over all cells equally, independent if they are fluid or not. Code generation is handled by the pystencils package [\[244,](#page-170-3) [247\]](#page-170-6). It uses symbolic manipulation with the SymPy algebra system to derive symbolically a stencil formulation from the continuous LBM collision operator. During this procedure several optimization techniques, such as common subexpression elimination and vectorization can be applied to generate highly efficient  $C/C++$  code. Additionally, optimized code for GPUs can be generated. Thus waLBerla with pystencils can achieve performance portabiliy to a wide range of different architectures, including CPUs and GPUs.

## **B.3.3. Numerical setups**

The three solvers were applied to the same swirler geometry of EM2C but they employ different meshes (Table [B.3\)](#page-142-0):  $AVBP_{pqs}$  uses body-fitted unstructured tetrahedral mesh with 18.1 M cells in total, while ProLB relies on cartesian unstructured mesh, offering a local refinement possibility but requiring up to 26.3 M grid elements, which amounts 21*.*4 M EFN to represent the same geometry. This tendency is exacerbated in WALBERLA, where the structured cartesian mesh is only able to refine whole blocks of the mesh, which leads to 39*.*3 M, or 22*.*6 M EFN cells overall.



### **Table B.3. –** Overall description of mesh parameters for the three solvers (*\* marks the number of EFN)*

A detailed representation of each grid, including swirler, injector and near-backplane region, is displayed in Fig. [B.3.](#page-143-0) It exhibits an axial cut for each code to show the local mesh structure: the swirler region has the highest resolution to predict the correct velocity field and pressure losses.

In this region AVBP<sub>*pgs*</sub> adopts a minimum cell parameter  $(\Delta x)$  of 80  $\mu$ m that increases along *z* up to the burner backplane with an average  $\Delta x \approx 180 \ \mu \text{m}$ . While ProLB mesh is refined through adaptive unstructured blocks of minimal mesh size  $\Delta x = 110$   $\mu$ m, waLBERLA uses a block of constant  $\Delta x = 110 \mu$ m in both swirler and injector. With these meshes, the time steps are adjusted to obtain CFL numbers based on the maximum convective velocity of the order of 0*.*1 for all codes.

 $\text{AVBP}_{\text{pos}}$  adopts Lax-Wendroff scheme [\[248\]](#page-170-7), second-order in both space and time. The CFL number (based on the modified sound speed) is set to 0*.*9. Temperature


<span id="page-144-0"></span>**Figure B.3. –** Mesh comparisons via ∆*x* contour maps for the three solvers: AVBP*pgs*, ProLB, WALBERLA. Differences among structured and unstructured grids, as well as between cubic and tetrahedral elements are highlighted.

and volumetric flow rate are fixed at the inlet, while ambient pressure (101325 Pa) with a proper relaxation coefficient is imposed at the outlet. The SIGMA model is used for subgrid Reynolds stresses [**?** ]. Both turbulent Prandtl number Pr and Schmidt number Sc are fixed to 0*.*6 and only one inert species representative of air is computed. The PGS parameters are set to obtain a maximum computational Mach number of 0*.*3.

While ProLB employs a H-RR collision operator combined with a DC mesh transition algorithm, WALBERLA is using a classical BGK collision model. Both solvers impose a one-seventh power law velocity profile at the inlet to match the experimental flow rate and a constant pressure of 1 bar at an extended outlet overlaid by a sponge layer to dump non-hydrodynamic reflection waves inside the domain. Walls are treated differently: ProLB uses a Grad's approximation and WALBERLA a bounce-back scheme to treat the "missing populations".

Since acoustics do not contribute significantly to the flow behavior, the nondimensionalized Newtonian sound speed  $c_s^*$ *s* is artificially minimized by being cautious that the maximal Mach Number does not exceed the critical value of 0*.*4 [\[249\]](#page-170-0):

$$
Ma_{\text{max}} = \frac{u_{\text{max}}}{c_s^*} \frac{\Delta t}{\Delta x} < 0.4. \tag{B.5}
$$

This requirement is similar to the CFL condition for classical Navier-Stokes numerical schemes [\[250\]](#page-170-1). This process intends to increase the time step to its maximal value and therefore allows to lower the computational time while the accuracy is still conserved.

