

FACULDADE DE ENGENHARIA DA UNIVERSIDADE DO PORTO

Experimental and numerical study of a natural gas burner with mixtures with hydrogen

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Mechanical Engineering Masters Specialization in Fluids and Energies

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Resumo

A transição para um sistema energético de baixo carbono exige novas soluções para reduzir as emissões de gases com efeito de estufa em dispositivos de combustão. O gás natural tem desempenhado um papel central devido à sua combustão relativamente limpa, mas continua a ser um combustível fóssil. A introdução de hidrogénio em sistemas a gás natural surge, por isso, como uma estratégia promissora, uma vez que o hidrogénio é um vetor energético livre de carbono que pode reduzir as emissões de CO_2 e, ao mesmo tempo, influenciar a estabilidade da chama e a formação de poluentes.

Esta dissertação investiga experimental e numericamente o comportamento de um queimador a gás natural operado com metano puro e com uma mistura de 80% CH_4 e 20% H_2 . Os testes experimentais foram realizados a cerca de 15kW, em condições próximas da estequiometria. As medições de temperatura mostraram as tendências esperadas, mas não permitiram retirar conclusões firmes sobre a temperatura adiabática de chama, devido ao posicionamento dos termopares e à incerteza de medição. As análises de gases confirmaram reduções de CO_2 com a adição de hidrogénio, enquanto os valores de NO_x apresentaram um comportamento ligeiramente variável entre combustíveis, sendo que os valores médios indicaram um pequeno aumento com a adição de hidrogénio. Os níveis de monóxido de carbono revelaram-se difíceis de quantificar de forma consistente, refletindo as limitações dos métodos de diagnóstico.

O estudo numérico foi inicialmente realizado nas condições experimentais, de forma a validar o modelo com os dados obtidos. Foram testadas duas geometrias tridimensionais. A geometria simplificada permitiu cálculos mais rápidos e forneceu uma primeira visão sobre o escoamento, mas representou mal a chama, com forma e posição diferentes das observações experimentais. Além disso, os campos de temperatura e as concentrações de espécies divergiram significativamente dos resultados obtidos com a geometria que incluía o sistema completo de injeção. Por contraste, esta geometria detalhada reproduziu com muito maior precisão o campo de temperaturas, a estrutura da chama e a formação de espécies, demonstrando a importância do detalhe geométrico para previsões realistas. Uma vez validado nas condições experimentais, o modelo confirmou o esperado aumento da temperatura adiabática de chama e a redução de CO_2 com hidrogénio, acompanhados por um aumento de NO_x .

Após a validação, o modelo foi alargado para condições de 11kW, que não puderam ser sustentadas experimentalmente. Neste caso foram testadas simulações bidimensionais e tridimensionais. As simulações 2D reproduziram razoavelmente a temperatura adiabática de chama, mas falharam na representação detalhada da estrutura da chama, enquanto as configurações 3D mantiveram a capacidade preditiva já observada nas condições experimentais. Os resultados a 11kW mostraram novamente temperaturas adiabáticas mais elevadas e redução de CO_2 com hidrogénio, mas neste caso acompanhados por uma diminuição de NO_x . As reduções anuais correspondentes de emissões de CO_2 foram de

aproximadamente 3,5 toneladas nas condições experimentais e 2,6 toneladas a 11kW.

De forma global, este trabalho demonstra a viabilidade do enriquecimento de gás natural com hidrogénio em queimadores do tipo doméstico, evidencia os compromissos entre redução de carbono e emissões de NO_x , e mostra a importância de combinar dados experimentais com CFD para uma análise fiável. Os resultados fornecem contributos relevantes para a integração de hidrogénio em sistemas de combustão existentes e para o esforço contínuo de descarbonização das tecnologias de energia térmica.

Abstract

The transition towards a low-carbon energy system requires new solutions to reduce greenhouse gas emissions in combustion devices. Natural gas has played a central role due to its relatively clean combustion, but it remains a fossil fuel. The introduction of hydrogen into natural gas systems is therefore emerging as a promising strategy, as hydrogen is a carbon-free energy carrier that can reduce CO₂ emissions while influencing flame stability and pollutant formation.

This dissertation investigates experimentally and numerically the behavior of a natural gas burner operated with pure methane and with a mixture of 80% CH₄ and 20% H₂. The experimental campaign was carried out at around 15kW under conditions close to stoichiometry. Temperature measurements showed the expected trends but did not allow firm conclusions on the adiabatic flame temperature, due to probe positioning and measurement uncertainty. Gas analysis confirmed reductions in CO₂ with hydrogen enrichment, while NO_x exhibited a modest variable behavior between fuels, with the averaged results indicating a slight increase with hydrogen addition. Carbon monoxide levels proved difficult to quantify consistently, reflecting the limitations of the diagnostic methods.

The CFD study was first performed at the experimental operating conditions, in order to validate the model against the experimental data. Two three-dimensional geometries were tested. The simplified domain provided faster calculations and some preliminary insight into the flow, but it predicted the flame poorly, with shape and position differing from the experimental observations. Moreover, the resulting temperature fields and species concentrations diverged significantly from those obtained with the geometry including the full injection system. By contrast, the detailed 3D geometry reproduced much more accurately the thermal field, the flame structure and the species formation, demonstrating the importance of geometric detail for realistic predictions. Once validated at the experimental operating conditions, the model confirmed the expected higher adiabatic flame temperature and lower CO₂ with hydrogen, accompanied by an increase in NO_x.

After validation, the model was extended to 11kW conditions, which could not be sustained experimentally. In this case, a two-dimensional and both three-dimensional geometries were tested. The 2D cases reproduced reasonably well the adiabatic flame temperature but failed to capture the detailed flame structure, while the 3D configurations retained the predictive capability already observed at experimental conditions. The results at 11kW again showed higher adiabatic flame temperature and reduced CO₂ with hydrogen, but in this case with a decrease in NO_x. The corresponding yearly reductions of CO₂ emissions were approximately 3.5 tons at experimental conditions and 2.6 tons at 11 kW.

Overall, this work demonstrates the feasibility of hydrogen enrichment in domestic-type burners, highlights the trade-offs between carbon reduction and NO_x emissions, and

shows the importance of combining experimental data with CFD for reliable analysis. The results provide useful insights for the integration of hydrogen into existing combustion systems and contribute to the ongoing effort of decarbonizing thermal energy technologies.

UN Sustainable Development Goals

The United Nations Sustainable Development Goals (SDGs) provide a global framework to achieve a better and more sustainable future for all. This thesis contributes to several SDGs by advancing hydrogen-enriched natural gas combustion for domestic ovens through experimental testing, CFD-based design, and engineering analysis focused on safety, efficiency, and emissions.

The specific Sustainable Development Goals addressed are:

SDG 3 Ensure healthy lives and promote well-being for all at all ages

SDG 7 Ensure access to affordable, reliable, sustainable and modern energy for all

SDG 9 Build resilient infrastructure, promote inclusive and sustainable industrialization and foster innovation

SDG 12 Ensure sustainable consumption and production patterns

SDG 13 Take urgent action to combat climate change and its impacts

Table 1: United Nations Sustainable Development Goals and their relevance to this thesis

SDG	Goal	Relevance to this Thesis
3	Ensure healthy lives and promote well-being for all at all ages	By reducing pollutant emissions (CO, NO _x) in domestic ovens through hydrogen-enriched combustion, this work contributes to improved indoor air quality and user safety.
7	Ensure access to affordable, reliable, sustainable and modern energy for all	Development and validation of a domestic burner capable of operating with methane–hydrogen blends (up to 20% H ₂) ensures compatibility with future energy infrastructures while promoting efficiency and cleaner energy use.
Continued on next page		

SDG	Goal	Relevance to this Thesis
9	Build resilient infrastructure, promote inclusive and sustainable industrialization and foster innovation	The thesis introduces design innovation through parametric modelling and CFD-based optimization, enabling robust, hydrogen-ready appliances and supporting industrial transition towards sustainable technologies.
12	Ensure sustainable consumption and production patterns	Preliminary life-cycle analysis highlights material and energy efficiency in appliance production, while promoting design for durability and end-of-life recyclability.
13	Take urgent action to combat climate change and its impacts	By demonstrating direct CO ₂ emission reductions via CH ₄ /H ₂ blending, this thesis supports decarbonization pathways and contributes to mitigating climate change.

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I would also like to thank Prof. Eliseu Monteiro for all the guidance and useful advice.

<Guilherme Moreira>

*“If you can see it here [points to his mind] and you have the courage enough to speak it...
It will happen”*

Conor McGregor

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Nomenclature

List of Acronyms

ANSYS	Engineering simulation software suite
CAD	Computer-Aided Design
CFD	Computational Fluid Dynamics
DNS	Direct Numerical Simulation
DO	Discrete Ordinates (radiation model)
EDC	Eddy Dissipation Concept (combustion model)
FVM	Finite Volume Method
HHV	Higher Heating Value
LHV	Lower Heating Value
LES	Large Eddy Simulation
PDF	Probability Density Function
RANS	Reynolds-Averaged Navier–Stokes
RMSE	Root Mean Square Error
ROM	Reduced-Order Mechanism (simplified chemistry)
RTE	Radiative Transfer Equation
SST	Shear Stress Transport (turbulence model)
WI	Wobbe Index

List of Symbols

T	Temperature [K]
p	Static pressure [Pa]
u	Velocity vector [m s^{-1}]
ρ	Density [kg m^{-3}]
μ	Dynamic viscosity [Pa s]
ν	Kinematic viscosity [$\text{m}^2 \text{s}^{-1}$]
k	Turbulent kinetic energy [$\text{m}^2 \text{s}^{-2}$]
ε	Turbulent dissipation rate [$\text{m}^2 \text{s}^{-3}$]
ω	Specific dissipation rate [s^{-1}]
k_t	Thermal conductivity [$\text{W m}^{-1} \text{K}^{-1}$]
c_p	Specific heat at constant pressure [$\text{J kg}^{-1} \text{K}^{-1}$]
h	Specific enthalpy [J kg^{-1}]
Y_i	Mass fraction of species i [–]
X_i	Mole fraction of species i [–]
$\dot{m}$	Mass flow rate [kg s^{-1}]

$\dot{Q}$	Heat transfer rate [W]
κ	Absorption coefficient [m^{-1}]
σ	Stefan–Boltzmann constant [$\text{W m}^{-2} \text{K}^{-4}$]
ε	Surface emissivity [–]
ϕ	Equivalence ratio [–]
λ	Excess-air ratio [–]
A	Area [m^2]
V	Volume [m^3]
L	Characteristic length [m]
D	Diameter [m]
Re	Reynolds number [–]
Pr	Prandtl number [–]
Nu	Nusselt number [–]

Chemical species

CH_4	Methane
H_2	Hydrogen
O_2	Oxygen
N_2	Nitrogen
CO	Carbon monoxide
CO_2	Carbon dioxide
H_2O	Water
NO	Nitric oxide
NO_2	Nitrogen dioxide
NO_x	Nitrogen oxides (NO and NO_2)

Units and prefixes

K	Kelvin (temperature)
$^{\circ}\text{C}$	Degree Celsius (temperature)
bar	Bar (pressure)
J	Joule (energy)
GJ	Gigajoule (energy)
W	Watt (power)
kW	Kilowatt (power)
s	Second (time)
yr	Year (time)
m	Meter (length)
cm	Centimeter (length)
mm	Millimeter (length)
g	Gram (mass)
mol	Mole (amount of substance)
kmol	Kilomole (amount of substance)
m^3	Cubic meter (volume)
ppm	Parts per million
%	Percent

Chapter 1

Introduction

1.1 Historical background of natural gas

The global energy transition is motivated by the need to reduce greenhouse gas emissions while ensuring security of supply. Natural gas has become one of the most widely used fuels due to its high efficiency and cleaner combustion compared with coal and oil. It is applied in power generation, industry and residential heating, representing about a quarter of global energy demand. In Portugal, the regular supply of natural gas was introduced in 1997, addressing not only the domestic sector but also electricity generation and industrial facilities. Despite its benefits, natural gas remains a fossil fuel and contributes significantly to CO₂ emissions. There are also concerns about methane, CH₄, leakage and nitrogen oxides, NO_x, formation during combustion.

1.2 Hydrogen enrichment in natural gas systems

The introduction of hydrogen as an energy carrier has been studied since the second half of the twentieth century, initially as a possible replacement for fossil fuels. Hydrogen, H₂, is a carbon-free fuel and when mixed with CH₄ it can directly reduce CO₂ emissions. International research programs have demonstrated that small fractions of hydrogen can be introduced into natural gas networks with limited technical modifications. Several European countries have already performed pilot projects where hydrogen is blended into the distribution grid in proportions that typically range from five to twenty percent by volume [1] [2]. In Portugal, the national hydrogen strategy launched in 2020 outlined the ambition of producing green hydrogen from renewable electricity and gradually injecting it into the natural gas system, particularly in industrial clusters located near renewable resources [3]. Studies on the integrity of natural gas infrastructure, such as the one presented by the Institute [4], have shown that existing pipelines can safely withstand hydrogen fractions up to around 20% mol/mol, which makes this concentration a particularly relevant case to investigate. This approach takes advantage of the existing infrastructure

and creates demand for hydrogen, although it can result in difficulties associated with material compatibility, safety standards and the need to guarantee a green origin for the hydrogen supplied. The successful integration of hydrogen therefore depends not only on technical adaptations to equipment and infrastructure but also on the large-scale development of renewable hydrogen production to ensure real decarbonization benefits.

1.3 Computational Fluid Dynamics in combustion research

The analysis of combustion processes has evolved from purely empirical observations to advanced numerical methods that allow detailed investigation of the phenomena involved. Computational Fluid Dynamics, commonly referred to as CFD, emerged in the second half of the twentieth century as computers became more powerful and capable of solving the equations of fluid mechanics numerically. Initially applied to aerodynamics and aerospace design, CFD rapidly expanded to energy systems, turbo-machinery, combustion, among others. Today it is a central tool in both academic research and industrial development [5].

In the field of combustion, CFD allows the simulation of complex interactions between fluid flow, heat transfer and chemical reactions. It provides access to local parameters such as velocity, temperature and species distribution, which can be difficult to obtain experimentally. This predictive capability makes CFD highly valuable for the design and optimization of burners and combustion chambers. Nevertheless, accurate results depend on the use of appropriate models for turbulence, chemical kinetics and radiation, and these models must always be validated against experimental data to ensure reliability.

1.4 Thesis structure and motivation

This thesis addresses these issues by experimentally and numerically investigating a natural gas burner operating with methane and a methane–hydrogen fuel blend. The second chapter provides a review of the relevant literature, followed by a third chapter that presents the experimental setup and the computational methodology. The experimental results are discussed in the fourth chapter, while the fifth chapter is dedicated to the CFD simulations and their validation. Finally, the sixth chapter summarizes the main findings and proposes directions for future research.

This work also has practical relevance for the energy and appliance industries. Burners operating with CH_4 and H_2 mixtures are directly applicable to domestic ovens, industrial furnaces and gas turbines. In the present work the burner under study is specifically integrated into a vertical drying oven installed in a Portuguese company.

Reducing CO₂ emissions in these configurations, without a complete redesign of the system is a major advantage. The insights obtained from this study support the integration of hydrogen into existing combustion technologies and contribute to the broader effort of decarbonizing industrial processes through the integration of renewable gases.

Chapter 2

Literature Review

2.1 Overview of Natural Gas

Natural gas is a gaseous blend with a composition that varies depending on its source, blending ratios, and quality. It is composed primarily of methane, CH₄, however, it may contain small quantities of other light hydrocarbons. In Table 2.1 it is shown the average composition of natural gas in Portugal according to Portgás[6], as well as its properties in Table 2.2 according to the same source.

Table 2.1: Average natural gas composition in Portugal in %mol [6]

Methane	Ethane	Propane	i-butane	n-butane	i-pentane	n-pentane	n-hexane	Nitrogen	CO ₂
90.05	6.4485	1.7445	0.234	0.2695	0.02	0.0105	0.01	0.5795	0.633

Table 2.2: Average natural gas properties in Portugal at ambient conditions [6]

Molecular Weight	Density [kg/m ³]	HHV [kWh/m ³]	LHV [kWh/m ³]	Wobbe Index [kWh/m ³]
17.919	0.8019	11.9	10.755	15.115

Lower Heating Value, LHV, and Higher Heating Value, HHV, are variables used to evaluate the energy content of fuels. LHV represents the amount of heat released by a fuel during its combustion, assuming that the water formed remains in a vapor state. On the other hand, HHV accounts for the heat released when the water vapor condenses back to liquid, therefore including the latent heat of vaporization [7]. Additionally, the Wobbe Index is a parameter that measures the interchangeability of fuels by comparing the combustion energy output of each one. Given by 2.1, with G_s being the fuel specific gravity, this index is essential to ensure that different fuels can be used in the same combustion system without altering the air-to-fuel ratio, maintaining efficiency [8].

$$I_w = \frac{HHV}{\sqrt{G_s}} \quad (2.1)$$

When undergoing combustion, natural gas emits chemical species such as NO_x , CO and CO_2 , which are some of the main pollutants that make the usage of this fuel so alarming. The main mechanism of NO_x formation is thermal NO_x , which means that, when subjected to higher combustion temperatures, natural gas tends to release more NO_x . In a complete combustion process most fuel carbon present in natural gas is converted to CO_2 , which translates in lower values for CO. Therefore, CO formation depends on combustion completion, meaning that a less complete combustion increases CO levels. However, the amount of CO emissions is insignificant compared to CO_2 levels, even in boilers with poor efficiency [9].

2.2 Hydrogen Properties and Its Effects on Combustion

The introduction of hydrogen in combustion has been under increasing study, mostly due to the gas properties and emission benefits, but also due to its abundance. In Table 2.3 it is presented hydrogen properties according to Cristello et al. [10].

Table 2.3: Properties of hydrogen at 1 bar pressure and 20°C temperature [10]

Molecular Weight	Density [kg/m^3]	HHV [kWh/m^3]	LHV [kWh/m^3]	Wobbe Index [kWh/m^3]
2.016	0.08	3.472	2.833	13.397

Although hydrogen's HHV and LHV values may seem low compared to the natural gas values, it is important to notice that its density is also ten times lower than that of the natural gas at the same conditions. That implies that measuring the LHV and HHV values in kWh/kg would translate into a superiority to the hydrogen's values, reassuring its qualities as a fuel.

On the other hand, while having a high specific energy, hydrogen's usage is primarily related to the reduced emissions that it generates while being burned. As can be seen in the works developed by Celtek and Pinarbasi [11], Meziane and Bentebbiche [12] and Yilmaz and Ilbas [13], mixing hydrogen with natural gas decreases CO and CO_2 emissions considerably. However, due to the increase in the adiabatic flame temperature caused by the addition of hydrogen, an increase in the thermal NO_x formation is also detected, translating into a big disadvantage.

The increase in the combustion temperature is not linear space-wise. As displayed by Yilmaz and Ilbas [13], even though with higher amounts of hydrogen in the mixture the adiabatic flame temperature increases, as the distance from the flame increases, at an axis and radial level, the temperature mixtures with higher amounts of hydrogen produce lower temperatures. This not only happens due to hydrogen's higher diffusivity and laminar speed, when compared to natural gas, but also due to the reduction in carbon dioxide

formation, which lowers radiative heat transfer and leads to a more dispersed distribution of thermal energy within the chamber. At the same time, the increased production of H₂O acts as a thermal sink due to its high specific heat capacity.

2.3 Numerical Modelling of Combustion

2.3.1 Introduction to CFD

Computational Fluid Dynamics, or CFD, has been increasingly used as a fundamental tool in engineering, capable of analyzing and predicting fluids mechanics, heat exchanges and chemical reactions. It consists in algorithms whose objective is to solve the governing equations that describe a given problem. These governing equations express laws of physics, more specifically the conservation of mass, the conservation of momentum and the conservation of energy. The differential formats of these equations are named the Navier-Stokes equations, which, considering a compressible flow, can be written as 2.2 for the conservation of mass, 2.3 for the conservation of momentum and 2.4 for the conservation of energy,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (2.2)$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g} \quad (2.3)$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot [\mathbf{u} (\rho E + p)] = \nabla \cdot (k \nabla T) + \nabla \cdot (\mathbf{u} \cdot \boldsymbol{\tau}) + \dot{q} \quad (2.4)$$

where ρ is the fluid density, $\mathbf{u}$ is the velocity vector, p denotes the pressure, $\boldsymbol{\tau}$ is the viscous stress tensor, $\mathbf{g}$ represents the body force, such as gravity, $E = e + \frac{1}{2}|\mathbf{u}|^2$ is the total energy per unit of mass, with e being the internal energy, k is the thermal conductivity, T is the temperature and $\dot{q}$ represents any heat sources, such as those from chemical reactions [14].

However, since these are differential equations, it is extremely difficult to solve them analytically, being only possible to do so in very specific and simple cases. So, in order to obtain an approximate solution it is necessary to use a discretization method, which approximates the differential equations using a system of non-linear algebraic equations. There are some different methods that allow to perform the discretization, being the most used ones the finite volume method, the finite difference method and the finite element method. Since ANSYS Fluent, as well as most CFD codes rely on the finite volume method, the other methods are only going to be explained briefly.

Finite Difference Method

The finite difference method approximates the derivatives in the governing differential equations by employing differences between values at discrete points on a structured grid. This approach is relatively straightforward to implement and is well suited to problems with simple, regular geometries. However, its application becomes more challenging in domains with complex boundaries or when unstructured meshes are required, as the accuracy and stability of the method can be compromised under such conditions [15].

Finite Element Method

The finite element method, on the other hand, subdivides the entire domain into a mesh of small, simple and mostly unstructured elements such as triangles, quadrilaterals, for 2D problems or tetrahedrons for 3D problems. Within each element, the solution is approximated by using locally defined interpolation functions, often referred to as shape functions. This method offers significant flexibility for handling complex geometries and varying material properties. However, it involves more computational work due to its unstructured grids, which makes the matrices of the linearized equations not as well structured as those for regular grids [15].