LES in ProLB are performed using a Shear-Improved Smagorinsky turbulence model (LES-SISM) [\[251\]](#page-170-2) which accounts for the dissipation of the unresolved turbulent scales through an eddy viscosity *νsgs*. This subgrid-scale eddy viscosity is introduced by locally shifting the relaxation time  $\tau^* = \tau + \tau_{sgs}$  in the collision operator in order to model the additional convection of momentum and energy through <span id="page-145-0"></span>the subgrid turbulent eddies. To enclosure this model, *νsgs* is computed via the strain-rate tensor.

waLBerla on the other hand employs a basic version of the Smagorinsky model  $\tau_{sgs} = (C_S \Delta)^2 |S|$ , in which the turbulent viscosity depends on the local strain rate tensor *S*, the Smagorinsky constant  $C_S$  and the filter length  $\Delta = 1$  in lattice units.

### **B.4. Comparison with experimental data**

The first quality indicator for swirler flows is the pressure loss ∆*p* through the swirler (Table [B.4\)](#page-144-0) which controls its performances in a real engine. ∆*p* is calculated between the pressure tap location (see Fig. [B.2\)](#page-138-0) and the outside ambient pressure.

$\Delta p$ (Pa)
$335 \pm 15$
330
368
313

**Table B.4. –** Injector head pressure losses due to swirler.

The agreement of AVBP*pgs* with the experiment is slightly better than for LBM codes, as expected for a code which uses body-fitting meshes. ProLB and waL-BERLA predict a  $\Delta p$  of 368 Pa and 313 Pa, respectively above and below the experimental confidence interval. To qualify codes, measuring the pressure loss is not sufficient, however, and the next sections focus on a detailed analysis of the velocity fields.

#### **B.4.1. PIV**

Velocity profiles are compared on two planes: the axial *zx* plane and the transverse plane  $z = 3.5$  mm (see Fig. [B.2\)](#page-138-0). In the first case data are displayed over a 40  $\times$ 50 mm<sup>2</sup> rectangular window symmetrically located with respect to the *z* axis. For the second, results are presented over a  $40 \times 40$  mm<sup>2</sup> squared area centered in the middle of the combustion chamber with sides oriented along *x* and *y* directions.

Furthermore local one-dimensional, velocity profiles extracted at constant *z* are also retrieved from both PIV data and simulations.

#### **B.4.1.1. Axial plane**

Fig. [B.4](#page-145-0) exhibits two rows of images: the top row shows the mean axial velocity component  $\bar{u}_z$ . The second one shows its RMS noted  $u_{z,RMS}$ . From left to right experimental data and numerical results are displayed, as specifically reported on top of each plot.

The experimental mean velocity contour map of Fig. [B.4](#page-145-0) highlights a large Inner Recirculation Zone (IRZ), typical of high swirling flows. This region of negative axial velocity is created by the vortex breakdown and is delimited by iso-velocity lines at  $\bar{u}_z = 0 \text{ m s}^{-1}$ . Moreover two high velocity branches develop in the wake of the injector annular channel, identified by isolines at  $8 \text{ m s}^{-1}$ .

The comparison with numerical results show that the three solvers properly capture the flow characteristics, for both width and intensity of the IRZ. Minor differences can be highlighted: the extension of the high mean velocity regions is slightly overestimated by LBM codes, where  $8 \text{ ms}^{-1}$  and  $4 \text{ ms}^{-1}$  isolines develop further

<span id="page-146-0"></span>

**Figure B.4.** – Contour map comparison of experimental and numerical results of the axial (*z*) component of the velocity on the axial plane. First row exhibits the mean velocity field  $\bar{u}_z$ , while second row displays the RMS distributions *uz,*RMS.

downstream than in experimental data. In addition, RMS maps obtained with the three solvers highlight less regular contour plots, potentially linked to averaging times which are much smaller in the LES than in the experiment. AVBP*pgs* shows slightly higher RMS with respect to other codes and experiment, especially in the high velocity region.

<span id="page-146-1"></span>The horizontal component  $(x)$  results (Fig. [B.5\)](#page-146-0) confirm the axial component conclusions of Fig. [B.4:](#page-145-0) the three solvers are able to match the experimental results and all solvers provide results which are within the experimental range of precision for PIV results (typically  $0.3 \text{ m/s}$  here). However Figures [B.4](#page-145-0) and [B.5](#page-146-0) are not sufficient to provide an appropriate evaluation of the precision: it is worth considering onedimensional profiles showing local  $\bar{u}_z$  and  $\bar{u}_x$  velocity profiles sectioning the axial plane at specific *z* locations.

Fig. [B.6](#page-147-0) displays mean and RMS profiles of  $\bar{u}_z$  and  $\bar{u}_x$ , where in the first row profiles are extracted at  $z = 5$  mm and in the second one at  $z = 15$  mm.

First, the  $\bar{u}_z$  profile reveals that experimental data are not exactly symmetric with respect to the *z* axis: the left-hand velocity peak is higher than the other, while simulations do not show the same differences. Numerical predictions show that at both *z* coordinates, the slope and the minimum of the axial velocity profile, which define the IRZ structure, are correctly represented. On the other hand the maximum axial velocity values at  $z = 15$  mm are slightly overestimated by LBM codes by roughly  $0.5 \text{ m s}^{-1}$ , which corroborates the little discrepancy highlighted in Fig. [B.4.](#page-145-0)  $\bar{u}_x$  profiles are generally hard to match in swirled flows since the mean velocity intensity is comparable to its RMS values. This emphasizes the fidelity of all simulations put in place. In fact the maximum difference between experimental data and simulations is only of the order of few tenths of meters per second. Furthermore, the RMS profiles for both  $\bar{u}_z$  and  $\bar{u}_x$  at both *z* coordinates confirm the AVBP<sub>*pgs*</sub>

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<span id="page-147-0"></span>

**Figure B.5.** – Contour map comparison of experimental and numerical results of the horizontal  $(x)$  component of the velocity on the axial plane. First row exhibits the mean velocity field  $\bar{u}_x$ , while second row displays the RMS distributions *ur,*RMS.

little overestimation at peak velocity locations, which in any case remains largely within the experimental accuracy margin.

Another way to accurately compare the codes is to compute the  $L^2$ -norm relative errors between the experimental and simulation values present in Fig. [B.4.](#page-145-0) These are given in the Tab. [B.5.](#page-146-1)

Code	$z=5$ mm			$z=15$ mm					
	$u_z$	$u_{z, \text{RMS}}$	$u_x$	$u_{x, \text{RMS}}$	$u_z$	$\bar{u}_{z, \text{RMS}}$	$\bar{u}_x$	$u_{x, \text{RMS}}$	$\langle \eta \rangle$
$AVBP_{pas}$	0.13		0.16 $0.16$	0.17	0.08		$0.14$ 0.39	0.17	0.17
ProLB	0.26		$0.15 \quad 0.21$		$0.16$ $0.26$	0.14	0.6	$0.15 \quad 0.24$	
WALBERLA	0.20	0.10	0.19	0.12	0.19	0.11	0.74	0.10	0.22

**Table B.5.**  $- L^2$ -norm relative error for each solver and each plot of the Fig. [B.4](#page-145-0) respectively. To give an overall comparison, the global error  $\langle \eta \rangle$  has been computed as the average of each plot error. Bold and emphasize errors shows the more and less accurate result respectively.

#### **B.4.1.2. Transverse plane**

Fig. [B.7](#page-148-0) displays  $\bar{u}_x$  and  $\bar{u}_y$  mean velocity profiles on the transverse plane  $z = 3.5$ mm.

The good agreement between computational and experimental velocity fields confirms the previous findings. Only a slight overestimation of absolute maximum and minimum for both  $\bar{u}_x$  and  $\bar{u}_y$  can be pointed out looking at iso-velocity lines of  $\pm$  $8 \ m.s^{-1}$ .

Furthermore the two high/low velocity symmetric patches result slightly counterclockwiserotated due to the square shape of the combustion chamber. Remarkably, the flow

<span id="page-148-0"></span>

**Figure B.6.** – Mean velocity profiles of  $\bar{u}_z$  and  $\bar{u}_x$  with related RMS at constant axial coordinate on the axial plane. First and second rows correspond to  $z =$ 5 mm and  $z = 15$  mm, respectively.

field is correctly captured by numerical computations.