Finite Volume Method

The finite volume method relies on an integral formulation of the conservation laws over control volumes. In this approach, the domain is subdivided into a finite number of contiguous cells, each bounded by surfaces or interfaces where fluxes of mass, momentum, energy, and species are computed. By integrating the governing equations over each control volume, this method ensures local conservation of the flow variables, since any flux leaving one volume must enter an adjacent one. At the cell level, these fluxes are typically interpolated from values stored at cell centers using schemes such as upwind or central differencing, which help maintain stability and accuracy in the solution. Numerical quadrature formulas approximate both surface and volume integrals, leading to a system of algebraic equations that must be solved, typically one per control volume. A key strength of the finite volume method is its inherent conservation property and its ability to handle both structured and unstructured meshes effectively, making it particularly suitable for simulating complex geometries and a broad spectrum of flow conditions, including compressible, incompressible, reactive, and multiphase flows. Its flexibility also facilitates the incorporation of turbulence models, heat transfer, including convection and radiation, and chemical kinetics. However, when compared to finite difference methods, this method may involve more intricate geometric bookkeeping, due to the three levels of approximation, which are integration, differentiation and interpolation, especially for highly irregular meshes. Despite this additional complexity, its accuracy, conservation

and adaptability has established the finite volume method as a mainstay in computational fluid dynamics [15].

2.3.2 Turbulence Modeling

Turbulence is an inherent feature of many fluid dynamic problems. Characterized by its chaotic and irregular fluctuations across a wide range of scales, it is one of the most complex and unpredictable phenomena within the broad spectrum of physical events governing the natural world.

In turbulent flows, energy is injected at large scales, generating coherent localized swirling motions named eddies, where the fluid circulates around a central point containing most of the kinetic energy. Nonlinear interactions cause these eddies to break into progressively smaller ones, through a process known as the energy cascade. This cascade continues until the smallest eddies, where viscous forces dominate, dissipate the energy as heat. As the energy cascades to finer scales, the increased number and reduced size of eddies create a larger interfacial area, significantly enhancing mixing. Consequently, turbulent flows achieve much higher rates of momentum, heat, and mass transfer compared to laminar flows. In combustion processes, turbulence is particularly critical as it promotes the rapid mixing of fuel and oxidizer, thereby affecting flame stability, reaction rates, and pollutant formation [14].

However, this complex, multi-scale behavior poses significant challenges for numerical modeling because resolving all turbulent scales directly is computationally prohibitive for most practical applications. To address these challenges, CFD employs a variety of turbulence models, ranging from Reynolds-Averaged Navier–Stokes, or RaNS, models that statistically represent the effects of turbulence, to Large Eddy Simulation, or LES, approaches that directly resolve the largest, most energetic eddies while modeling the smaller scale turbulence using the RaNS technique, and even Direct Numerical Simulation, or DNS, in cases where computational resources and problem characteristics permit full resolution of all turbulent scales. A graphic insight to the behavior of these models is exhibited in Figure 2.1. These modeling strategies form a bridge between the underlying physics of turbulence in combustion and practical engineering simulations, enabling accurate predictions of complex reactive flows in industrial applications [15].

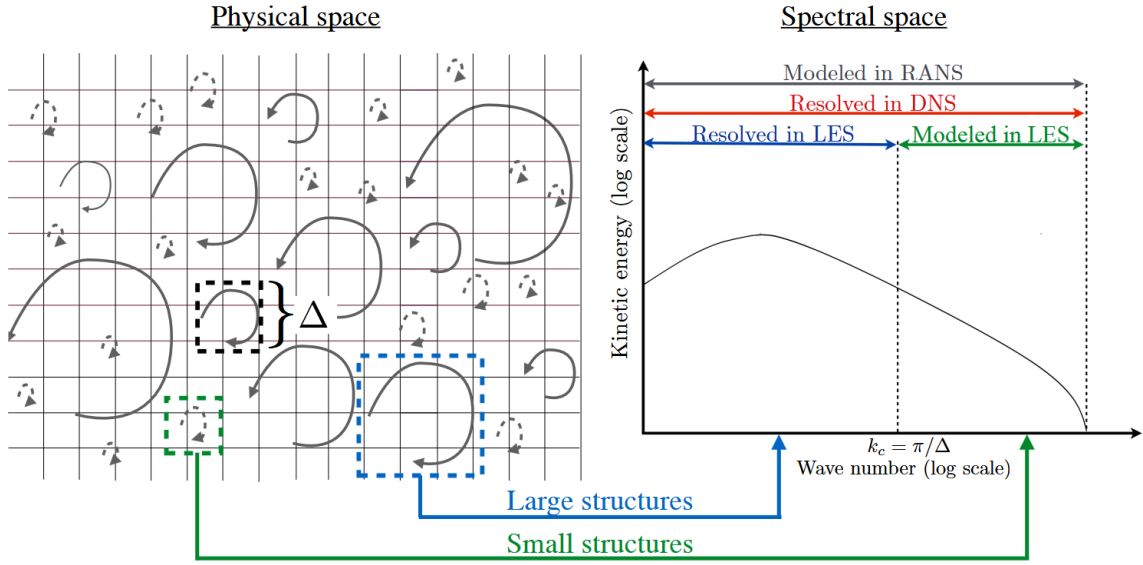


Figure 2.1: Comparison of DNS, LES and RANS simulation techniques on an idealized non-reacting homogeneous and isotropic turbulent flow [16]

DNS

DNS is the most fundamental and accurate approach to simulating turbulent flows. It resolves all scales of motion, from the large energy-containing eddies down to the smallest dissipative structures, by solving the full Navier–Stokes equations without any turbulence model. This method captures every detail of the turbulent flow field, providing comprehensive insight into the physics of turbulence and its interaction with combustion processes. However, DNS is extremely computationally expensive since the required grid resolution increases dramatically with the Reynolds number, limiting its application to simple geometries and low-to-moderate Reynolds numbers. Due to that expense it is rarely employed in CFD applications [15].

LES

LES represents a compromise between DNS and Reynolds-Averaged methods. It explicitly resolves the larger turbulent structures, which contain most of the kinetic energy, while modeling only the smaller scales using subgrid-scale models, diminishing the computational needs compared to DNS. This approach captures the unsteady, three-dimensional features of turbulent combustion that are critical for accurately predicting flame dynamics and pollutant formation. Although LES requires fewer grid points than DNS, it remains computationally intensive and is generally applied when capturing unsteady flow features is essential, especially in high Reynolds number or complex geometries. However, with advancements in computational capacities, it is gradually becoming more established in contemporary CFD research [15].

RaNS

While methods such as DNS and LES offer detailed unsteady flow information, their high computational cost often makes RaNS the preferred approach for practical engineering problems. RaNS typically employs a single two-equation turbulence model, such as k - ε , k - ω , and k - ω SST, to provide an efficient balance between computational cost and accuracy in predicting mean flow properties.

In RaNS approaches, the instantaneous flow variables are decomposed into a time-averaged mean and a fluctuating component, i.e., $u_i = U_i + u'_i$, where U_i is the mean velocity and u'_i represents the turbulent fluctuations. When the Navier–Stokes equations are averaged in time, additional terms arise, notably the Reynolds stress tensor $\bar{\tau}_{ij} = -\rho \overline{u'_i u'_j}$, which accounts for momentum transfer due to turbulence. Since these extra terms cannot be expressed solely in terms of the mean quantities, closure models are required; a common approach is the eddy-viscosity hypothesis, which relates the Reynolds stresses to the mean strain rate through a turbulent viscosity μ_t [15].

One of the most widely used two-equation models is the k - ε model. In this formulation, the turbulent viscosity is computed as

$$\mu_t = C_\mu \rho \frac{k^2}{\varepsilon}, \quad (2.5)$$

where k is the turbulent kinetic energy and ε is its dissipation rate. The model includes transport equations for k and ε , which account for production, diffusion, and dissipation of turbulent energy. Although the k - ε model is robust and well validated for many industrial flows, it sometimes encounters difficulties in flows with strong adverse pressure gradients or separation [15].

An alternative is the k - ω model, which employs the specific dissipation rate ω , with $\omega \approx \varepsilon/k$, instead of ε . The turbulent viscosity in this model is given by

$$\mu_t = \rho \frac{k}{\omega}, \quad (2.6)$$

which generally yields improved accuracy in the near-wall region, though it may be sensitive to free-stream conditions [15].

To combine the advantages of both formulations, the k - ω Shear Stress Transport, SST, model was developed. This model blends the k - ω formulation near walls with the k - ε formulation in the free stream through a blending function, typically denoted as F_1 , thereby improving predictions in flows with separation and adverse pressure gradients. The k - ω SST model has become one of the most versatile tools for simulating turbulent combustion in complex engineering applications [17].

2.3.3 Species Transport Modelling

Species transport models are vital in simulating combustion as they govern the evolution of chemical species through convection, diffusion, and chemical reactions. These models are essential for predicting flame structure, heat release, and pollutant formation, and the choice of model depends on the level of chemical detail required and the available computational resources. Even though it is possible to use species transport models in various types of problems, the most correct model to use in combustion applications is the volumetric reactions one, which takes into account simultaneous chemical reactions occurring in the fluid phase.

In order to solve the conservation equations for chemical species, it is necessary to predict the local mass fraction of each species, Y_i , which can be calculated by solving the following convection-diffusion equation for the i^{th} species:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \vec{u} Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i \quad (2.7)$$

where R_i is the net rate of production of species i by chemical reaction and S_i is the rate of creation by addition from the dispersed phase plus any other defined sources. $\vec{J}_i$ is the mass diffusion flux, which manifests different forms depending on the flow's turbulent nature [17].

2.3.3.1 Chemistry Models

Inside the volumetric model of species transport it is also necessary to select the chemistry models that will compute the reaction rate terms, R_i , displayed in equation 2.7. The characteristics of those models are going to be explained briefly, however it is important to notice that inside of every model explained there is the option to choose the Chemistry Solver. The Chemistry Solver will either let the species evolve according to the kinetic mechanism chosen, which is explained in the next chapter, or introduce complementary ways to solve the chemical reactions. In the first three models explained, lies an option to let the reactions relax to chemical equilibrium, by driving the species composition to its equilibrium state, instead of using a solver [17].

Finite-Rate Kinetics Model

The finite-rate kinetics model directly solves the species conservation equations by computing reaction source terms from detailed Arrhenius expressions. This approach offers a very detailed description of the chemical kinetics, capturing complex reactions and intermediate species with high fidelity. However, because it requires solving stiff, multi-step reaction mechanisms, it is computationally expensive and typically suited to laminar flows or scenarios where detailed kinetics are critical [17].

Eddy-Dissipation Model

The eddy-dissipation model simplifies the chemistry by assuming that turbulent mixing controls the overall reaction rate, so the reaction proceeds as soon as fuel and oxidizer are mixed by turbulent eddies. This assumption makes the ED model computationally efficient, which is particularly attractive for high-temperature, non-premixed flames where reactions occur almost instantaneously. However, this model tends to oversimplify the kinetics and does not capture the formation of intermediate species or radicals as accurately as the finite-rate kinetics approach. Thus, while the ED model reduces computational cost significantly, it does so at the expense of chemical detail [18].

Finite-Rate/Eddy-Dissipation Model

The finite-rate/eddy-dissipation model combines the strengths of both the finite-rate and the eddy-dissipation models to provide a more accurate representation of reaction rates in turbulent flows. It calculates both the Arrhenius reaction rate and the turbulent mixing rate, selecting the slower of the two rates to govern the overall reaction rate, which ensures that the limiting process is appropriately captured. This approach is particularly effective in scenarios where both chemical kinetics and turbulence play significant roles and while being more precise than the eddy-dissipation model, it does not increase the computational needs as drastically as the finite-rate or the EDC model [18].

Eddy-Dissipation Concept Model

The eddy-dissipation concept model enhances the basic ED approach by accounting for finite-rate chemical kinetics within small, well-mixed turbulent structures inside each computational cell. These fine scales are treated as tiny reactors, where detailed chemical reactions are solved over a characteristic time scale that reflects both turbulent mixing and reaction kinetics. The EDC model therefore offers improved predictions of intermediate species and radicals compared to the ED model. Nevertheless, this increased accuracy comes with higher computational cost and greater numerical stiffness. In essence, the EDC model strikes a balance between the finite-rate kinetics model and the ED model [19].

Composition PDF Transport Model

For turbulent flames where local species concentrations exhibit significant fluctuations due to turbulence–chemistry interactions, the composition Probability Density Function, PDF, transport model provides a statistical approach. Instead of solving only for mean values, this model captures the full distribution of species concentrations, offering a nuanced prediction of flame behavior and pollutant formation. While this approach delivers a more detailed description of the turbulence–chemistry coupling than the ED or EDC

models, it also increases the complexity and computational cost. Compared to previous models, the composition PDF model is best suited for flows where understanding the variability of species concentrations is essential [17].

2.3.4 Kinetic Mechanisms Modelling

In order to properly replicate a combustion model in CFD it is required a detailed knowledge of the involved chemical reactions, reaction rates, and associated thermal and fluid dynamic effects. These phenomena are mathematically described by kinetic mechanisms, which can be introduced into the CFD code, allowing it to predict the system behaviour. Kinetic mechanisms provide insights into key aspects for a combustion problem, such as species formation and consumption, heat release rates and interaction with other physical processes. However, since combustion's chemical reactions may be extensive and complex, some of these mechanisms focus on reducing them to essential chemical interactions, reducing computational needs while maintaining its accuracy, detail and precision. Therefore, kinetic mechanisms can be divided into two categories, detailed mechanisms and reduced mechanisms.

Detailed kinetic mechanisms involve a large amount of reactions and species, offering high accuracy and comprehensive representation of chemical processes, however simulating this mechanisms requires significant computational resources, making them impractical for real-time applications or large-scale simulations. On the other hand, reduced models are simplified versions of the detailed mechanisms, designed to capture essential features of the combustion process, by focusing on key reactions, making simulations faster and more practical. Nevertheless, since reduced mechanisms are often developed for specific types of combustion, they possess limited validity outside the range of conditions for which they were designed, such as temperature, pressure and fuel composition [20].

Gri-Mech [21], San Diego Mechanism [22] and USC-Mech [23] are some of the most famous and extensively researched detailed mechanisms, however as seen in the works of Ji et al. [24] and Meziane and Bentebbiche [12] they still lack accuracy when it comes to hydrogen reactions, being preferable to utilize step reaction schemes directly developed to simulate hydrogen-methane reactions. In the studies of Li et al. [25] a comparison was made between detailed and reduced kinetic mechanisms specifically for CH₄ and H₂ combustion, with the reduced mechanisms having solid performances when compared to the detailed ones. In the work developed by Azevedo [26], it is presented a reduced kinetic mechanism built focusing on hydrogen presence in combustion, that revealed excellent results when compared to other detailed (USC-Mech, Gri-Mech and San Diego) and reduced (ROM [27]) mechanisms.

2.3.5 Radiation Modeling

Radiation plays an important role in combustion, specially when in it comes to high-temperature environments, due to the changes it provokes in the temperature field. It is fundamental not only to predict the formation of certain hydrocarbon-fuel combustion products, such as H_2O , CO_2 and CO , as a result of their high absorptivities and emissivities in the near infrared zone, but also to predict the thermal NO_x formation, since the kinetics of these molecules are extremely sensitive to temperature [28].

ANSYS Fluent offers six different radiation models in order to simulate this phenomenon correctly, namely the Discrete Transfer, P-1, Rosseland, Surface-to-Surface, Monte Carlo and Discrete Ordinates radiation models. Each model as its advantages and limitations, however, according to the works of Ge et al. [29] and Gamil et al. [30], as well as ANSYS own theory guide [17], the Discrete Ordinates model is the most feasible option when it comes to combustion problems. Therefore, only this model will be covered in this chapter.

Discrete Ordinates

The Discrete Ordinates radiation model is a deterministic method used to solve the Radiative Transfer Equation, or RTE, for a finite number of discrete solid angles. This model objective is to transform the RTE into a transport equation for radiation intensity, which will then be solved using methods similar to those employed for fluid flow and energy equations. The RTE is considered a field equation in the $\vec{s}$ direction and its general form is given by [17]:

$$\nabla \cdot (I(\vec{r}, \vec{s}) \vec{s}) + (a + \sigma_s) I(\vec{r}, \vec{s}) = an^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(\vec{r}, \vec{s}') \Phi(\vec{s} \cdot \vec{s}') d\Omega' \quad (2.8)$$

where $I(\vec{r}, \vec{s})$ represents the radiation intensity, a the absorption coefficient, σ_s the scattering coefficient, n the refractive index, σ the Stefan-Boltzmann constant and T the temperature. The Discrete Ordinates model then discretizes the directional component of the RTE into a finite set of solid angles, transforming it into a set of transport equations for specific wavelengths [29]:

$$\frac{dI_{i,\eta}}{ds_i} = \kappa_\eta I_{b\eta} - \kappa_\eta I_{i,\eta} - \sigma_\eta I_{i,\eta} + \frac{\sigma_\eta}{4\pi} \sum_{j=1}^N I_{j,\eta}(\hat{s}_j) \Phi_\eta(\hat{s}_j \cdot \hat{s}_i) d\Omega_i \quad (2.9)$$

where η denotes the wavelength in question, $I_{i,\eta}$ represents the radiation intensity in the direction $\hat{s}_i$, κ_η the absorption coefficient, $I_{b\eta}$ the blackbody intensity and Φ_η the scattering phase function.

The Discrete Ordinates model becomes particularly useful when simulating radiative heat transfer in complex geometries and in applications involving high optical thicknesses and scattering, while also being able to handle both gray and non-gray radiation. In spite of its advantages, it may not be suitable for problems with weak coupling between energy

and radiation intensities, or when solving enthalpy equations instead of temperature ones [17].

2.3.6 CFD Software

CFD software vary significantly in their capabilities, user interfaces, and computational requirements. Some are known for their comprehensive features and user-friendly interfaces that make them suitable for both academic research and industrial applications. Others offer open-source flexibility, allowing users to customize the code for specific needs, without any financial costs, which is particularly advantageous for research and development or low-cost environments. The choice of CFD solver often depends on the specific requirements of the simulation, including the complexity of the geometry, the need for customization, and the available computational resources. In order to perform this work ANSYS Fluent was the chosen solver, therefore it will be the only one reviewed.

ANSYS Fluent

ANSYS Fluent is one of the most used computer programs to model fluid flows, heat transfer and chemical reactions in complex geometries. Written in the C language, this program is able to resolve the stated problems with efficiency and flexibility. ANSYS Fluent also works in a client/server architecture, which means that remote simulations in powerful compute servers is a reality. On a meshing level, ANSYS Fluent is extremely versatile, meaning that it's able to solve problems using unstructured meshes, with diverse cell shapes, in complex geometries with relative ease, not only supporting mesh creation but also imported meshes [31]. All subsequent operations, including setting boundary conditions, defining fluid properties, executing the solution and refining the mesh are performed within Fluent's solution mode. On top of that, Fluent also possesses refined post-processing tools that enhances solution analysis and workflow.

2.4 Experimental Analysis of Hydrogen and Natural Gas Combustion

When developing a CFD model it's of great importance to verify that the simulation results are according to the experimental data obtained when testing the exact same installation in a real world scenario, making the experimental tests and analysis critical for the model success. The experimental analysis of hydrogen and methane combustion has been studied for a longer time than the CFD analysis. Therefore there is substantially more information about experimental practice, enhancing the ability to compare and verify the results of a new experimental study, as well as the understanding of the most accurate methodologies.

When it comes to hydrogen-methane combustion most authors vary not only the hydrogen concentration, as in the works of Yilmaz and Ilbas [13], but also the mixture equivalence ratio, as presented by Hu et al. [32] and Nemitallah et al. [33], enabling a more complete and detailed analysis of the air mass flow influence in the combustion. On the other hand, most works aim to measure not only the temperature profile obtained, but also the levels of pollutants formation, with some variation in the choice of pollutants measured, with CO, CO₂ and NO_x being the most common [13] [34] [33]. There is also the concern to analyze some other factors such as flashback limits, heat release rates and flame thickness and in spite of being less common, these properties are still studied in some works [32] [33].

The equipment used, the quality of the installation and the way properties are measured have significant impact in the results obtained. For temperature measurements, thermocouples are the most common choice. Usually installed along the axis, they may vary in type, with some authors choosing R-Type [13] [33], K-Type [35] and even Traveling thermocouples [32]. In order to obtain pollutant formation it's necessary to utilize a gas analyzer, however the analyzer choice varies a lot in between works, making it impossible to detect which are the most common. Mass flow controllers are also essential in the installation in order to control the burner power and the mass flows of each mixture component.

Even though there are differences between installations and equipments, most studies obtain similar results when analyzing the trends followed by some properties while varying the mixture content and/or burner power, which leads to prove that the experimental analysis of hydrogen-methane combustion is well studied and established.

Chapter 3

Materials and Methods

This chapter introduces the problem investigated, as well as the experimental and computational approaches made in order to fully understand, measure and simulate the system.

3.1 Problem Description

This work focus on the experimental and CFD analysis of a RIELLO 40 FS 3 (35 kW) burner, with the objective to validate the CFD model with the experimental measurements made. In order to achieve this objective a system was set up, where two containers with different methane and hydrogen compositions were tested, more precisely one container with a molar basis of 100% methane and another with 80% methane mixed with 20% hydrogen. At the same time, CFD simulations were made utilizing the same fuels, starting with simplified versions and progressing to more complex and trustworthy models in order to achieve a more complete results analysis. Both the experimental and CFD analysis were planned to be conducted at an output power of 11kW with 30% excess air. In Figure 3.1, are displayed photographs of the experimental setup used during the tests, courtesy of INEGI.

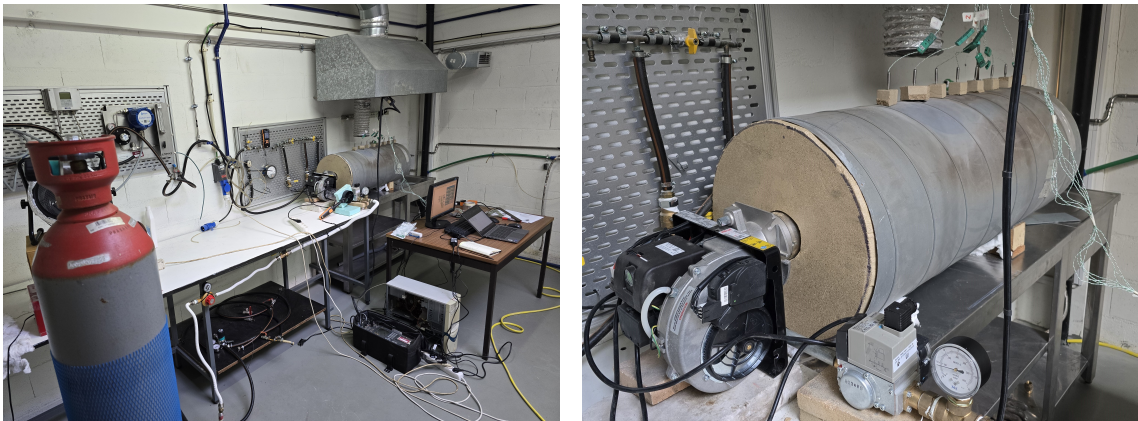


Figure 3.1: Setup used during the experimental tests

Also, in Figure 3.2 is presented a diagram revealing the overall logic of the experimental setup, while in Figure 3.3 are presented the combustion chamber's detailed measurements and thermocouples and gas analyzer probe positioning.

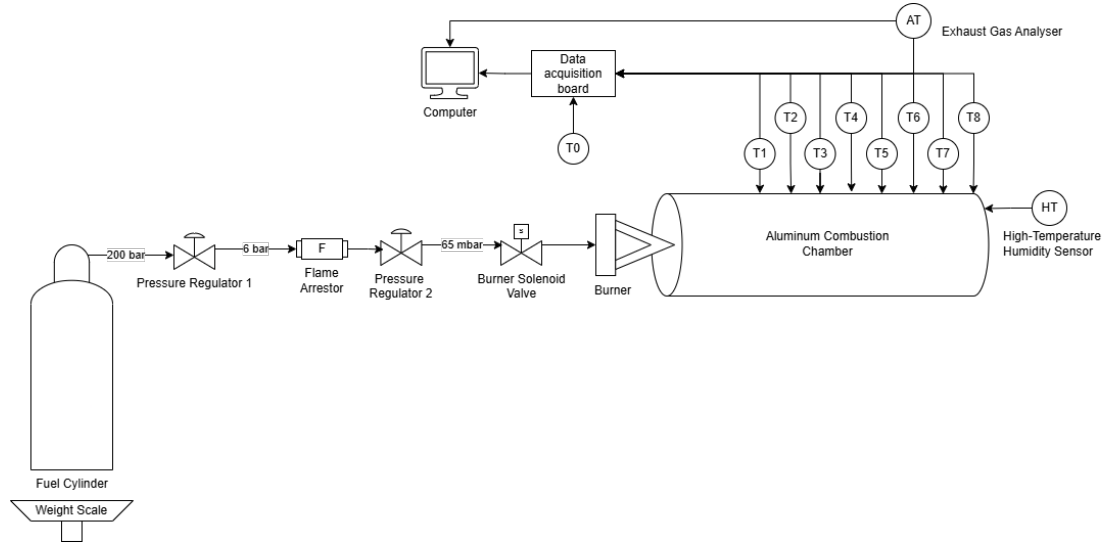


Figure 3.2: Schematic representation of the experimental setup logic

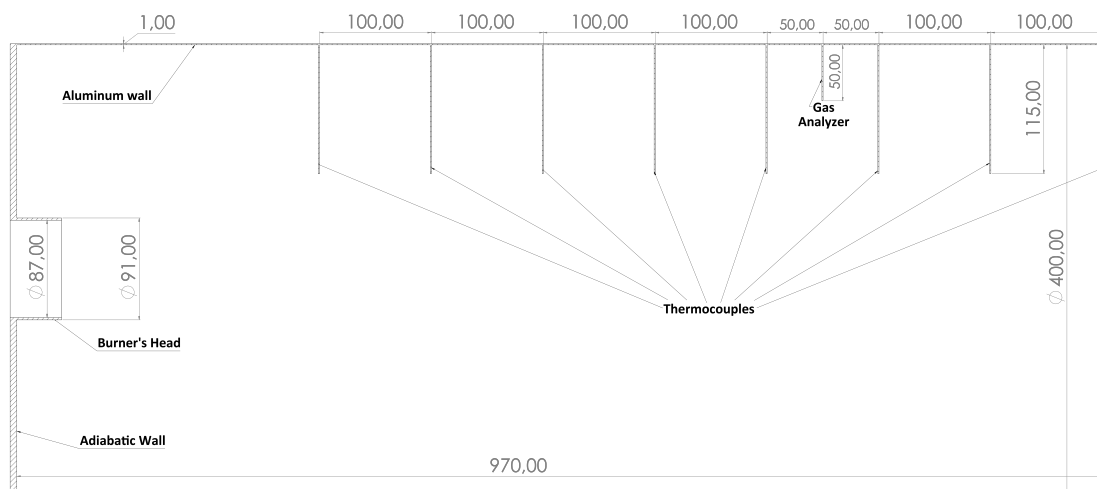


Figure 3.3: Section view of the combustion chamber

3.2 Computational Approach

As denoted before, the first iterations of the CFD analysis were simple, starting with 2D axisymmetric simulations, progressing into simplified 3D simulations and ending with detailed 3D ones, where the full injection system was explicitly modeled. In both the 2D and simple 3D simulations an homogeneous fuel and air mixture will be considered. For

each type of simulation, different geometries and meshes were developed and different models were selected, which will be all explained in the next sections.

In order to be able to calculate the properties surrounding CH₄ and H₂ combustion, as well as to obtain the necessary input variables for ANSYS Fluent, a calculation tool was developed. By inputting the CH₄ and H₂ molar fractions, the burner's thermal power, and the desired excess air percentage, the tool provided outputs such as the fuel/gas and air mass flow rates, individual species mass flows, species mass fractions in the fuel, air, and total mixture, and stoichiometric values for comparison. The gas properties used in the calculations are defined in Chapter 2. It is important to notice that, if desired, it was possible to easily redefine which variables to input, which allowed to shape the tool around any present variable/parameter. The calculations in the tool are based on the following chemical and mathematical equations

$$Y_i = \frac{X_i M_i}{X_{\text{CH}_4} M_{\text{CH}_4} + X_{\text{H}_2} M_{\text{H}_2}} \quad (3.1)$$

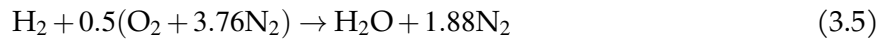
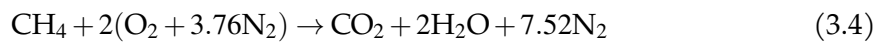
With X_{CH_4} and X_{H_2} being the fuel's molar fractions of methane and hydrogen, respectively, Y_i the corresponding mass fractions, M_i the corresponding molar masses and with i being either CH₄ or H₂. Considering the lower heating values of methane and hydrogen as LHV_{CH_4} and LHV_{H_2} , described in Tables 2.2 and 2.3, the fuel's LHV is calculated by:

$$\text{LHV}_{\text{fuel}} = Y_{\text{CH}_4} \cdot \text{LHV}_{\text{CH}_4} + Y_{\text{H}_2} \cdot \text{LHV}_{\text{H}_2} \quad (3.2)$$

Given the desired burner's thermal power as $\dot{Q}$, in kW, the required fuel mass flow rate, in kg/s, is:

$$\dot{m}_{\text{fuel}} = \frac{\dot{Q}}{\text{LHV}_{\text{fuel}}} \quad (3.3)$$

Considering the following stoichiometric combustion reactions:



the required stoichiometric air moles per mole of fuel can be calculated as:

$$\left(\frac{n_{\text{air}}}{n_{\text{fuel}}} \right)_{\text{CH}_4} = 2 \cdot (1 + 3.76) = 9.52 \quad (3.6)$$

$$\left(\frac{n_{\text{air}}}{n_{\text{fuel}}} \right)_{\text{H}_2} = 0.5 \cdot (1 + 3.76) = 2.38 \quad (3.7)$$

which can then be used to calculate the stoichiometric air-to-fuel mass ratio:

$$\left(\frac{m_{\text{air}}}{m_{\text{fuel}}} \right)_{\text{stoich}} = \frac{(X_{\text{CH}_4} \cdot 9.52 + X_{\text{H}_2} \cdot 2.38) \cdot M_{\text{air}}}{X_{\text{CH}_4} \cdot M_{\text{CH}_4} + X_{\text{H}_2} \cdot M_{\text{H}_2}} \quad (3.8)$$

Considering λ the excess air fraction in decimal form, the real air-to-fuel mass ratio becomes:

$$\left(\frac{m_{\text{air}}}{m_{\text{fuel}}}\right)_{\text{real}} = \left(\frac{m_{\text{air}}}{m_{\text{fuel}}}\right)_{\text{stoich}} \cdot (1 + \lambda) \quad (3.9)$$

which can then be used to determine the real air mass flow, for a given fuel mass flow $\dot{m}_{\text{fuel}}$:

$$\dot{m}_{\text{air}} = \dot{m}_{\text{fuel}} \cdot \left(\frac{m_{\text{air}}}{m_{\text{fuel}}}\right)_{\text{real}} \quad (3.10)$$

The chemical and mathematical equations presented above consider an ideal situation, where the air present in the combustion process is completely dry. However, in reality, that is not the case, being necessary to also determine the amount of gaseous H_2O present in the air, which can be achieved by the following equations,

$$\dot{m}_{\text{H}_2\text{O}} = \frac{\omega}{\dot{m}_{\text{air}}} \quad (3.11)$$

$$\dot{m}_{\text{total air}} = \dot{m}_{\text{H}_2\text{O}} + \dot{m}_{\text{air}} \quad (3.12)$$

where ω is the humidity ratio, in $\text{kg}_{\text{H}_2\text{O}}/\text{kg}_{\text{air}}$, calculated using the CoolProp database plugin [36] in calculation, which uses as inputs the ambient temperature, the relative humidity and the pressure. The ambient temperature was obtained during the experimental tests, while the relative humidity was obtained resorting to the national weather database for the experimental test day. The pressure was considered to be atmospheric pressure. With the total air and fuel mass flows calculated and the corresponding mass fractions, individual species mass flows can be determined, which leads to a versatile analysis of the CH_4 and H_2 burning process.

On the other hand, another calculation tool was developed to accurately calculate the convective heat transfer coefficient associated with heat loss from the outer surface of the combustion chamber wall, which consisted of a cylindrical aluminum duct, to the surrounding air. The duct is subjected to forced convection, due to the air flow provoked by the exhaust system placed above it, however the heat transfer coefficient value varies according to the duct surface temperature. Therefore it is necessary to formulate h as a function of surface temperature, in order to insert the formula in the ANSYS boundary conditions and allow the solver to correctly calculate the heat transfer coefficient value. The calculation tool was built according to the Nusselt formulation for a *Circular Cylinder in Cross Flow* exhibited by Bergman and Lavine [37], which can be described by the following equations:

$$h = \frac{k \text{Nu}_D}{D} \quad (3.13)$$

where h represents the convection heat transfer coefficient, k the thermal conductivity of

air, Nu_D the Nusselt number and D the duct's diameter,

$$\overline{Nu}_D = 0.3 + \frac{0.62 Re_D^{1/2} Pr^{1/3}}{[1 + (0.4/Pr)^{2/3}]^{1/4}} \left[1 + \left(\frac{Re_D}{282000} \right)^{5/8} \right]^{4/5} \quad (3.14)$$

where Re_D stands for the Reynolds number and Pr the Prandtl number, which can be written as:

$$Re_D = \frac{v D}{\nu} \quad (3.15)$$

$$Pr = \frac{\nu}{\alpha} \quad (3.16)$$

with ν representing the air's kinematic viscosity, α the air's thermal diffusivity and v the air stream's velocity. The calculation was made for superficial temperatures between 303.15K and 2423.15K, an air stream temperature equal to 295.15K and an air velocity of 3m/s, measured during the experimental tests. The following expression was obtained:

$$h = 1.5381 \cdot 10^{-19} T_s^6 - 1.5144 \cdot 10^{-15} T_s^5 + 6.2062 \cdot 10^{-12} T_s^4 - 1.3757 \cdot 10^{-8} T_s^3 + 1.7943 \cdot 10^{-5} T_s^2 - 1.4160 \cdot 10^{-2} T_s + 14.8277 \quad (3.17)$$

and its curve is represented in Figure 3.4.

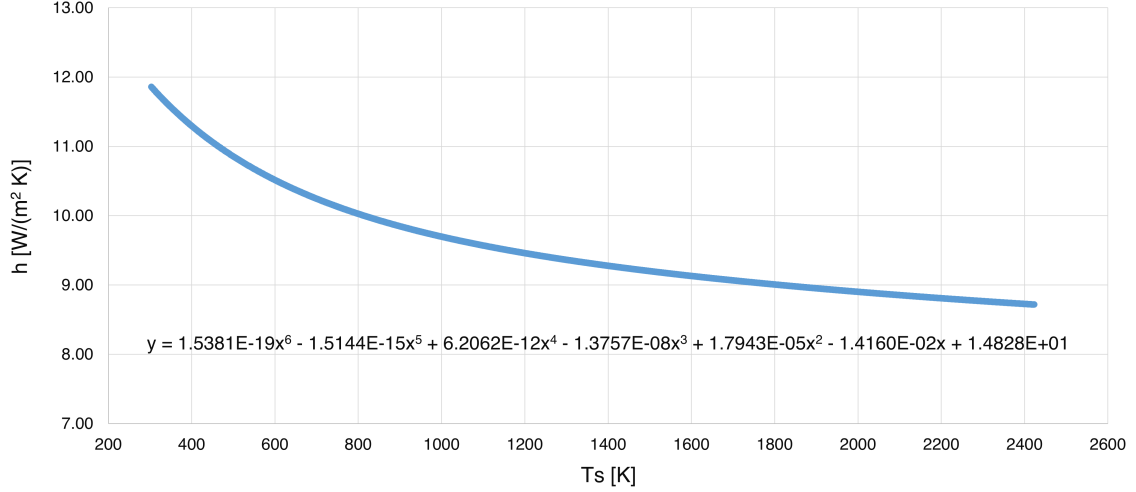


Figure 3.4: Variation of the convection heat transfer coefficient h with surface temperature T_s

It is also important to justify why heat transfer through conduction within the cylinder wall is negligible in this situation. In order to proceed, it is required to calculate the Biot number, that can be defined as:

$$Bi = \frac{h L_C}{k} \quad (3.18)$$

where h is the convection heat transfer coefficient, obtained in the calculation tool, k the

thermal conductivity of aluminum and L_c the characteristic length for conduction. For thin-walled cylinders, where radial heat conduction dominates, the wall thickness t serves as the appropriate characteristic length, meaning $L_c = t = 0.001\text{m}$. The thermal conductivity of aluminum was considered to be $k = 237\text{W/mK}$. As explained by Bergman and Lavine [37], if $\text{Bi} \leq 0.1$ then internal conduction is sufficiently fast to maintain a nearly uniform temperature distribution throughout the solid, meaning that there is no formation of temperature gradients in the duct's wall, therefore confirming that heat transfer through conduction is negligible. When calculating the Biot number for the range of values exhibited in Figure 3.4, the maximum value obtained is $5.00 \cdot 10^{-5}$, meaning it is correct to neglect conduction in the duct's wall.

3.2.1 2D Simulations

As referred above, the 2D simulations were axisymmetric, with the geometry representing only the system's upper half, as can be seen in Figure 3.5. In this Figure were drawn colored lines in order to better describe the defined boundaries. The corresponding names and boundary types can be found in Table 3.1.

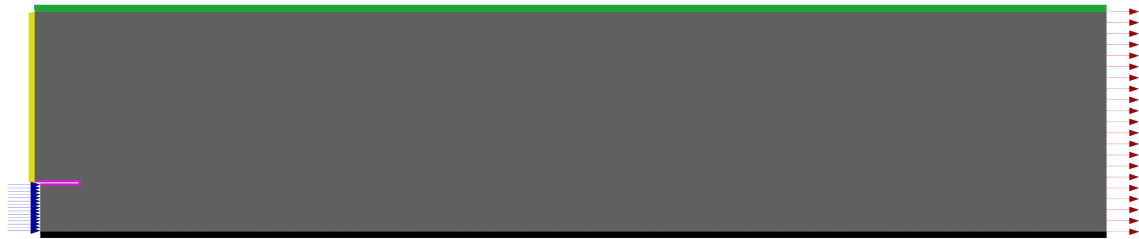


Figure 3.5: Geometry designed for the 2D approach

Table 3.1: Boundaries defined in the 2D geometry

Color and Shape	Boundary Name	Type
Green Line	Aluminum Wall	Wall
Yellow Line	Adiabatic Wall	Wall
Pink Line	Burner's Head	Wall
Black Line	Axis	Axis
Blue Arrows	Mix Inlet	Mass Flow Inlet
Red Arrows	Outlet	Pressure Outlet

The mesh, displayed in Figure 3.6, was built utilizing ANSYS Mechanical. It was composed by 195675 cells, with more than an element per mm^2 . Quality wise the mesh had an average orthogonal quality of 1 and an average skewness of $6.1554 \cdot 10^{-4}$, which is considered a perfect result following the ANSYS meshing guidelines [38], that state that these

values range from 0 to 1, with 1 being an ideal value for orthogonal quality and 0 ideal for skewness.

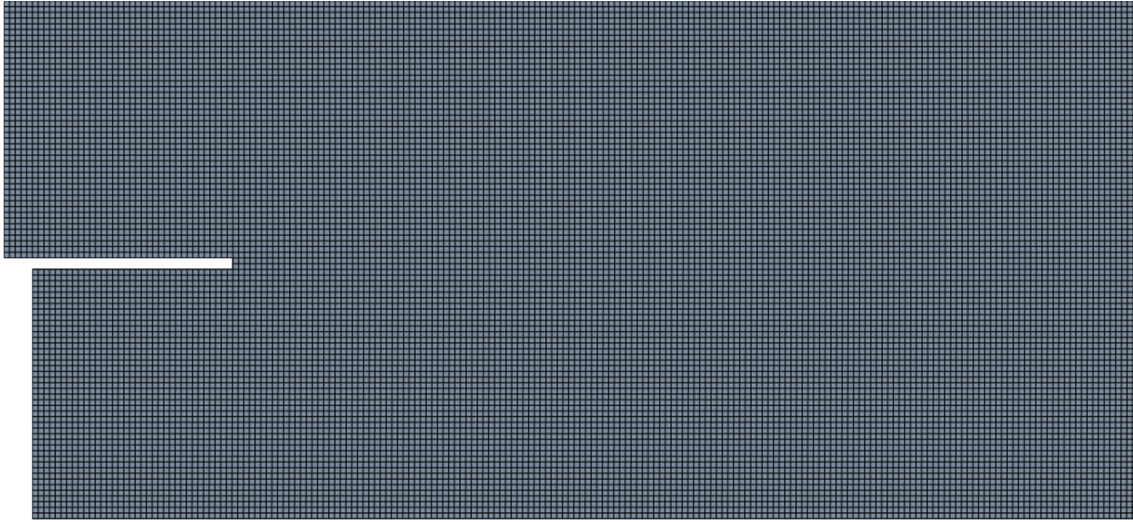


Figure 3.6: Mesh developed for the 2D approach

It is important to notice that, in Figure 3.6, only part of the geometry is represented, since otherwise the cells wouldn't be visible in a clear manner. The horizontal gap represented in Figure 3.6 corresponds to the pink line in Figure 3.5.

In ANSYS, the set of input variables displayed varies depending on the selected boundary condition type. Therefore, in Table 3.3 it is presented an overview of the boundaries exhibited in Table 3.1, together with the corresponding input variables and the specific values assigned to each. For improved clarity, only the most relevant or modified variables are included in the table, all the other parameters were left at their default values and therefore are not listed. It is also important to notice that the Mix Inlet mass flow and species mass fractions vary according to the gas composition being tested, therefore the values for this variables are listed in Table 3.2 for a better clarification. As stated previously, the inlet mixture is an homogeneous composition of fuel and air, where the species mass fractions are calculated in the first calculation tool mentioned, by dividing the individual species mass flow for the air plus fuel total mass flows. In order to calculate the H_2O mass fraction, a relative humidity of 70% was arbitrated.

Table 3.2: Mix Inlet properties for the different gas compositions tested

Properties	100% Methane	80% Methane 20% Hydrogen
Mix Inlet Mass Flow [kg/s]	$5.184 \cdot 10^{-3}$	$5.115 \cdot 10^{-3}$
Mix O ₂ Mass Fraction	0.22010	0.22040
Mix N ₂ Mass Fraction	0.72420	0.72510
Mix H ₂ O Mass Fraction	0.01321	0.01322
Mix CH ₄ Mass Fraction	0.04244	0.03999
Mix H ₂ Mass Fraction	–	0.00126

Table 3.3: Boundary conditions selected for the 2D approach

Boundary Name	Variable	Value
Aluminum Wall	Thermal Conditions	Convection
	Heat Transfer Coefficient	Equation 3.17
	Free Stream Temperature	25°C
	Wall Thickness	0.001m
Adiabatic Wall	Thermal Conditions	Heat Flux
	Heat Flux	0 W/m ²
Burner's Head	Thermal Conditions	Heat Flux
	Heat Flux	0 W/m ²
Axis	-	-
Mix Inlet	Turbulent Intensity	10%
	Total Temperature	25°C
	Mass Flow Rate	Table 3.2
	Species Mass Fractions	Table 3.2
Outlet	Backflow Turbulent Intensity	5%
	Backflow Total Temperature	25°C
	O ₂ Mass Fraction	0.230
	N ₂ Mass Fraction	0.756
	H ₂ O Mass Fraction	0.014
	Boundary Condition Radiation Type	Transparent

The remaining models chosen to replicate the combustion process in the 2D approach

can be found in Table 3.4. They were selected based on the theory explained in Chapter 2. In Table 3.5 are presented the formulations chosen to calculate the mixture properties. It is important to notice that non referred variables are left at default.