#### **B.4.2. Power Spectral Density (PSD) of axial velocity**

In addition to the mean and RMS values, it is also interesting to look at axial velocity spectra and compute Power Spectral Density (PSD) from local time signals: PSD are obtained experimentally from LDV velocity signals acquired along the *x* axis: from  $x = -15$  mm to  $x = 15$  mm with 0.5 mm step. It is worth mentioning that in contrast with simulations, measurements have been performed without combustion chamber. However it has been verified that experimental mean and RMS axial velocity are comparable with both PIV data the numerical predictions obtained in confined configuration. This feature is attributed to the weak impact of the confinement on the flow structure close to the injector outlet, at  $z = 3$  mm.

<span id="page-148-1"></span>Simulations and experimental signals are extracted for axial velocity over a span of 120 ms in order to share the same numerical frequency resolution of 8*.*3 Hz. Even though the upper-limiting frequency of the spectra is mathematically fixed by the sampling frequency, this limit could be misleading since oil particles used to seed the flow act like a low-pass filter, not responding to high perturbation frequencies. In the present case, the cut-off frequency of the small oil particles is of the order of 4 kHz: above this value, experimental spectra can not be physically considered.

Fig. [B.8](#page-149-0) displays the PSD at two locations (values in  $mm$ ):  $P = (3, 0, 3)$  is located in the wake of the central bluff-body and  $Q = (7, 0, 3)$  lies in the shear layer of the swirling jet (Fig. [B.2\)](#page-138-0). The gray scale marks the fact that at high frequencies only numerical results can be interpreted.

For the present flow rate, experimental PSD results (left column in Fig. [B.8\)](#page-149-0) do not exhibit peaks associated to coherent structures such as Precessing Vortex Cores (PVC) which are frequently found in swirling flows [\[252,](#page-170-3) [253,](#page-170-4) [254,](#page-171-0) [255\]](#page-171-1). Similarly

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<span id="page-149-0"></span>

**Figure B.7.** – Contour map comparison among experimental and numerical results on transverse plane. The first row exhibits mean velocity component  $\bar{u}_x$ , while second row displays the mean velocity component  $\bar{u}_y$ .

all three simulations do not reveal any peak related to hydrodynamic modes. The PSD decay above 1 kHz shows that calculations exhibit a higher dissipation with respect to experimental results, maybe due to the LES subgrid model used in the three codes. Limited differences are observed among codes at point  $P$ . For point  $Q$ , a difference emerges in the high frequency range: the two LBM codes introduce less dissipation than the finite volume solver but it is difficult to say if this is physically right or not.

## **B.5. Comparison of computational costs**

The code performances are given by Table [B.6.](#page-148-1) A first parameter, which is independent of mesh size and time step is the reduced computational time, i.e. the time required to perform one cell update. The last line of Table [B.6](#page-148-1) displays a second parameter which is the most important one for the user: the total CPU time required by each code to compute 1 ms of physical time.

Code	$\mathbf{AVBP}_{\mathit{pqs}}$	ProLB	waLBerla
Time step [s]	$4.4 \times 10^{-7}$	$8.5 \times 10^{-7}$	$7.1 \times 10^{-7}$
Equivalent Fine Fluid Nodes	18,1	21,4	22,6
ſМ			
CPU time per iteration [ms]	83	90	24
Reduced computational time	- 1.67	1.50	0.38
$[\mu \text{s} \text{ iteration}^{-1} \text{ cell}^{-1} \text{ core}]$			
$Cost \quad 1 \quad ms \quad physical \quad time$	19.1	10.6	3.4
[CPU <sub>h</sub> ]			

**Table B.6.** – Comparison of computational efficiency of the three different solvers on a 360 cores run.

For Table [B.6,](#page-148-1) all outputs and post-processing routines are disabled: only the



<span id="page-150-0"></span>**Figure B.8.** – Axial velocity spectra of kinetic energy for the different solvers at  $P =$ (3*,* 0*,* 3) (top row) and *Q* = (7*,* 0*,* 3) (bottom row).

fluid solver itself is considered. All codes run on 360 processes on a cluster which uses a Intel Xeon Gold 6140 Skylake chipset.

Table [B.6](#page-148-1) shows that the LBM solvers are faster than the finite volume solver but the speed ratios are not different by orders of magnitude: the fastest code waLBerla goes 5 times faster than the AVBP*pgs* solver.