Table 3.4: Models selected for the 2D approach

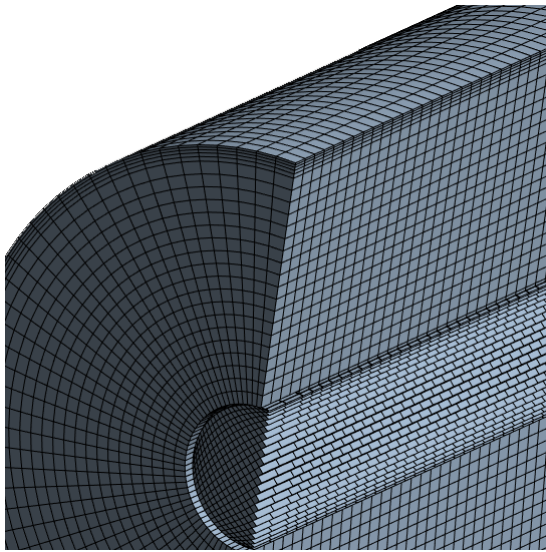
Model Type	Selected Options
Solver Type	Pressure-based, Steady, Axisymmetric
Energy equation	Enabled
Viscous Model	Standard k- ϵ , Standard wall functions
Radiation Model	Discrete Ordinates, Theta and Phi: Divisions=10, Pixels=8
Species Model	Species Transport, Volumetric, Finite-Rate/Eddy-Dissipation, Relax to Chemical Equilibrium, Diffusion Energy Source, Thermal Diffusion
CHEMKIM Mechanism	POA mechanism
Pressure-Velocity Coupling	Coupled
Discretization Schemes	Second Order Upwind (Pressure, Density, Momentum, Energy, Species)
	First Order Upwind (Turbulent Kinetic Energy, Turbulent Dissipation Rate, Discrete Ordinates)
Relaxation Factors	0.75 (Pressure, Density, Momentum, Energy, Species, Turbulent Kinetic Energy, Turbulent Dissipation Rate)
	1 (Body Forces, Turbulent Viscosity, Discrete Ordinates)
Initialization	Standard, Turbulent Kinetic Energy=1, Turbulent Dissipation Rate=1 O ₂ =0.230, N ₂ =0.756, H ₂ O=0.014, Temperature=25°C Other Values=0

Table 3.5: Formulations selected to calculate the mixture properties in the 2D simulations

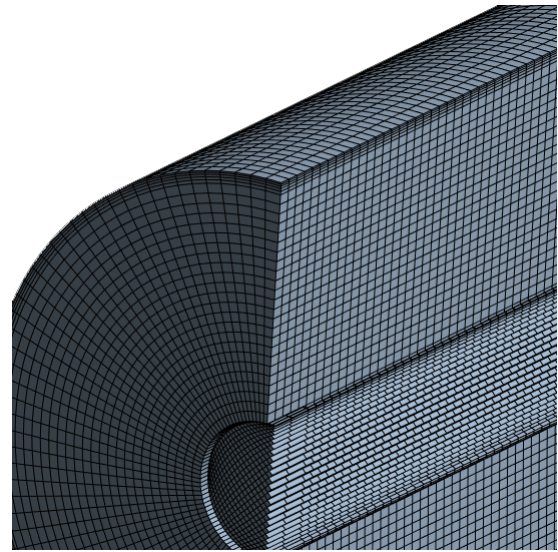
Mixture Property	Formulation
Density	Ideal Gas
Specific Heat	Mixing Law
Thermal Conductivity	Mass Weighted Mixing Law
Viscosity	Mass Weighted Mixing Law
Thermal Diffusion Coefficient	Kinetic Theory
Absorption Coefficient	WSGGM Domain Based

3.2.2 Simple 3D Simulations

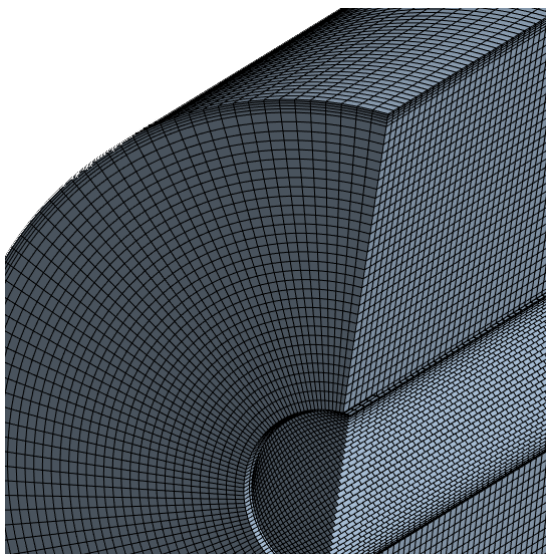
To introduce the study of 3D simulations, a simple 3D geometry and multiple meshes were developed. The geometry is considerably simple, consisting of a revolve applied to the 2D Geometry, Figure 3.5, around the axis boundary. Since 3D simulations are considerably more computational expensive than 2D simulations, a mesh independence test was made in order to analyze which was the optimal mesh resolution. Therefore 6 meshes were developed, utilizing ANSYS Mechanical, ranging from 250 thousand to 3 million cells. This 6 meshes are represented in Figure 3.7.



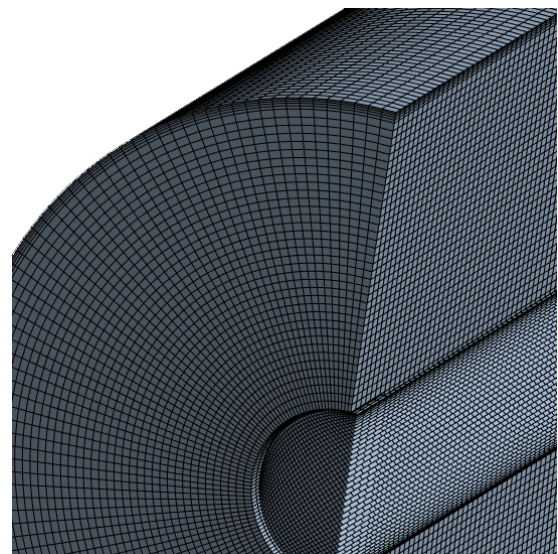
(a) 250 000 cell mesh



(b) 500 000 cell mesh



(c) 1 000 000 cell mesh



(d) 1 500 000 cell mesh

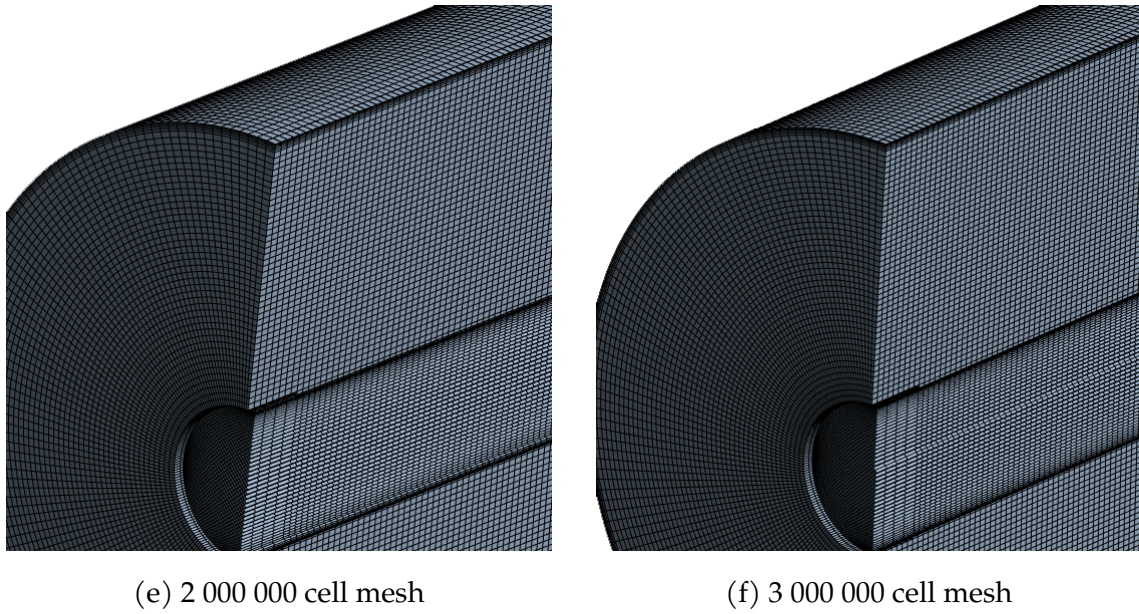


Figure 3.7: Meshes used for the mesh independence test

In Table 3.6 are shown the average skewness and orthogonal quality levels for each mesh. As referred before, following the ANSYS mesh guidelines [38], these values range from 0 to 1, with 0 being the ideal value for skewness and 1 the ideal value for orthogonal quality.

Table 3.6: Average Skewness and Orthogonal Quality levels for the meshes used for the mesh independence test

Quality Parameters	250 thousand cell mesh	500 thousand cell mesh	1 million cell mesh	1.5 million cell mesh	2 million cell mesh	3 million cell mesh
Skewness	0.064126	0.060275	0.057555	0.055662	0.055036	0.053981
Orthogonal Quality	0.97293	0.97442	0.97520	0.97587	0.97603	0.97648

As can be seen by the results presented in the table, and as expected, the mesh quality levels increase with the mesh size. The meshes were tested for the 100% methane fuel. The boundary conditions, models selected and the formulations selected to calculate mixture properties are exhibited in Tables 3.7, 3.8 and 3.9, respectively.

Table 3.7: Boundary conditions selected for the simple 3D approach

Boundary Name	Variable	Value
Aluminum Wall	Thermal Conditions	Mixed
	Heat Transfer Coefficient	Equation 3.17
	Free Stream Temperature	25°C
	External Emissivity	0.7
	External Radiation Temperature	25°C
	Wall Thickness	0.001m
Adiabatic Wall	Thermal Conditions	Heat Flux
	Heat Flux	0 W/m ²
Burner's Head	Thermal Conditions	Heat Flux
	Heat Flux	0 W/m ²
Mix Inlet	Turbulent Intensity	10%
	Total Temperature	25°C
	Mass Flow Rate	Table 3.2
	Species Mass Fractions	Table 3.2
	Coordinate System	Local Cylindrical
	Tangential-Component of Flow Direction	0.3
	Axial-Component of Flow Direction	0.7
Outlet	Backflow Turbulent Intensity	5%
	Backflow Total Temperature	25°C
	O ₂ Mass Fraction	0.230
	N ₂ Mass Fraction	0.756
	H ₂ O Mass Fraction	0.014
	Boundary Condition Radiation Type	Transparent

The changes made in the Mix Inlet boundary conditions, when compared to the 2D simulations setup, served as a way to simulate a swirl effect. For the Aluminum Wall boundary, an additional radiation model was enabled to account for the radiative heat transfer, enabling the inclusion of a wider range of the involved heat transfer. It is, again, important to notice that, for both tables, every non-listed variable/parameter was left at default.

Table 3.8: Models selected for the simple 3D approach

Model Type	Selected Options
Solver Type	Pressure-based, Steady, Gravity ($Y=-9.81 \text{ m/s}^2$)
Energy equation	Enabled
Viscous Model	Standard k- ϵ , Standard wall functions, Full Buoyancy Effects
Radiation Model	Discrete Ordinates, Theta and Phi: Divisions=10, Pixels=8
Species Model	Species Transport, Volumetric, Finite-Rate/Eddy-Dissipation, Relax to Chemical Equilibrium, Diffusion Energy Source, Thermal Diffusion
CHEMKIM Mechanism	POA mechanism
Pressure-Velocity Coupling	Coupled
Discretization Schemes	Second Order Upwind (Pressure, Density, Momentum, Energy, Species) First Order Upwind (Discrete Ordinates, Turbulent Kinetic Energy, Turbulent Dissipation Rate)
Relaxation Factors	0.75 (Energy, Species) 0.5 (Turbulent Kinetic Energy, Turbulent Dissipation Rate) 0.3 (Pressure, Momentum, Density) 1 (Body Forces, Turbulent Viscosity, Discrete Ordinates)
Initialization	Standard, Turbulent Kinetic Energy=1, Turbulent Dissipation Rate=1 $O_2 = 0.230$, $N_2=0.756$, $H_2O=0.014$, Temperature=25°C Other Values=0

Table 3.9: Formulations selected to calculate the mixture properties in the simple 3D simulations

Mixture Property	Formulation
Density	Ideal Gas
Specific Heat	Mixing Law
Thermal Conductivity	Mass Weighted Mixing Law
Viscosity	Mass Weighted Mixing Law
Thermal Diffusion Coefficient	Kinetic Theory
Absorption Coefficient	WSGGM Domain Based

In order to proceed with the mesh independence test, average temperatures were calculated, in ANSYS CFD-Post, from six representative zones of the domain: along the central axis, along two lines vertically aligned and parallel to the axis at the bottom and top of the combustion chamber, at a mid-plane cutting through the axis, at the outlet face, and over the entire volume of the chamber. Afterwards an error analysis was made for every

mesh size in each zone, in order to understand the temperature values convergence as the mesh size increases. The equation used to calculate the relative error is the following,

$$\text{Relative Error [\%]} = \left| \frac{T_i - T_I}{T_I} \right| \times 100 \quad (3.19)$$

with T_i and T_I representing the average temperature for each zone, obtained with mesh i and the most refined mesh I , respectively. In this case I represents the 3 million cell mesh. As shown in Table 3.10, only from the 2 million cell mesh onward the relative errors are, consistently, below 0.1%, which is a reliable benchmark to determine if the solution has converged. Therefore, it is correct to assume that the 2 million cell mesh is independent and offers the best compromise between accuracy and computational cost.

Table 3.10: Simple 3D Mesh independence test results

Number of Mesh Cells	Parameter	Bottom Line	Top Line	Axis Line	Total Volume	Axial Mid-Plane	Outlet Plane
250 000	Average Temperature [K]	511.369	668.343	669.078	529.015	618.028	420.997
	Relative Error	0.78442%	0.73298%	3.82057%	0.45746%	0.06112%	0.08939%
500 000	Average Temperature [K]	515.972	675.168	674.652	532.275	621.603	421.754
	Relative Error	0.10865%	0.28072%	3.01931%	1.07652%	0.51697%	0.26936%
1 000 000	Average Temperature [K]	518.463	677.372	685.827	531.433	621.072	420.859
	Relative Error	0.59195%	0.60807%	1.41291%	0.91662%	0.43111%	0.05658%
1 500 000	Average Temperature [K]	513.134	671.482	696.269	526.074	617.884	420.429
	Relative Error	0.44198%	0.26675%	0.08812%	0.10102%	0.08441%	0.04565%
2 000 000	Average Temperature [K]	515.002	672.896	695.907	526.844	618.510	420.464
	Relative Error	0.07955%	0.05674%	0.03608%	0.04520%	0.01682%	0.03733%
3 000 000	Average Temperature [K]	515.412	673.278	695.656	526.606	618.406	420.621

With the mesh independence test finished and with the results for the 100% CH₄ fuel gathered, another simulation was made, using the 2 million cell mesh, for a fuel molar composition of 80% CH₄ + 20% H₂. The models, boundary conditions and formulations presented in this sub-chapter's tables are valid for both fuels.

3.2.3 Detailed 3D Simulations

In order to create a more accurate geometry in the simulations, it was necessary to design and include the burner's injection system into ANSYS. This was done in two steps, a pre-decessor simulation where the fuel injection system was simulated separately, without

combustion involved, to understand the fuel's mass flux behavior inside it and a successor simulation, with the combustion chamber and detailed injection system together to test the full combustion process. Through this process the entire system was faithfully represented.

Predecessor Simulation

As referred above, this step focused on studying the behavior of the fuel injection system, equipped with 8 primary outlets and 6 secondary outlets. This will be achieved by inputting the total required fuel mass flow, in the injector's inlet, in order to retrieve the mass flow exiting through each of the injector's outlet. This analysis was carried out individually for each fuel composition, since they both require different fuel mass flows. The geometry and mesh were provided by INEGI, with the mesh independence test already made. The selected mesh had a total of 264630 cells, an average orthogonal quality of 0.95816 and an average skewness of 0.04119. Both the geometry and mesh are represented in Figure 3.8. Also, in Figure 3.9 is exhibited a schematic of the fuel injection system operation, provided by INEGI.

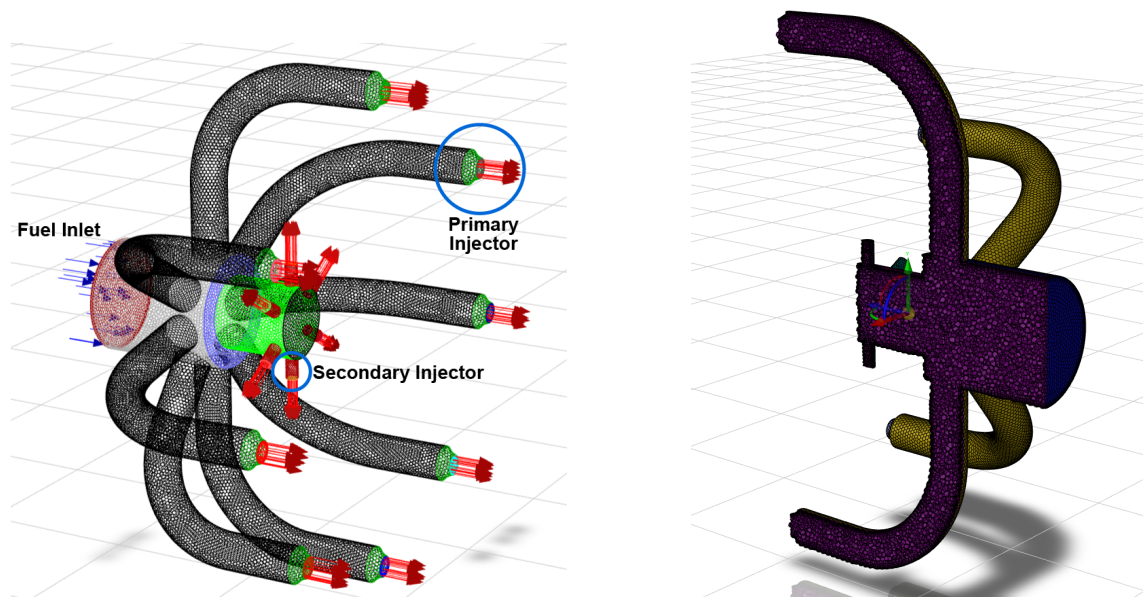


Figure 3.8: Predecessor simulations geometry and mesh

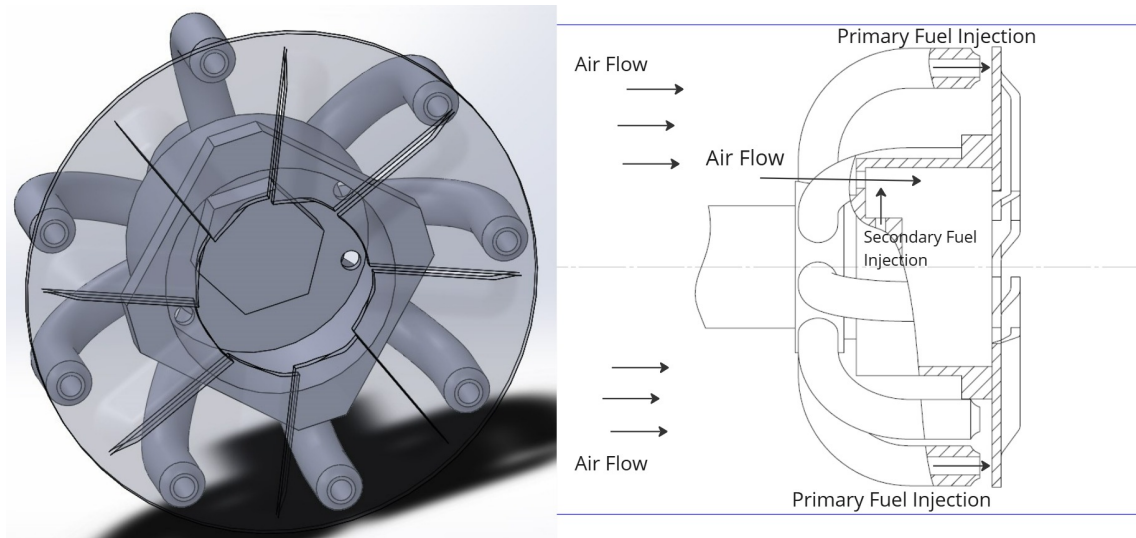


Figure 3.9: Schematic of the fuel injection system operation

In Tables 3.11, 3.12, 3.13 and 3.14 are represented the models, formulations and boundary conditions selected in order to study the way fuel circulates and splits through the injector's pipes and outlets. As for the above tables, every non listed variable in the following tables was left at default.