#### **B.5.1. Scaling**

In addition to the computational cost at a fixed number of cores, scalability is an important question in HPC: the strong scaling behaviour of the three codes was tested here from 36 to 900 cores. We measure the parallel efficiency E by relating the the computational time per iteration  $T_P$  on a given number of cores  $N_P$  to the time per iteration  $T_{36}$  on 36 cores, which is equivalent one full node on the utilized architecture.

$$
E = \frac{36}{N_P} \frac{T_{36}}{T_P} \tag{B.6}
$$

Figure [B.9](#page-150-0) shows that AVBP scales almost ideally over the whole range of cores, while the LBM solvers efficiencies drop by  $30-40\%$  when increasing the number of cores by a factor of 25. In this particular configuration, parallel scalability is controlled by the spatial distribution of grid cells to achieve an even workload balance among all processes. In AVBP there are few constraints on the decomposition of the computational domain as long as the surface area between subdomains is kept at a minimum. Moreover, AVBP remains efficient even when only a few thousand mesh nodes are handled by each core.

ProLB preserves performance up to 72 cores but then loses efficiency beyond 144 cores because of an increase in waiting time: the solver has an optimum scalability

estimated between  $10^5$  and  $10^6$  fluid elements per core to efficiently manage industrial configurations that require much larger grids. In other words, while weak scaling works well in ProLB, the present strong scaling exercise is more difficult since the order of magnitude of fluid elements per core is  $10^4$  at 900 cores.

In WALBERLA whole blocks are assigned to each core. When using an excessive amount of cores, there are not enough blocks per process to find an even workload distribution. On the other hand WALBERLA exhibits excellent weak scaling until almost half a million cores  $[245, 246]$  $[245, 246]$ . Furthermore in the LBM scheme the different levels of refinement have to be executed sequentially. This is an inherent obstacle to achieving even workload distribution and it limits strong scaling capabilities. The strong scaling limit of the LBM codes may affect the overall conclusion: at 900 cores, ProLB becomes less efficient than AVBP. WALBERLA maintains the lowest computation time over the whole range of cores (Fig. [B.9\)](#page-150-0).



**Figure B.9.** – Parallel performance of the three codes up to 900 cores, normalized by the performance at 36 cores.

## **B.6. Conclusions**

One finite volume and two Lattice-Boltzmann solvers suitable for Large Eddy Simulation have been compared in terms of accuracy and CPU efficiency in a swirling flow, a typical aeronautical application.

The fidelity of the three solvers was demonstrated by comparing numerical and experimental PIV data in terms of: injector head pressure losses, mean and RMS velocity profiles and axial velocity spectra. Despite minor differences, the three solvers provide very similar and accurate results: the discrepancies with respect to experimental results are limited to the tenth of  $ms^{-1}$  on velocity profiles. For pressure losses, the finite volume solver using body-fitted meshes captures the experimental result very well (330 Pa for AVBP*pgs* versus 335 Pa for the experiment) but the two LBM codes results, using structured meshes are also close to measurements (368 Pa for ProLB and 313 Pa for WALBERLA). These results confirm that LES formulations provide high accuracy results for swirled flows, much better than usual RANS codes especially in terms of RMS data for all components. Furthermore LDV data at two specific locations are used to create PSD analysis of axial velocity: the three solvers as well as the LDV data do not reveal any hydrodynamic mode. Moreover, AVBP*pgs* shows higher numerical dissipation in the high frequency range with respect to LBM solvers.

Strong scaling tests from 36 to 900 cores reveal that the finite volume solver maintains its performance, whereas the LBM codes exhibit some loss in efficiency as the workload per core decreases. On 360 cores the CPU times necessary to compute 1 ms of physical time are: 3.4 for WALBERLA, 10.6 for ProLB and 19 CPU hours for  $\text{AVBP}_{\text{pqs}}$ . The three solvers offer similar orders of magnitude in terms of absolute performance, especially considering the fact that the finite volume solver carried more equations (energy and chemical species) as well as much more complex thermochemical models.

Finally, a point which has been left for further studies is the importance of the mesh quality on the results. The results shown in the paper were obtained with useroptimized meshes which play a crucial role in the final results, maybe as important as the solvers themselves. AMR (Automatic Mesh Refinement) is clearly a topic to address in future works.

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