Table 3.11: Fuel Inlet properties for the different gas compositions tested

Properties	100% Methane	80% Methane 20% Hydrogen
Fuel Inlet Mass Flow [kg/s]	$2.200 \cdot 10^{-4}$	$2.110 \cdot 10^{-4}$
Fuel CH ₄ Mole Fraction	1	0.8
Fuel H ₂ Mole Fraction	-	0.2

Table 3.12: Formulations selected to calculate the mixture properties in the predecessor simulations

Mixture Property	Formulation
Density	Ideal Gas
Specific Heat	Mixing Law
Thermal Conductivity	Mass Weighted Mixing Law
Viscosity	Mass Weighted Mixing Law

Table 3.13: Boundary conditions selected for the predecessor simulation

Boundary Name	Type	Variable	Value
Fuel Inlet	Mass Flow Inlet	Turbulent Intensity	10%
		Total Temperature	25°C
		Mass Flow Rate	Table 3.11
		Species Mole Fractions	Table 3.11
Outlets	Pressure Outlet	Backflow Turbulent Intensity	5%
		Backflow Total Temperature	25°C
		O ₂ Mass Fraction	0.230
		N ₂ Mass Fraction	0.756
		H ₂ O Mass Fraction	0.014

Table 3.14: Models selected for the predecessor simulation

Model Type	Selected Options
Solver Type	Pressure-based, Steady, Gravity ($Y=-9.81 \text{ m/s}^2$)
Energy equation	Enabled
Viscous Model	Standard k- ϵ , Standard wall functions, Full Buoyancy Effects
Species Model	Species Transport, Diffusion Energy Source
Pressure-Velocity Coupling	Coupled
Discretization Schemes	Second Order Upwind (Pressure, Density, Momentum, Energy, Species)
	First Order Upwind (Turbulent Kinetic Energy, Turbulent Dissipation Rate)
Relaxation Factors	0.75 (Energy, Species, Turbulent Kinetic Energy, Turbulent Dissipation Rate)
	0.5 (Pressure, Momentum)
	0.25 (Density)
	1 (Body Forces, Turbulent Viscosity)
Initialization	Standard, Turbulent Kinetic Energy=1, Turbulent Dissipation Rate=1
	O ₂ = 0.230, N ₂ =0.756, H ₂ O=0.014, Temperature=25°C
	Other Values=0

With the simulations finished, it was then necessary to calculate the percentages of fuel flowing in each injector's outlet. For that purpose, CFD-Post was used to determine

the total fuel mass flux in each outlet. The values were then transferred to an calculation tool where they were subjected to the following equation:

$$\text{Outlet Mass Flow [\%]} = \frac{\text{Outlet Mass Flow [kg/s]}}{\text{Fuel Inlet Mass Flow [kg/s]}} \cdot 100 \quad (3.20)$$

The results obtained in the calculation tool revealed that each primary injector outlet had an average of 10.457%, of the fuel's total mass flow, and each secondary injector outlet an average of 2.724%. The values in between primary injectors, between secondary injectors and in between different fuel compositions were extremely similar, therefore it is safe to assume mean values, differing only between primary and secondary outlets.

Successor Simulation

In this step both the detailed injection system and combustion chamber were simulated together. It is important to note that the fuel injection system not only determines the fuel distribution, but also affects the airflow. In combination with the turbulator located immediately after the primary injectors, as seen in Figure 3.9, it influences the mixing between air and fuel, thereby directly affecting the combustion process. Therefore, its accurate modeling is of extreme importance. The geometry was provided by INEGI, however, unlike in the previous step, the mesh had not yet been developed. Thus, a mesh independence test was also necessary. Therefore, seven different meshes were designed, using Fluent Meshing, ranging from 1.7 million cells to 10 million. Every mesh had a minimal orthogonal quality above 0.15, an average orthogonal quality above 0.95 and an average skewness below 0.05. Average temperatures were calculated following the same measure zones and process defined in the simple 3D simulation's mesh independence test. The boundary conditions, selected models, selected formulations to calculate mixture properties and results obtained are displayed in Tables 3.16, 3.17, 3.18 and 3.19, respectively. The mass flows obtained for each primary and secondary fuel inlet, following the results acquired in the predecessor simulations, are displayed in Table 3.15 along with the respective mole fractions.

Table 3.15: Air and fuel mass flows used in the detailed 3D simulations

Properties	100% Methane	80% Methane 20% Hydrogen
Primary Inlet Fuel Mass Flow [kg/s]	$2.301 \cdot 10^{-5}$	$2.206 \cdot 10^{-5}$
Secondary Inlet Fuel Mass Flow [kg/s]	$5.993 \cdot 10^{-6}$	$5.748 \cdot 10^{-6}$
Fuel CH ₄ Mole Fraction	1	0.8
Fuel H ₂ Mole Fraction	-	0.2
Air Inlet Mass Flow [kg/s]	$4.964 \cdot 10^{-3}$	$4.904 \cdot 10^{-3}$

Table 3.16: Boundary conditions for the detailed 3D simulations

Boundary Name	Variable	Value
Aluminum Wall	Thermal Conditions	Mixed
	Heat Transfer Coefficient	Equation 3.17
	Free Stream Temperature	25°C
	External Emissivity	0.7
	External Radiation Temperature	25°C
	Wall Thickness	0.001m
Adiabatic Wall	Thermal Conditions	Heat Flux
	Heat Flux	0 W/m ²
Burner's Head	Thermal Conditions	Heat Flux
	Heat Flux	0 W/m ²
Air Inlet	Turbulent Intensity	10%
	Total Temperature	25°C
	Mass Flow Rate	Table 3.15
	O ₂ Mass Fraction	0.230
	N ₂ Mass Fraction	0.756
	H ₂ O Mass Fraction	0.014
Primary Fuel Inlet	Turbulent Intensity	10%
	Total Temperature	25°C
	Mass Flow Rate	Table 3.15
	Species Mole Fractions	Table 3.15
Secondary Fuel Inlet	Turbulent Intensity	10%
	Total Temperature	25°C
	Mass Flow Rate	Table 3.15
	Species Mole Fractions	Table 3.15
Outlet	Backflow Turbulent Intensity	5%
	Backflow Total Temperature	25°C
	O ₂ Mass Fraction	0.230
	N ₂ Mass Fraction	0.756
	H ₂ O Mass Fraction	0.014
	Boundary Condition Radiation Type	Transparent

Table 3.17: Models selected for the detailed 3D simulations

Model Type	Selected Options
Solver Type	Pressure-based, Steady, Gravity ($Y=-9.81 \text{ m/s}^2$)
Energy equation	Enabled
Viscous Model	Standard k- ϵ , Standard wall functions, Full Buoyancy Effects
Radiation Model	Discrete Ordinates, Theta and Phi: Divisions=10, Pixels=8
Species Model	Species Transport, Volumetric, Finite-Rate/Eddy-Dissipation, Relax to Chemical Equilibrium, Diffusion Energy Source, Thermal Diffusion
CHEMKIM Mechanism	POA mechanism
Pressure-Velocity Coupling	Coupled
Discretization Schemes	Second Order Upwind (Pressure, Density, Momentum, Energy, Species) First Order Upwind (Discrete Ordinates, Turbulent Kinetic Energy, Turbulent Dissipation Rate)
Relaxation Factors	0.5 (Turbulent Kinetic Energy, Turbulent Dissipation Rate, Species) 0.3 (Pressure, Momentum, Density, Energy) 1 (Body Forces, Turbulent Viscosity, Discrete Ordinates)
Initialization	Standard, Turbulent Kinetic Energy=1, Turbulent Dissipation Rate=1 $O_2 = 0.230$, $N_2=0.756$, $H_2O=0.014$, Temperature=25°C Other Values=0

Table 3.18: Formulations selected to calculate the mixture properties in the detailed 3D simulations

Mixture Property	Formulation
Density	Ideal Gas
Specific Heat	Mixing Law
Thermal Conductivity	Mass Weighted Mixing Law
Viscosity	Mass Weighted Mixing Law
Thermal Diffusion Coefficient	Kinetic Theory
Absorption Coefficient	WSGGM Domain Based

Table 3.19: Detailed 3D simulations mesh independence test results

Number of Mesh Cells	Parameter	Bottom Line	Top Line	Axis Line	Total Volume	Axial Mid-Plane	Outlet Plane
2 000 000	Average Temperature [K]	527.666	676.361	768.366	557.740	646.694	431.636
	Relative Error	0.21880%	0.25410%	2.38355%	0.21796%	0.96564%	0.22860%
4 000 000	Average Temperature [K]	527.761	677.455	769.307	560.577	640.191	433.894
	Relative Error	0.20082%	0.09276%	2.50839%	0.72773%	0.04965%	0.29333%
5 000 000	Average Temperature [K]	527.538	677.277	766.889	559.884	640.852	433.998
	Relative Error	0.24299%	0.11901%	2.18674%	0.60321%	0.05355%	0.31736%
6 300 000	Average Temperature [K]	527.401	676.601	777.328	562.201	644.043	434.800
	Relative Error	0.26890%	0.21870%	3.57772%	1.01954%	0.55175%	0.50274%
7 000 000	Average Temperature [K]	532.474	680.841	741.154	558.659	639.627	432.535
	Relative Error	0.69040%	0.40659%	1.24241%	0.38309%	0.13770%	0.02080%
8 500 000	Average Temperature [K]	527.645	675.212	759.258	555.209	639.013	432.471
	Relative Error	0.22276%	0.42355%	1.16992%	0.23683%	0.07806%	0.27761%
10 000 000	Average Temperature [K]	528.823	678.084	750.478	556.527	640.509	432.625

It is important to note that, unlike the simple 3D simulations, those conducted in this step did not fully converge due to the simulation's high complexity level. Therefore, a limited iteration approach was adopted, by running each simulation for 1000 iterations, after which the results were evaluated, providing a fair comparison between meshes. Also unlike the simple 3D simulations, in this case there is not a clear convergence of values, even when running meshes with as much as 10 million cells. However, from the 7 million cell mesh onward every error was below 1.3%, which is already a considerably good value when taking into account the complexity and sensitivity provoked by the full injection system presence. Therefore the 7 million cell mesh was the one selected to run the remaining simulations. From Figure 3.10 to Figure 3.13 are exhibited the geometry and the selected mesh for this step.

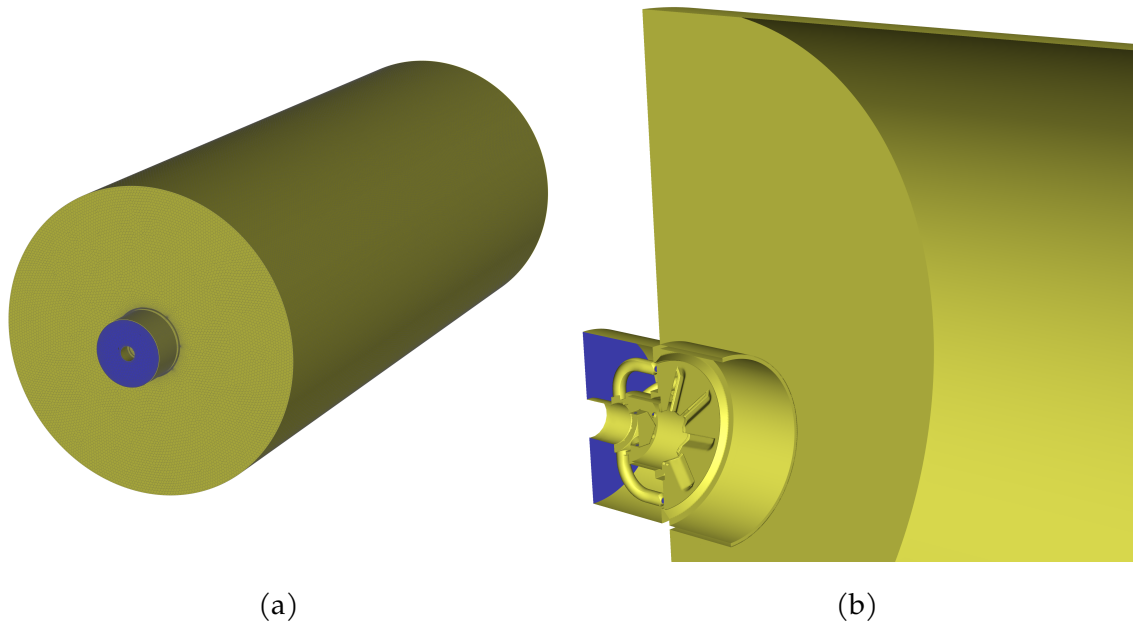


Figure 3.10: Overview of the geometry used in the detailed 3D simulations

In Figure 3.10 (a) is possible to visualize the combustion chamber as well as the Air Inlet boundary, defined with a blue color. In Figure 3.10 (b) is presented a vertical cut through the chamber axis, where is possible to observe the whole injection system, composed by the fuel injection system studied in the predecessor simulations, the turbulator which ensures a swirl effect into the flame and the cylindrical walls surrounding the system representing the burner's head. As stated above, the air enters the injection system through the blue circular crown, while the fuel enters the fuel injection system through the hole in the middle of the circular crown. Air and fuel then meet right before the turbulator, where the fuel exits the fuel injection system's outlets. In Figures 3.11 (a) and (b) is represented a close up picture of the front and back side, respectively, of the full injection system geometry, however the circular crown representing the Air Inlet boundary is no longer visible in order to be possible to fully observe the path taken by the air as it enters the injection system.

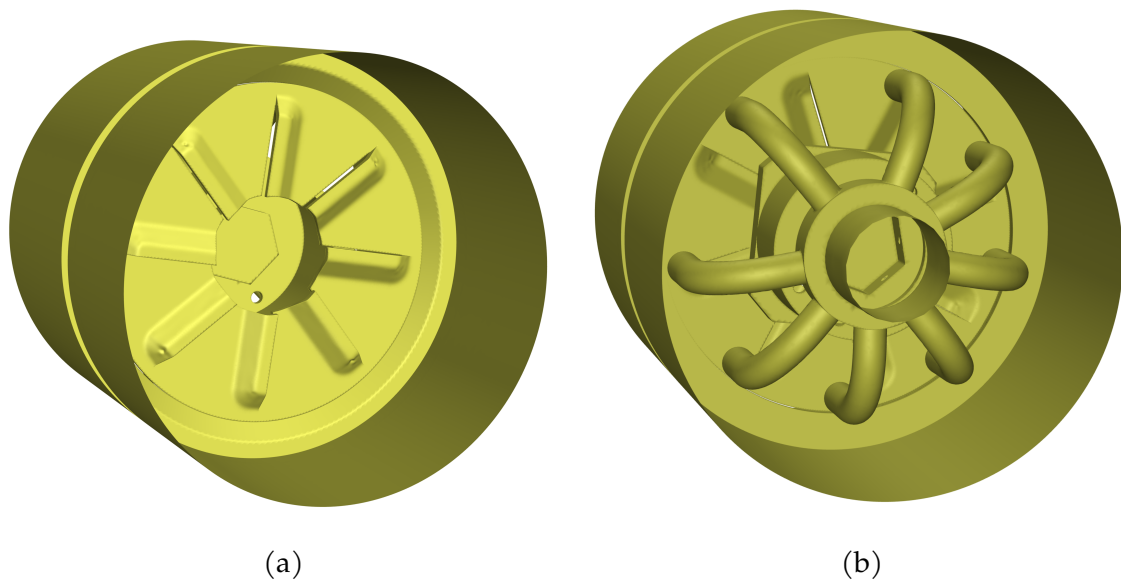


Figure 3.11: Close up pictures of the geometry representing the injection system

The mesh was then developed in Fluent Meshing, using the Watertight Geometry Workflow. A Poly-Hexcore fill was selected, along with an Aspect Ratio Offset feature in the most critical zones, in order to correctly capture the phenomena happening inside the boundary layers. The result was a mesh with around 7 million cells, an average cell orthogonal quality of 0.975 and an average cell skewness of 0.022. In Figure 3.12 is possible to visualize the mesh through a vertical cut aligned with the chamber axis.

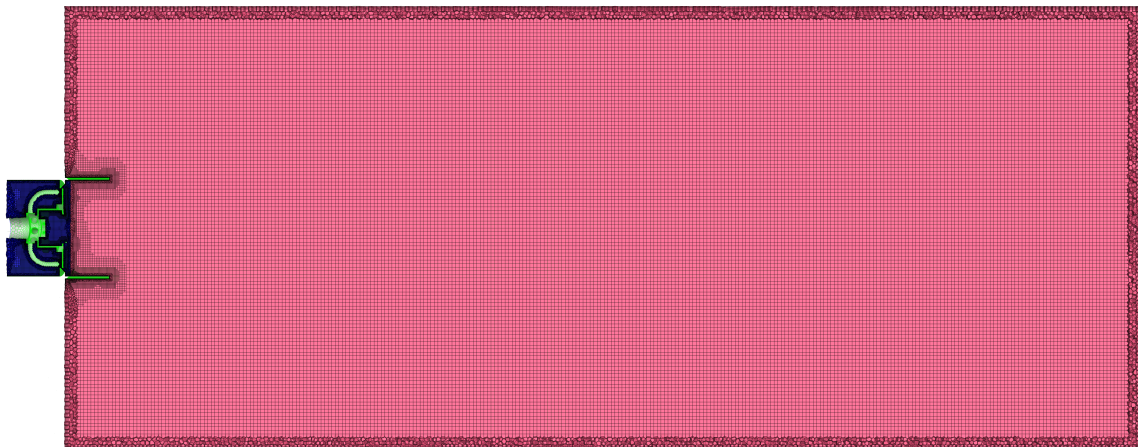


Figure 3.12: Detailed 3D simulation mesh overview

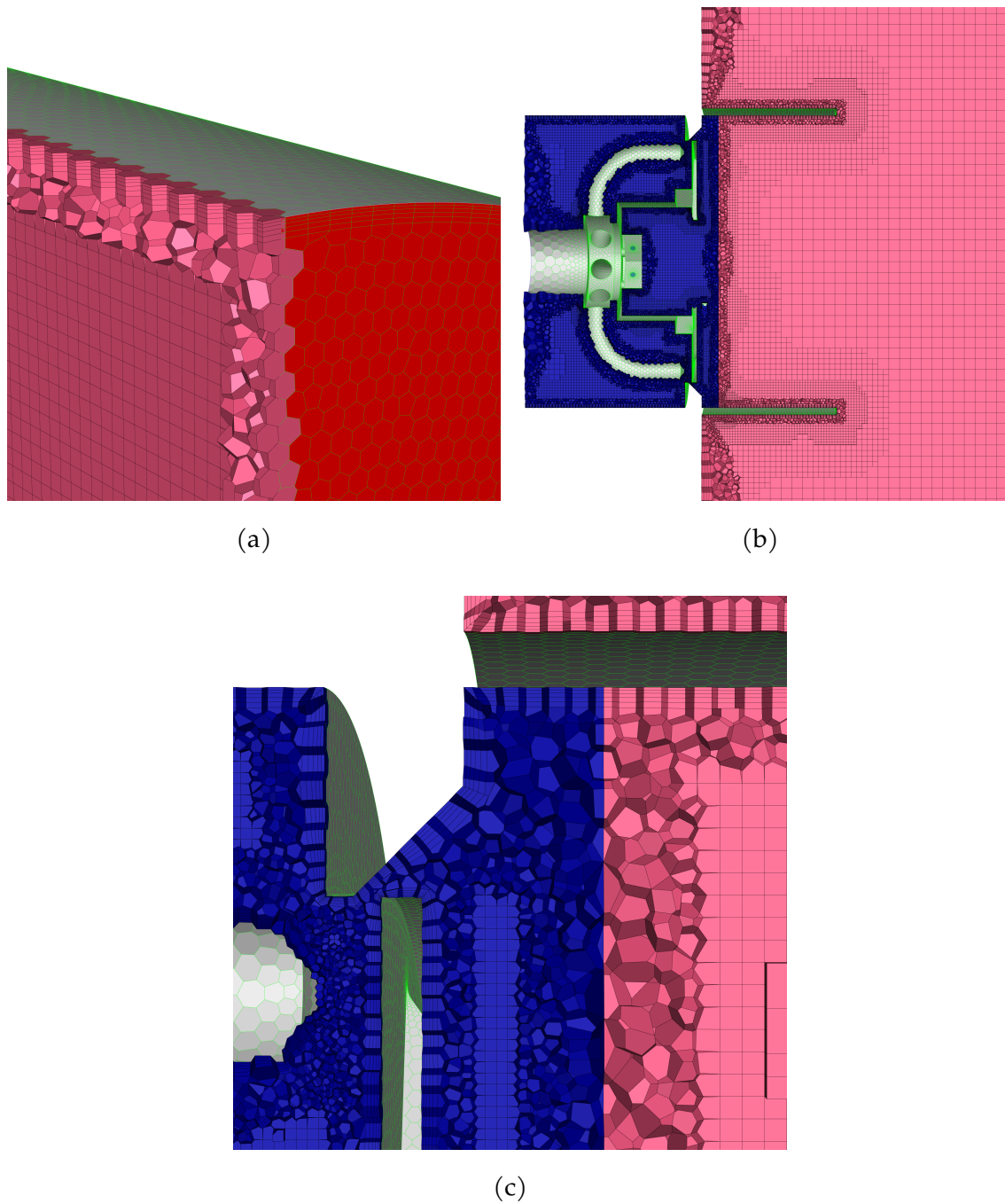


Figure 3.13: Detailed 3D simulation mesh details

In Figure 3.13 (a) is possible to observe some of the features of the Poly-Hexcore and Aspect-Ratio Offset actuating near the Outlet and Aluminum Wall boundaries, represented with red and grey colors respectively. Through Figures 3.13 (b) and (c) is also possible to understand the mesh versatility when there is the need for detail in tight spaces, such as the space between the fuel primary outlets and the turbulator, as represented in (c).

3.3 Experimental Tests Setup

As mentioned before, a system was built in order to successfully analyze the combustion of methane and hydrogen in a cylindrical combustion chamber with a RIELLO 40 FS3 burner attached. As presented in Figure 3.1, gas containers with different hydrogen and methane compositions were connected to the burner through a series of gas pipes and valves in order to safely proceed with the experimentation. The burner was surrounded with an aluminum cylindrical duct, serving as an horizontal combustion chamber, with an internal diameter of 400 mm and a wall thickness of 1 mm. In between the burner's head and the aluminum duct was placed a vermiculite ring that served as an adiabatic wall. On top of the aluminum duct, nine holes were made where eight K-type thermocouples and one Madur GA-21 plus gas analyzer probe were mounted in them, in order to measure the temperature throughout the chamber axis and evaluate the exhaust gas chemical composition. In Figure 3.3 is possible to analyze the detailed positions for better understanding. Furthermore, there is an exhaust system placed over the burner and aluminum chamber, that contributed not only for safety increase, but also for an augmented air flow speed surrounding the chamber.

In order to measure the power produced by the burner, the containers' weight was measured multiple times during the experimental procedures, with variable time intervals in between weight measurements. This permitted the recurrent calculation of the gas mass flow throughout the experimental tests and, therefore, the calculation of the power being produced by the burner. On the other hand, since the air mass flow was also a necessary variable, a series of empirical tests were made, in order to relate the burners air inlet port opening with the air mass flow going through it. After some iterations a correlation was achieved, which enabled the control of the air mass flow through the scale present in the air inlet port, which was always reassured by the usage of a digital anemometer in every iteration. With the intent to record and analyze the measurements made, the thermocouples and the Madur GA-21 plus exhaust gas analyzer were connected to a computer where the data was stored along with the exact times at which the experiments took place, promoting a smoother data analysis process.

Thermocouples are the most used devices when it comes to temperature measurements, due to their compromise between robustness, accuracy, ease of use and price. However, it is important to take into account that the temperature read by a thermocouple does not exactly represent the gas temperature, as seen in the work of Li et al. [39], it represents actually the thermocouple's bead temperature, which results from its energy balance. Therefore, a calculation tool was developed in order to calculate the gas temperature based on the thermocouple's readings. It is important to notice that, even though there exists some heat transfer through the wires, a simpler approach considering only the

bead's heat transfer was chosen. For that the following energy balance was considered,

$$\dot{Q}_{\text{in}} = \dot{Q}_{\text{out}} \quad (3.21)$$

where $\dot{Q}_{\text{in}}$ and $\dot{Q}_{\text{out}}$ represent the heat gained and lost by the bead, respectively. Considering,

$$\dot{Q}_{\text{in}} = \dot{Q}_{\text{conv}} = hA(T_{\text{gas}} - T_{\text{tc}}) \quad (3.22)$$

$$\dot{Q}_{\text{out}} = \dot{Q}_{\text{rad}} = \varepsilon\sigma A(T_{\text{tc}}^4 - T_{\text{surr}}^4) \quad (3.23)$$

the following correlation was obtained:

$$T_{\text{gas}} = T_{\text{tc}} + \frac{\varepsilon\sigma(T_{\text{tc}}^4 - T_{\text{surr}}^4)}{h} \quad (3.24)$$

where h represents the convective heat transfer coefficient, ε the emissivity of the thermocouple's bead surface, σ the Stefan-Boltzmann constant, T_{tc} the temperature measured by the thermocouple, T_{surr} the temperature of the radiative surroundings and T_{gas} the gas temperature. The thermocouple's bead emissivity value was considered to be 0.75, a normal value for a Nickel-Chromium alloy. The surrounding temperature was considered to be the average aluminum chamber temperature, obtained through the CFD simulation for the respective case in study. In order to calculate h , the convective heat transfer coefficient, the Nusselt equation for a spherical body was considered, since the bead has a spherical shape with a diameter of 1mm. The following equations were exhibited by Bergman and Lavine [37],

$$h = \frac{k \text{Nu}_D}{D} \quad (3.25)$$

$$\overline{\text{Nu}}_D = 2 + 0.6 \text{Re}_D^{1/2} \text{Pr}^{1/3} \quad (3.26)$$

$$\text{Re}_D = \frac{v D}{\nu} \quad (3.27)$$

$$\text{Pr} = \frac{\nu}{\alpha} \quad (3.28)$$

with h representing the bead's convection heat transfer coefficient, k the thermal conductivity of combustion products, Nu_D the Nusselt number, ν the combustion products' kinematic viscosity, α the combustion products' thermal diffusivity, v the combustion products' velocity and D the bead's diameter. These properties were also obtained through the CFD simulation, by creating a spherical volume with a 1cm radius surrounding the coordinates of the thermocouple's bead position and retrieving the average values for that volume. Even though collecting data through the CFD simulation in order to correct experimental values may not be the most correct approach, it was the only one possible.

Chapter 4

Experimental Tests Results

Due to limitations during the experiments it became necessary to revise the original plan. Even though the initial objective was to test the burner using a power of 11kW and 30% excess air, no such thing was possible due to instability caused by the burner when operating at low power values. Therefore, the burner's power was increased and the excess air percentage was reduced to values closer to stoichiometry, in order to achieve a more stable combustion and, consequently, enabling a more reliable data acquisition. In spite of these adversities, it was still possible to simulate the new conditions through the CFD model due to the flexibility of the numerical methodology, as seen in the next chapter.

As stated before, the data was acquired through eight thermocouples and one gas analyzer, for fuels with compositions of 100% CH₄ and 80% CH₄-20% H₂. Also, both the air and fuel mass flows were acquired through the steps exhibited in the previous chapter. This chapter is divided between temperature and species data, in order to promote a direct comparison between fuels as soon as the results are presented. Therefore it is necessary to present the burner's power and mass flow rates for each test. The following table summarizes those values.

Table 4.1: Experimental tests power and mass flow rates

Fuel	Power [kW]	Air Mass Flow [kg/s]	Fuel Mass Flow [kg/s]	Mass-Based Excess Air [%]
100% CH ₄	14.80	0.004740	0.000296	-6.423
80% CH ₄ 20% H ₂	14.81	0.004758	0.000284	-5.015

4.1 Temperature Analysis

As stated before, the eight thermocouples were placed in holes made on top of the aluminum chamber, as displayed in Figure 3.3. The values were recorded automatically in a computer in intervals of 5 seconds and average values were calculated. The results are exhibited in the following table,

Table 4.2: Average temperatures measured by the thermocouples

Fuel	Tamb [K]	T1 [K]	T2 [K]	T3 [K]	T4 [K]	T5 [K]	T6 [K]	T7 [K]	T8 [K]
100% CH ₄	307.17	990.99	811.64	656.55	640.80	634.13	620.04	593.50	506.45
80% CH ₄ 20% H ₂	304.71	921.56	886.51	686.07	641.33	635.56	626.79	607.83	525.96

where Tamb represents the ambient temperature, T1 the first thermocouple starting on the left and T8 the last, with the others following the same order. In Tables 4.3 and 4.4 are also represented the maximum and minimum temperatures, respectively, captured by the thermocouples during the test, enhancing the interpretation of each thermocouple's temperature range.

Table 4.3: Maximum temperatures measured by the thermocouples

Fuel	Tamb [K]	T1 [K]	T2 [K]	T3 [K]	T4 [K]	T5 [K]	T6 [K]	T7 [K]	T8 [K]
100% CH ₄	308.57	1044.82	879.26	686.22	667.99	655.98	641.49	611.86	543.56
80% CH ₄ 20% H ₂	305.79	985.94	924.11	719.66	663.86	657.90	645.73	634.91	548.51

Table 4.4: Minimum temperatures measured by the thermocouples

Fuel	Tamb [K]	T1 [K]	T2 [K]	T3 [K]	T4 [K]	T5 [K]	T6 [K]	T7 [K]	T8 [K]
100% CH ₄	304.56	956.39	767.05	632.73	618.46	619.63	606.78	574.11	458.30
80% CH ₄ 20% H ₂	303.35	828.68	833.30	643.32	611.20	608.63	599.38	576.49	482.86

In Figure 4.1 are displayed the average, maximum and minimum temperatures for each fuel in each thermocouple.

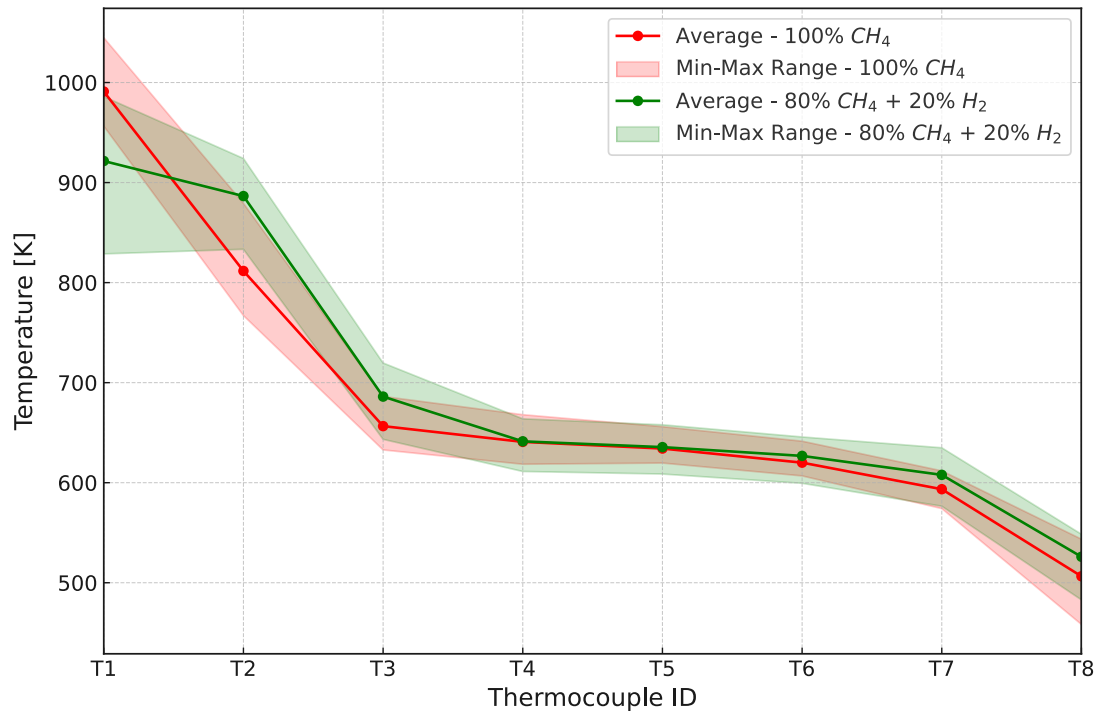


Figure 4.1: Temperatures measured by the thermocouples

It is important to notice that these values are the ones measured by the thermocouples. As explained in the previous chapter a correction is necessary in order to adapt them and estimate the experimental gas temperature. Therefore, a correction was made based on the process stated in the previous chapter. In tables 4.5, 4.6 and 4.7 are displayed the corrected average, maximum and minimum temperatures, respectively.

Table 4.5: Corrected average experimental temperatures

Fuel	T1 [K]	T2 [K]	T3 [K]	T4 [K]	T5 [K]	T6 [K]	T7 [K]	T8 [K]
100% CH ₄	1265.21	927.09	706.70	702.44	693.93	666.84	624.75	509.56
80% CH ₄ 20% H ₂	1122.97	1059.14	752.07	704.45	697.23	677.97	645.89	534.96

Table 4.6: Corrected maximum experimental temperatures

Fuel	T1 [K]	T2 [K]	T3 [K]	T4 [K]	T5 [K]	T6 [K]	T7 [K]	T8 [K]
100% CH ₄	1319.05	994.71	736.37	729.63	715.78	688.29	643.11	546.67
80% CH ₄ 20% H ₂	1187.35	1096.74	785.66	726.98	719.57	696.90	672.98	557.51

Table 4.7: Corrected minimum experimental temperatures

Fuel	T1 [K]	T2 [K]	T3 [K]	T4 [K]	T5 [K]	T6 [K]	T7 [K]	T8 [K]
100% CH ₄	1230.62	882.5	682.88	680.10	679.43	653.58	605.36	461.41
80% CH ₄ 20% H ₂	1030.09	1005.93	709.32	674.32	670.30	650.55	614.56	491.86

In Figure 4.2 are also represented the average, maximum and minimum corrected temperatures for each thermocouple.

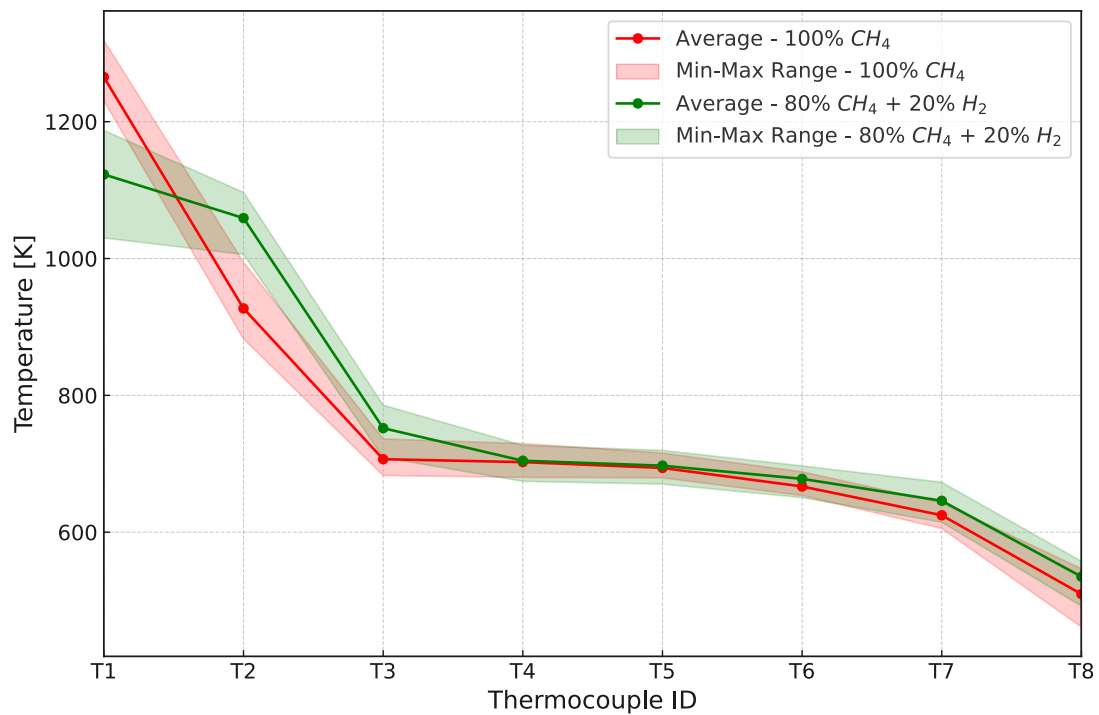


Figure 4.2: Corrected experimental temperatures

Even though at first sight the experimental results do not seem to be according to bibliography, there are some factors that explain the nature of these results. Since it is known that hydrogen enriched fuel tends to have higher adiabatic flame temperature, it was expected to see the first thermocouple with a higher temperature for the 80% CH₄ + 20% H₂ fuel. Even though that is not the case, it is important to remember that the position of the first thermocouple is nowhere near the flame core and, therefore, no conclusions can be made about the adiabatic flame temperature in this case. Also, as displayed in Table 4.1, it is clear that a higher amount of air and fuel mixture was entering the combustor during the 80% CH₄ + 20% H₂ tests, which translates into a higher mixture velocity, possibly pushing the thermal plume forward when compared with 100% CH₄ fuel tests, therefore

explaining the higher temperature for the methane-hydrogen mixture near the second thermocouple zone.

Also, it is noticeable that temperature amplitudes for each thermocouple were substantially bigger for the 80% CH₄ + 20% H₂ tests when comparing with 100% CH₄ fuel tests, specially for the first and second thermocouples. This arises from the burner's power variations when performing the tests. As explained above, the data was acquired during a certain time interval, in which the burner's power average values calculated were the ones exhibited in Table 4.1. However, the power variations during the tests were not discriminated when presenting the mean value, with fluctuations being much higher during the methane-hydrogen fuel tests. For reference, the maximum and minimum power levels considered for the data analysis of the 100% CH₄ fuel were 15.183 and 13.793 kW respectively, while for the 80% CH₄ + 20% H₂ the maximum and minimum were 15.700 and 13.495 kW, respectively. Those fluctuations were not intentional, nor operator induced, they were most likely caused by the usage of a nearly empty fuel tank during the 80% CH₄ + 20% H₂ tests and/or wear-related valve failure. In fact, variations in the calculated burner power were noticed throughout the tests, without any changes in knobs positions of the mass flow controllers and valves. There was the option to select a smaller time interval, with smaller variation in power levels, however bigger time intervals were preferred to reduce uncertainty in the scale measurements. As explained above, a scale was used to measure the fuel tank weight during the tests. With the weight variation during the test's duration, the fuel mass flux was calculated. It was given priority to a reduced uncertainty rather than to a more concise range of power levels.

4.2 Species Formation Analysis

As shown in Figure 3.3, the Madur GA-21 Plus probe was positioned between thermocouples five and six to measure the local species mole fractions. In Table 4.8 is represented the average values measured during the tests for each fuel. It is important to notice that the gas analyzer measures the chemical species in a dry basis.

Table 4.8: Average species mole fractions values measured during the experimental tests

Fuel	O ₂ [%]	CO ₂ [%]	NO _x [ppm]
100% CH ₄	16.86	3.10	17.96
80% CH ₄ 20% H ₂	16.74	3.10	18.58

CO mole fraction data was also acquired, however it was revealed to be highly unstable, presenting abnormal variations throughout the tests with relative deviations from the mean of up to 250%, ranging from 0 to 27 ppm. Therefore the readings were considered unreliable for quantitative comparison or model validation. It is important to notice that

NO_x mole fractions values also revealed modest variability throughout the tests, within typical uncertainty, contrasting with O₂ and CO₂ mole fractions which remained considerably constant. In Figure 4.3 are represented the average, maximum and minimum CO₂, O₂ and NO_x mole fractions values for the 100% CH₄ and the 80% CH₄ + 20% H₂ fuels respectively. In Table 4.9 are represented those same values for a more precise analysis.

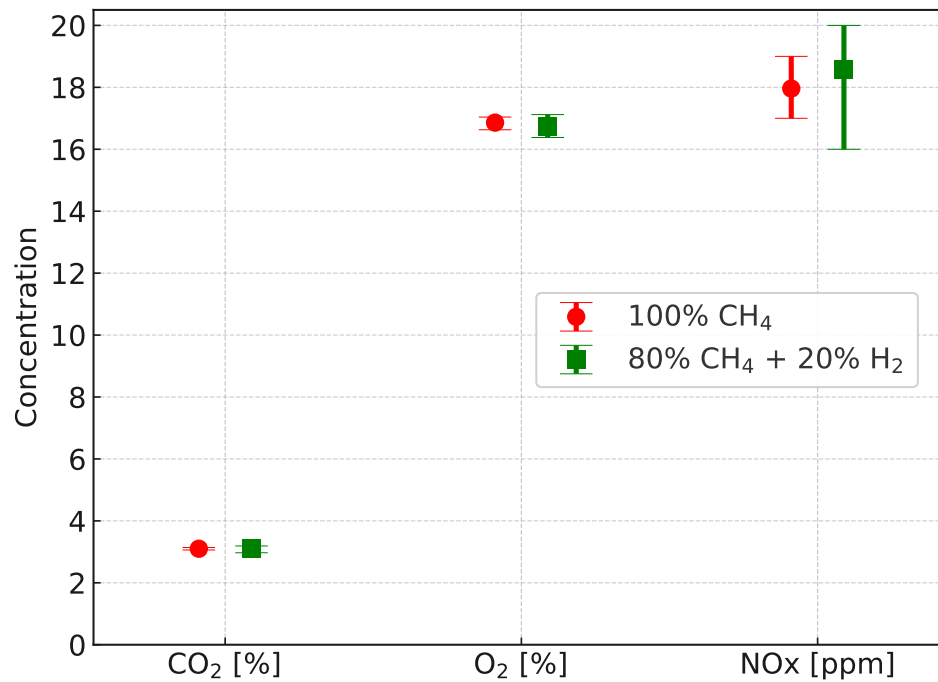


Figure 4.3: Experimental CO₂, O₂ and NO_x mole fractions values

Table 4.9: Maximum and minimum experimental species mole fractions

Fuel	Parameter	O2 [%]	CO2 [%]	NO _x [ppm]
100% CH ₄	Maximum Value	17.04	3.14	19.00
	Minimum Value	16.63	3.06	17.00
80% CH ₄ 20% H ₂	Maximum Value	17.12	3.19	20.00
	Minimum Value	16.38	2.97	16.00

As can be seen, for the 100% CH₄ fuel NO_x mole fractions ranged from 17 to 19 ppm, while for the 80% CH₄ + 20% H₂ fuel they ranged from 16 to 20 ppm. Although through an relative mean deviation analysis these are bigger variations than those of CO₂ and O₂ mole fractions, if an absolute value analysis is made, the variation of NO_x mole fractions are substantially smaller. It is important to notice that, once again, a bigger amplitude of

values was detected for the methane-hydrogen fuel, reassuring the influence of a bigger power level range. This factor may explain the similarities in between CO_2 average mole fraction levels that, according to bibliography, were supposed to be lower for the 80% $\text{CH}_4 + 20\% \text{H}_2$ fuel. When it comes to NO_x mole fractions it is noticeable a slight increase when introducing hydrogen into the fuel, which is in line with the literature, even though a bigger increase was expected.

When analyzing the O_2 mole fractions it is clear that the gas analyzer is not only measuring the combustion products, but also being influenced by outside air. Since the system was set up for a fuel rich combustion, if no outside air was entering the chamber, the O_2 mole fraction would be expected to be zero in the flame core. However, due to the end of the combustion chamber being open and in direct contact with ambient air, a backflow phenomena takes place, where outside air enters the combustion chamber due to pressure gradients caused by the extremely hot combustion products exiting the chamber. This was confirmed not only through CFD simulations, as seen in next chapter, but also experimentally, since temperature measurements made at the chamber outlet revealed really high temperatures on the top, as expected due to the low density and high temperature of combustion products, and close to ambient temperatures at the bottom, where the outside air was entering the chamber. This backflow affects not only O_2 levels but also the mole fractions of all species, which contributes for a dilution of CO_2 and NO_x , explaining the low fluctuations observed in the mole fractions of these species when introducing hydrogen into the fuel.

Chapter 5

Computational Results

This chapter is divided in three sections. The first presents the experimental CFD simulations' results, while also discussing the validation of the model. The second exhibits the results of the 11kW simulations, while the final section compares and discusses the differences and similarities between the experimental and 11kW CFD simulations. This way the results are presented in a smoother and more concise way, contributing for the overall flow of the argument.

5.1 Experimental Simulations and Model Validation

In order to validate the CFD model with the experimental results, it was necessary to recreate the operating conditions experienced during the tests and set them up in ANSYS Fluent. Therefore, some of the settings displayed in the tables presented in Chapter 3 were modified. Since the model validation was made for both 3D geometries, the simple and the detailed, in the following tables will be presented the changes made for both cases. The variables that do not appear on these tables remain as described in Chapter 3. It is important to remember that, as stated in Chapter 3, every simulation using the simple 3D geometry fully converged according to Fluent's default criteria, while the simulations considering the full injection system were terminated at around 1000 iterations or when the residuals reached stable values close to $1e-3$, which was the convergence criteria.

Table 5.1: Variables changed in the simple 3D simulations for model validation

Parameter	100% CH ₄	80% CH ₄ + 20% H ₂
Free Stream Temperature [K]	307.17	304.71
External Radiation Temperature [K]	307.17	304.71
Mix Inlet Total Temperature [K]	307.17	304.71
Mix Inlet Mass Flow Rate [kg/s]	$5.036 \cdot 10^{-3}$	$5.042 \cdot 10^{-3}$
Mix Inlet CH ₄ Mass Fraction	$5.766 \cdot 10^{-2}$	$5.381 \cdot 10^{-2}$
Mix Inlet H ₂ Mass Fraction	-	$1.691 \cdot 10^{-3}$
Mix Inlet O ₂ Mass Fraction	$2.153 \cdot 10^{-1}$	$2.167 \cdot 10^{-1}$
Mix Inlet N ₂ Mass Fraction	$7.083 \cdot 10^{-1}$	$7.128 \cdot 10^{-1}$
Mix Inlet H ₂ O Mass Fraction	$1.881 \cdot 10^{-2}$	$1.501 \cdot 10^{-2}$
Backflow Total Temperature [K]	307.17	304.71
Outlet O ₂ Mass Fraction	$2.284 \cdot 10^{-1}$	$2.294 \cdot 10^{-1}$
Outlet N ₂ Mass Fraction	$7.516 \cdot 10^{-1}$	$7.547 \cdot 10^{-1}$
Outlet H ₂ O Mass Fraction	$1.996 \cdot 10^{-2}$	$1.589 \cdot 10^{-2}$

Table 5.2: Variables changed in the detailed 3D simulations for model validation

Parameter	100% CH ₄	80% CH ₄ + 20% H ₂
Free Stream Temperature [K]	307.17	304.71
External Radiation Temperature [K]	307.17	304.71
Primary/Secondary Fuel Inlet Total Temperature [K]	307.17	304.71
Primary Fuel Mass Flow Rate [kg/s]	$3.095 \cdot 10^{-5}$	$2.971 \cdot 10^{-5}$
Secondary Fuel Mass Flow Rate [kg/s]	$8.063 \cdot 10^{-6}$	$7.738 \cdot 10^{-6}$
Air Relative Humidity	0.60	0.55
Air Inlet Total Temperature [K]	307.17	304.71
Air Inlet Mass Flow Rate [kg/s]	$4.740 \cdot 10^{-3}$	$4.758 \cdot 10^{-3}$
Air Inlet O ₂ Mass Fraction	$2.284 \cdot 10^{-1}$	$2.294 \cdot 10^{-1}$
Air Inlet N ₂ Mass Fraction	$7.516 \cdot 10^{-1}$	$7.547 \cdot 10^{-1}$
Air Inlet H ₂ O Mass Fraction	$1.996 \cdot 10^{-2}$	$1.589 \cdot 10^{-2}$
Backflow Total Temperature [K]	307.17	304.71
Outlet O ₂ Mass Fraction	$2.284 \cdot 10^{-1}$	$2.294 \cdot 10^{-1}$
Outlet N ₂ Mass Fraction	$7.516 \cdot 10^{-1}$	$7.547 \cdot 10^{-1}$
Outlet H ₂ O Mass Fraction	$1.996 \cdot 10^{-2}$	$1.589 \cdot 10^{-2}$

The data analysis was made through ANSYS CFD-Post, where sphere volumes, with a radius of 1 cm, were created. The spheres' centers were aligned with the thermocouples' bead and the gas analyzer probe positions, so that the extracted values could better represent the experimental measurements. This process made it possible to account for measurement errors, such as thermocouple/probe displacement, caused by flow velocity,

instabilities or small uncertainties in the positioning during the tests. Furthermore, averaging the temperature field and species mole fractions over a finite volume, rather than a single point, can help reduce mesh discretization errors.

This section will be further divided into two subsections, one approaching temperatures results and the other analyzing species formation, since these are the two different results used to validate the model.

5.1.1 Temperature Analysis

The average temperature values calculated for each sphere are represented in Tables 5.3 and 5.4, for the simple 3D and detailed 3D simulations respectively.

Table 5.3: Average temperature values calculated for the experimental simple 3D simulation

Fuel	T1 [K]	T2 [K]	T3 [K]	T4 [K]	T5 [K]	T6 [K]	T7 [K]	T8 [K]
100% CH ₄	1918.94	1084.73	506.771	572.533	624.338	663.576	677.556	541.435
80% CH ₄ 20% H ₂	1940.18	1057.24	506.516	572.238	623.572	662.645	676.161	532.722

Table 5.4: Average temperature values calculated for the experimental detailed 3D simulation

Fuel	T1 [K]	T2 [K]	T3 [K]	T4 [K]	T5 [K]	T6 [K]	T7 [K]	T8 [K]
100% CH ₄	1723.32	1256.99	629.319	643.721	687.208	715.103	718.662	609.531
80% CH ₄ 20% H ₂	1750.72	1245.83	622.061	641.549	686.444	714.883	717.868	605.154

For a better visual comparison, in Figures 5.1 and 5.2 are presented comparisons between the temperature profiles obtained in the experimental tests and both CFD simulations.

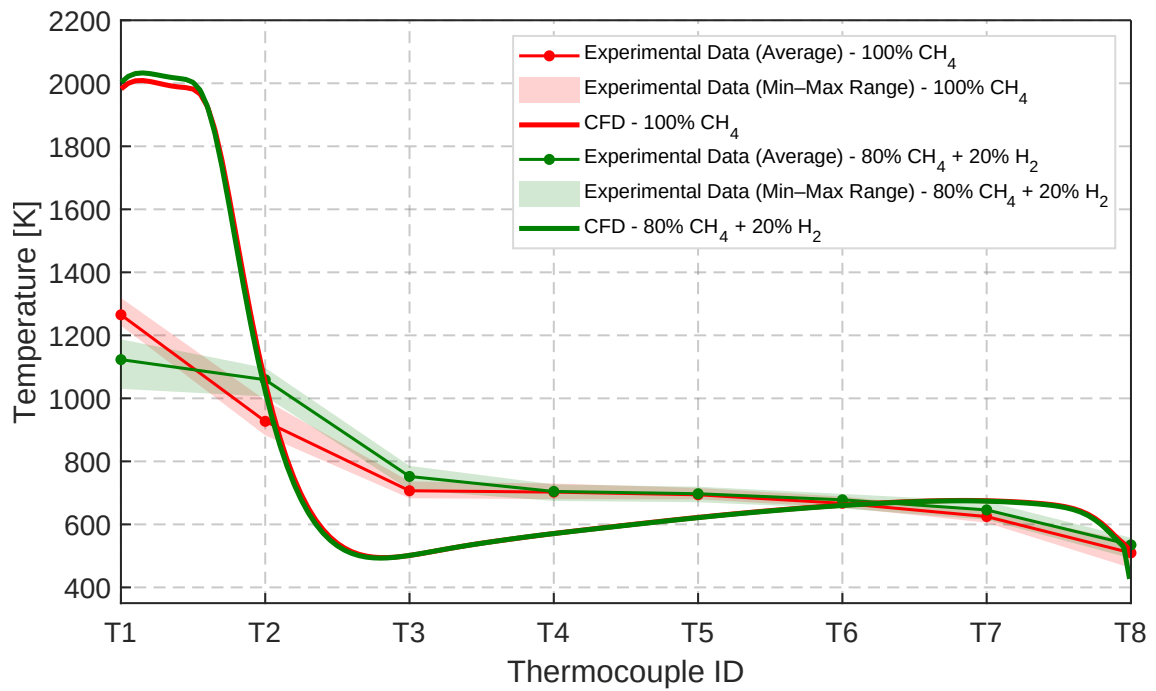


Figure 5.1: Comparison between the temperature profiles of the experimental tests and the simple 3D simulation

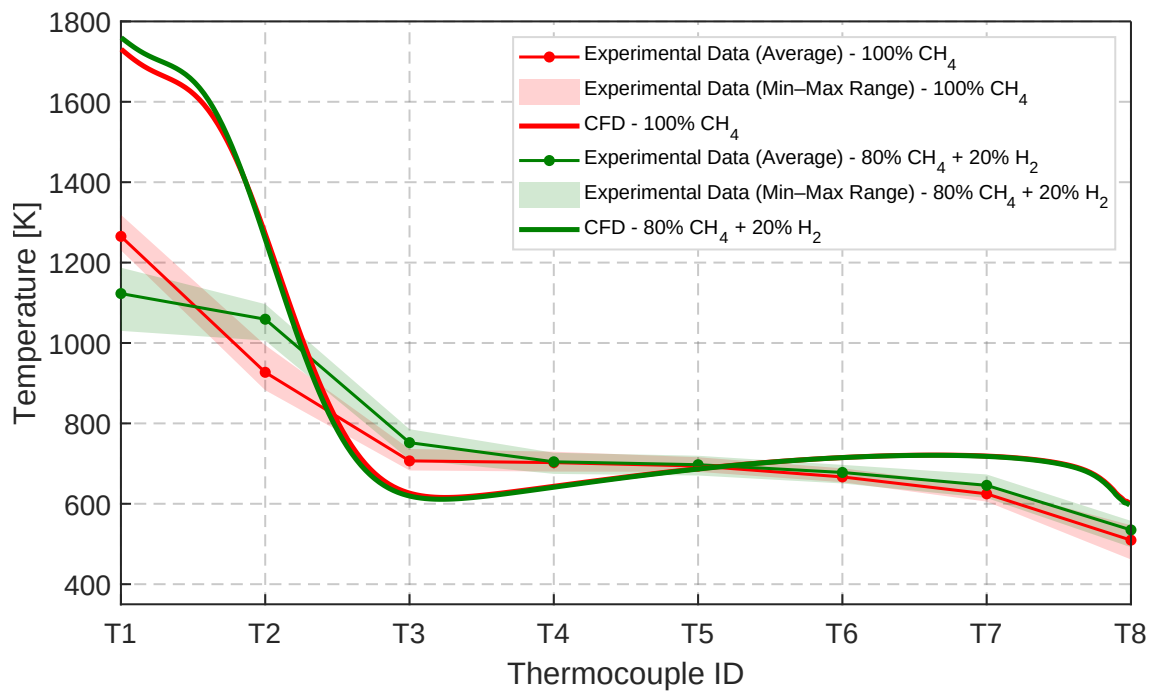


Figure 5.2: Comparison between the temperature profiles of the experimental tests and the detailed 3D simulation

As can be seen, both CFD simulations over predicted temperature levels in the first two thermocouples, which was to be expected due to the high temperature gradients caused

by the flame presence near them, which become extremely difficult for the CFD to replicate. However, as the distance from the flame increases the model's predictive accuracy improves, with CFD temperature profiles assuming a very similar shape to that of the experimental tests one.

In order to better understand the differences between the temperatures obtained in the CFD models and the experimental tests, an relative error analysis is presented in Tables 5.5 and 5.6, for both models. It is important to note that errors were calculated not only for average experimental temperatures, but also for the respective maximum and minimum values. In order to calculate these errors, the following equation was used,

$$\text{Relative Error [\%]} = \frac{T_{\text{CFD}} - T_{\text{EXP}}}{T_{\text{EXP}}} \times 100 \quad (5.1)$$

where T_{CFD} represents the temperature obtained through the simulation and T_{EXP} the temperature obtained through the experimental test.

Table 5.5: Errors between the temperatures obtained through the simple 3D simulation and the experimental tests

Fuel	Type of Experimental Measure	T1	T2	T3	T4	T5	T6	T7	T8
100% CH ₄	Average Temperature	+53.29%	+17.13%	-29.68%	-19.79%	-11.06%	-1.34%	+7.89%	+5.58%
	Maximum Temperature	+46.97%	+9.16%	-32.46%	-22.74%	-13.74%	-4.38%	+4.83%	-1.55%
	Minimum Temperature	+57.65%	+23.06%	-27.28%	-17.20%	-9.18%	+0.65%	+11.33%	+16.52%
80% CH ₄ 20% H ₂	Average Temperature	+74.41%	+0.04%	-34.18%	-19.80%	-11.53%	-3.12%	+4.16%	-1.14%
	Maximum Temperature	+64.87%	-3.39%	-36.93%	-22.26%	-14.25%	-5.73%	-0.02%	-5.11%
	Minimum Temperature	+90.30%	+5.35%	-30.31%	-16.26%	-8.02%	+0.93%	+9.44%	+7.46%

Table 5.6: Errors between the temperatures obtained through the detailed 3D simulation and the experimental tests

Fuel	Type of Experimental Measure	T1	T2	T3	T4	T5	T6	T7	T8
100% CH ₄	Average Temperature	+36.21%	+35.58%	-10.95%	-8.36%	-0.97%	+7.24%	+15.03%	+19.62%
	Maximum Temperature	+30.65%	+26.37%	-14.54%	-11.77%	-3.99%	+3.90%	+11.75%	+11.50%
	Minimum Temperature	+40.04%	+42.43%	-7.84%	-5.35%	+1.15%	+9.41%	+18.72%	+32.10%
80% CH ₄ 20% H ₂	Average Temperature	+55.90%	+17.63%	-17.29%	-8.93%	-1.55%	+5.45%	+11.14%	+13.12%
	Maximum Temperature	+47.45%	+13.59%	-20.82%	-11.75%	-4.60%	+2.58%	+6.67%	+8.55%
	Minimum Temperature	+69.96%	+23.85%	-12.30%	-4.86%	+2.41%	+9.89%	+16.81%	+23.03%

In order to further synthesize the temperature errors, and Root Mean Square Error (RMSE) was calculated for each measurement type. RMSE is a statistical metric that

quantifies the overall deviation between simulated and experimental values and can be calculated through the following equation,

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (x_i)^2} \cdot 100 \quad (5.2)$$

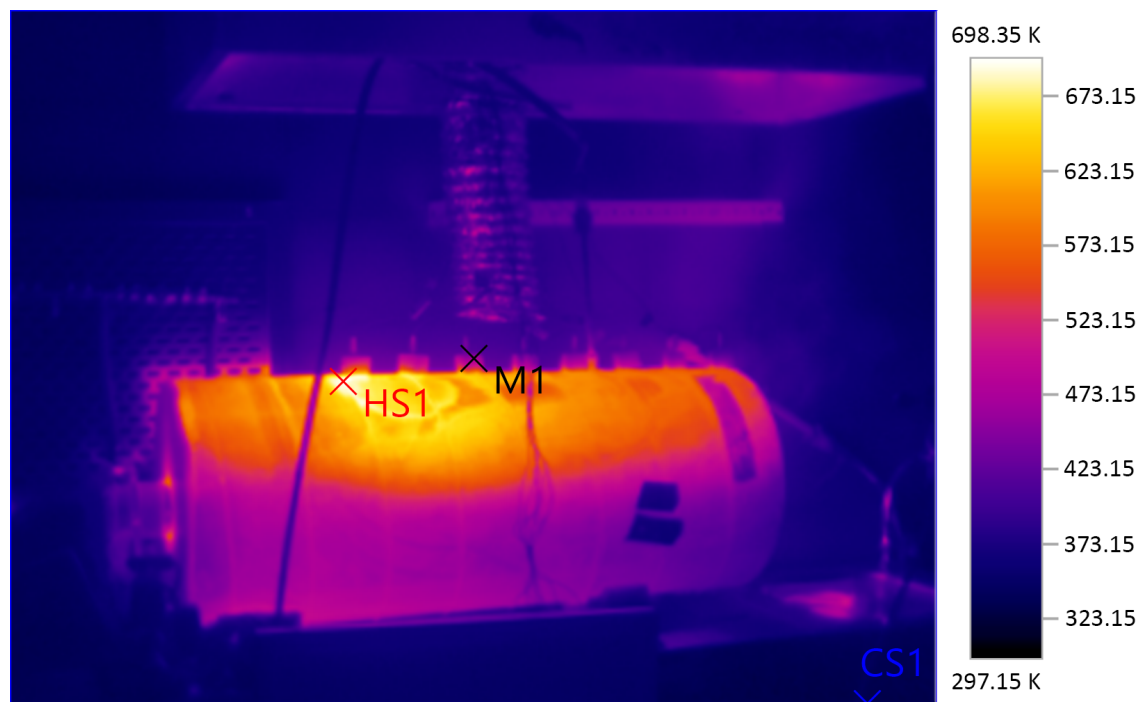
where n is the total number of thermocouples and x_i the error obtained in the previous tables in decimal form. In Table 5.7 are presented the RMSE values obtained for each geometry and fuel.

Table 5.7: RMSE values between experimental tests and both 3D simulations

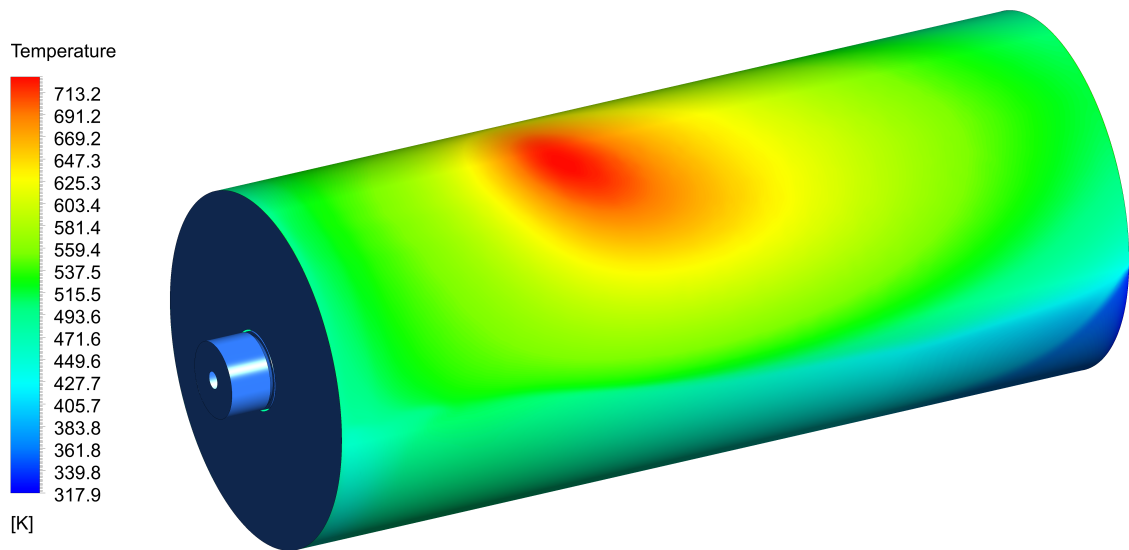
Fuel	Type of Experimental Measure	Simple 3D Simulation RMSE	Detailed 3D Simulation RMSE
100% CH ₄	Average Temperature	24.04%	20.71%
	Maximum Temperature	22.62%	16.90%
	Minimum Temperature	25.94%	24.91%
80% CH ₄ 20% H ₂	Average Temperature	30.12%	22.76%
	Maximum Temperature	28.15%	19.85%
	Minimum Temperature	34.60%	28.62%

As expected the detailed 3D simulation was superior in every situation, due to its increased complexity, geometry detail and mesh refinement. It was also able to go under the 20% RMSE threshold for the maximum temperature values for each fuel. It is important to note that, in the simple 3D simulation, the CFD temperature values were also closer to the experimental maximum values. Both simulations revealed increased difficulties when dealing with the methane-hydrogen fuel, probably due to the added complexity brought by having two different species as a fuel and also due to the larger variations observed in the experimental testing of this fuel. However, the detailed 3D simulation reacted better to the addition of hydrogen, since its RMSE values increased a lot less than the simple 3D values.

On another note, there are also some temperature related visual representations important to validate the CFD model. During the experimental tests, certain phenomena were captured in pictures that were also observed in the simple 3D and detailed 3D simulations. In Figure 5.3 (a) is represented a thermography taken to the combustion chamber during the experimental tests, courtesy of INEGI, while in (b) is a contour taken in ANSYS representing the temperature of the combustion chamber.



(a)



(b)

Figure 5.3: Comparison between experimental and CFD combustion chamber temperature profiles

As can be observed, the temperature profile between both cases is extremely similar. When analyzing the thermography, a maximum temperature of 698.35K is revealed, differing only 29.92K from the maximum temperature obtained in the CFD models, 728.27K, representing an error of only 4.28%, therefore contributing for the CFD model validation.

This phenomena can be observed in both simple 3D and detailed 3D simulations.

Also, in Figure 5.4 (a) is shown a picture, provided by INEGI, taken to the burner's head during the experimental tests, through the chamber's open outlet. In this picture can be observed small blue flames near the burner's head wall. These blue flames represent fuel rich zones that agglomerate due to the position of the primary fuel injectors, combined with the turbulator and injection system geometries. In (b) is possible to observe the same effect happening in the detailed 3D simulation, with the agglomerations taking almost the same positions represented in (a). This phenomena was not possible to observe in the simple 3D simulations, since the geometry used did not contemplate neither the turbulator nor the injection system.

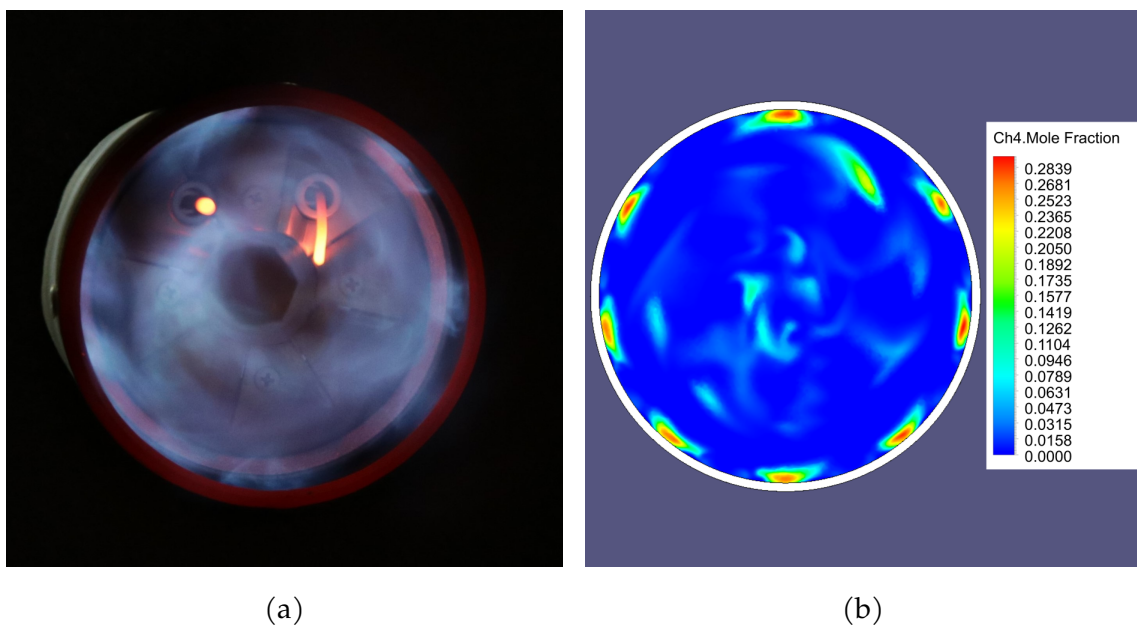


Figure 5.4: Comparison between experimental and CFD CH₄ agglomerations

In addition, in Figure 5.5 (a) and (b) is represented a temperature profile of a vertical plane passing through the combustion chamber axis, in the detailed 3D simulation, for the 100% CH₄ and 80% CH₄ + 20% H₂ fuel, respectively. In this figures are also presented the sphere volumes used in representation of the thermocouples and the gas analyzer probe.

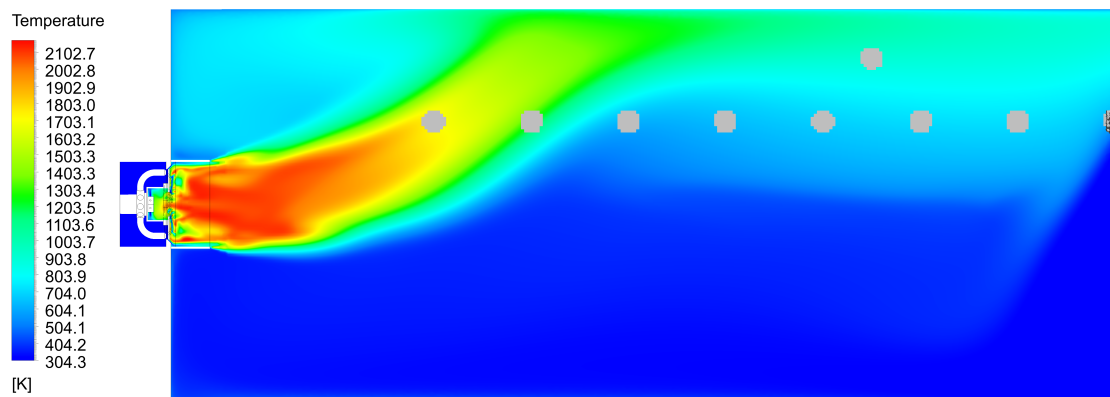
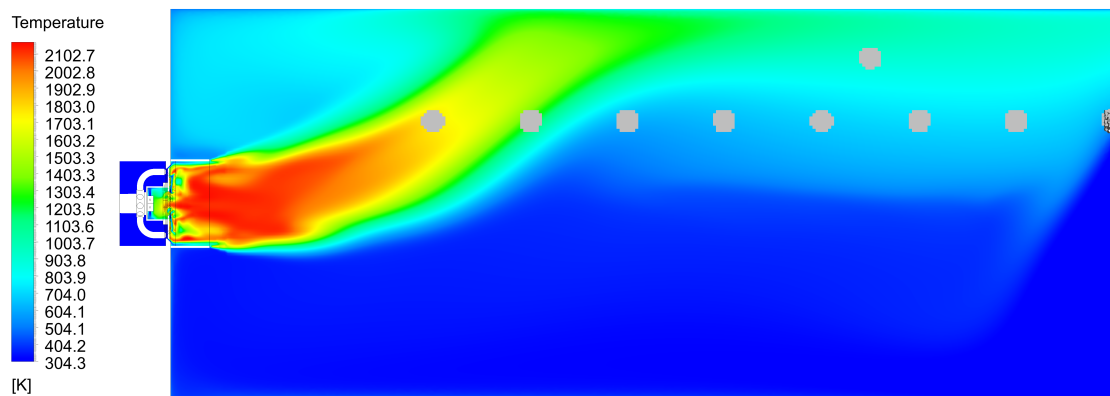
(a) 100% CH₄ fuel(b) 80% CH₄ + 20% H₂ fuel

Figure 5.5: Comparison between the experimental detailed 3D simulation vertical axial plane's temperature profiles for the 100% CH₄ and 80% CH₄ + 20% H₂ fuels

As can be seen in this figures, the first two thermocouples are, in fact and as stated above, under influence of aggressive thermal gradients due to flame proximity. Also, it is possible to verify that the thermal plume advances slightly further for the methane-hydrogen fuel. On the other end of the combustion chamber, is possible to detect the backflow effect, with cooler air entering through the bottom of the outlet and the hotter air exiting through the top. Therefore, it is possible to conclude that most of the temperature related phenomena observed in the experimental tests is also observed in the detailed 3D simulation. As for the simple 3D simulations there is a slightly indication of advancement in the thermal plume movement, however its effect is not as prominent as in the detailed 3D simulations.

5.1.2 Species Formation Analysis

As done in the temperature analysis, CFD Post was used to create a sphere volume, representing the gas analyzer probe, in order to capture the properties to be studied. Therefore,

average mole fractions of O₂, CO₂, NO_x and H₂O were calculated and are exhibited in Tables 5.8 and 5.9, for both the simple 3D and detailed 3D simulations respectively.

Table 5.8: Simple 3D simulation experimental species mole fractions on a wet-basis

Fuel	O ₂ [%]	CO ₂ [%]	H ₂ O [%]	NO _x [ppm]
100% CH ₄	12.97	3.35	9.75	46.72
80% CH ₄ 20% H ₂	13.15	3.11	9.43	43.65

Table 5.9: Detailed 3D simulation experimental species mole fractions on a wet-basis

Fuel	O ₂ [%]	CO ₂ [%]	H ₂ O [%]	NO _x [ppm]
100% CH ₄	13.28	3.21	9.47	14.62
80% CH ₄ 20% H ₂	13.47	2.97	9.13	16.43

Since the mole fractions shown above are expressed on a wet basis, they must be converted to a dry basis in order to allow a proper comparison with the experimental results, as the gas analyzer also reports mole fractions on a dry basis. The formulation to do so is as follows,

$$Y_i^{\text{dry}} = \frac{Y_i^{\text{wet}}}{1 - Y_{\text{H}_2\text{O}}^{\text{wet}}} \quad (5.3)$$

where Y_i^{wet} is the molar fraction of the species i in a wet basis, $Y_{\text{H}_2\text{O}}^{\text{wet}}$ is the molar fraction of the water in a wet basis and Y_i^{dry} represents the mole fraction of the species i in a dry basis. In Tables 5.10 and 5.11 are represented the O₂, CO₂ and NO_x mole fractions in a dry basis, for both the simple 3D and detailed 3D simulations respectively.

Table 5.10: Simple 3D simulation experimental species mole fractions on a dry-basis

Fuel	O ₂ [%]	CO ₂ [%]	NO _x [ppm]
100% CH ₄	14.37	3.71	51.77
80% CH ₄ 20% H ₂	14.32	3.44	48.20

Table 5.11: Detailed 3D simulation experimental species mole fractions on a dry-basis

Fuel	O ₂ [%]	CO ₂ [%]	NO _x [ppm]
100% CH ₄	14.67	3.54	16.15
80% CH ₄ 20% H ₂	14.82	3.27	18.08

For a better visual analysis, in Figures 5.6 and 5.7 are represented comparisons between the species mole fractions obtained in the experimental tests and both CFD simulations.

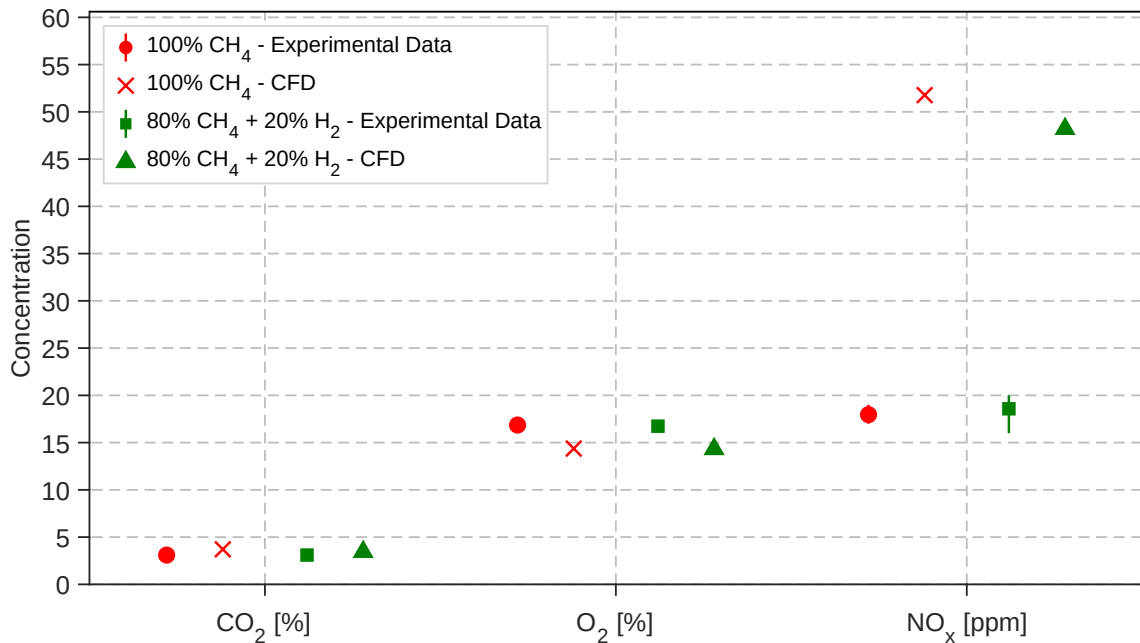


Figure 5.6: Comparison between the species mole fractions obtained in the experimental tests and the simple 3D simulation

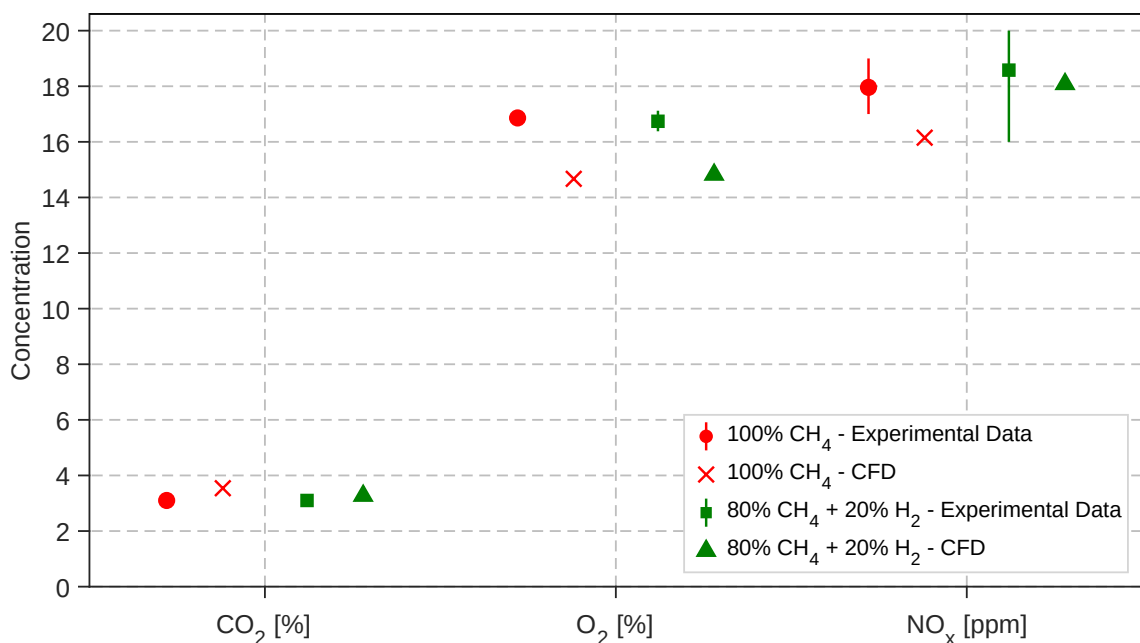


Figure 5.7: Comparison between the species mole fractions obtained in the experimental tests and the detailed 3D simulation

As seen through the tables and figures above, the simple 3D simulation predicted good

values for the O₂ and CO₂ mole fractions, however completely over predicted NO_x mole fractions. On the other hand, the detailed 3D simulation had better results predicting all three mole fractions. For a clearer understanding of the differences between the mole fractions predicted by the CFD models and those measured experimentally an relative error analysis is presented in Tables 5.12 and 5.13, for the simple 3D and detailed 3D simulations, respectively. In order to calculate these errors, the following equation was used,

$$\text{Relative Error [\%]} = \frac{Y_{\text{CFD}} - Y_{\text{EXP}}}{Y_{\text{EXP}}} \times 100 \quad (5.4)$$

where Y_{CFD} represents the mole fraction obtained in the simulation and Y_{EXP} the mole fraction obtained in the experimental tests.

Table 5.12: Errors between the mole fractions obtained through the simple 3D simulation and the experimental tests

Fuel	O ₂	CO ₂	NO _x
100% CH ₄	-14.78%	+19.95%	+188.26%
80% CH ₄ 20% H ₂	-14.44%	+10.87%	+159.36%

Table 5.13: Errors between the mole fractions obtained through the detailed 3D simulation and the experimental tests

Fuel	O ₂	CO ₂	NO _x
100% CH ₄	-12.98%	+14.37%	-10.09%
80% CH ₄ 20% H ₂	-11.45%	+5.57%	-2.70%

As described by these tables, both the simple 3D and the detailed 3D simulations had smaller errors when calculating mole fractions for the methane-hydrogen fuel. However, the simple 3D simulation proved to be completely unreliable for predicting NO_x mole fractions, with errors almost as big as 200%. It is also important to note that, in the detailed 3D simulation, every error was able to go under the 15% error threshold.

Another important aspect to consider is the percentage variation in the mole fractions of the chemical species when hydrogen is introduced into the fuel. In order to calculate the variations the following equation was used,

$$\text{Mole Fraction Variation [\%]} = \frac{Y_{80\%CH_4+20\%H_2} - Y_{100\%CH_4}}{Y_{100\%CH_4}} \cdot 100 \quad (5.5)$$

where $Y_{80\%CH_4+20\%H_2}$ represents the species mole fraction for the methane-hydrogen fuel and $Y_{100\%CH_4}$ represents the species mole fraction for the 100% CH₄ fuel. The results are presented in Table 5.14.

Table 5.14: Experimental species mole fractions variation when introducing hydrogen into the fuel

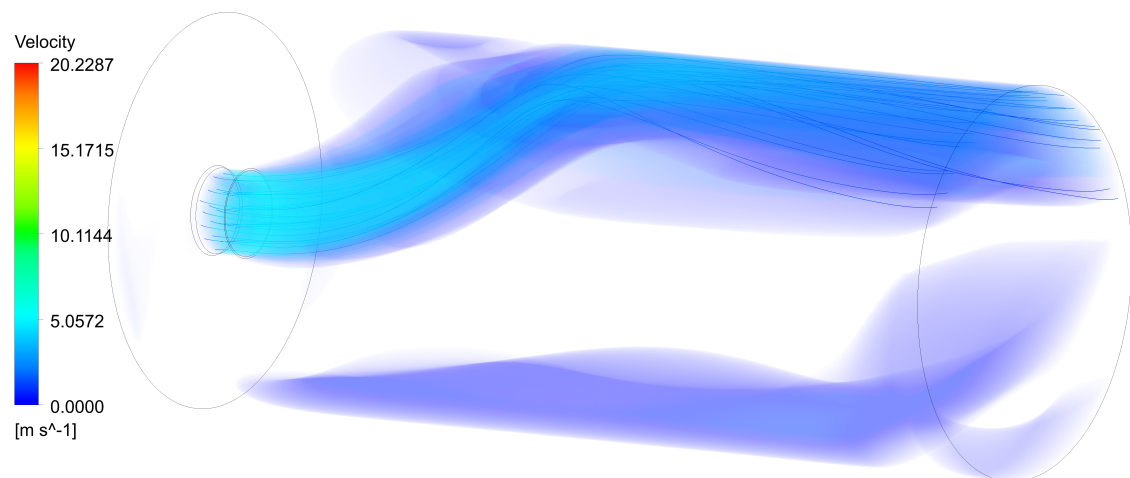
Source	O ₂	CO ₂	NO _x
Experimental Average Values	-0.746%	+0.132%	+3.467%
Simple 3D Simulation Values	-0.351%	-7.444%	-6.910%
Detailed 3D Simulation Values	+1.004%	-7.576%	+11.970%

As the values presented in the table suggest, the simple 3D simulation had slightly better results for the variations of O₂ and CO₂ mole fractions, even though the detailed 3D simulation also presented good results. The NO_x variation was badly predicted by the simple 3D simulation, as expected, however the values presented by the detailed 3D simulation were satisfying.

It is important to notice that the CO mole fraction was also analyzed, but the model presented residual values for it, which goes into the encounter of the instability found when measuring it experimentally and, therefore, was not considered in this model validation.

Velocity Maps

In order to further analyze the the fluid flow differences between both 3D simulations, due to the presence of the injection system, in Figures 5.8 (a) and (b) are represented the 100% CH₄ 3D velocity renders and velocity streamlines for the simple 3D and detailed 3D simulations, respectively.



(a) Simple 3D simulation

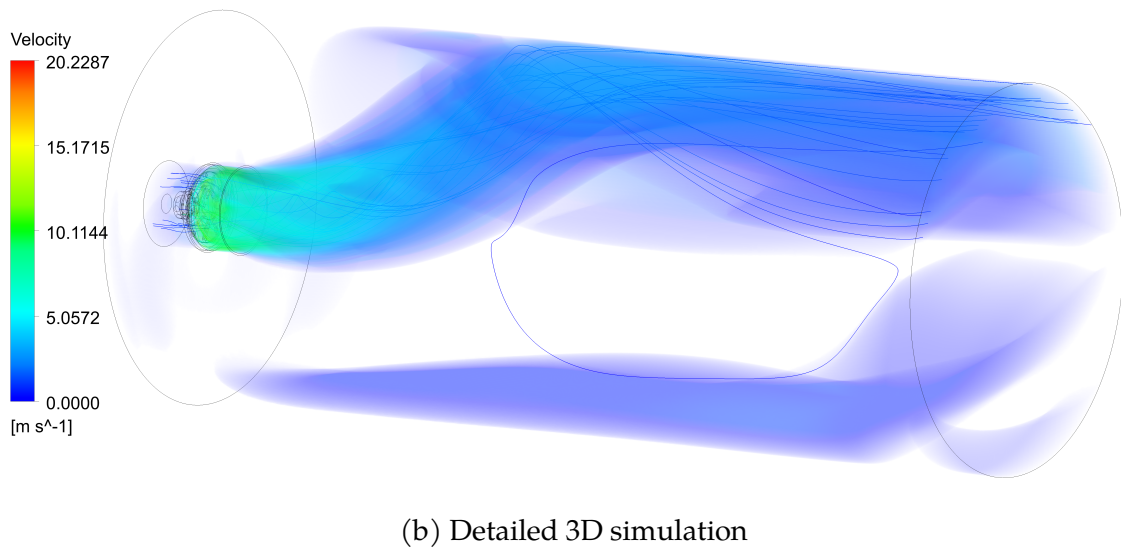


Figure 5.8: 3D velocity render for both 3D geometries and 100% CH₄ fuel

As can be seen in the figures, while the simple 3D simulations have a smooth velocity gradient throughout the whole flow, the detailed 3D simulation have a larger field, as well as higher velocities near the injector's exit, contributing for bigger velocity gradients near the flame core. Also, it is noticeable a bigger velocity field near the chamber's outlet for the detailed 3D simulation, revealing a considerable influence on the backflow's intensity.

5.2 Simulations At 11kW

As in the previous section, this section is divided into two subsections, one dedicated to the analysis of temperature and the other to the analysis of species formation, in order to provide a clearer understanding of the results. Also, in both analysis, a comparison between the 2D and both 3D geometries will be carried out, in order to understand the model's differences and to determine if simplified simulations are justified. The simulations in this chapter were carried out for the conditions and models exhibited in Chapter 3, with the most relevant operational parameters being a burner's power of 11kW, an excess air ratio of 30%, an ambient temperature of 25°C, or 298.15K, and a relative humidity of 70%.

5.2.1 Temperature Analysis

Before comparing the results, it is important to note that the results for the 100% methane fuel may differ slightly from those reported in the mesh independence tests performed

for the simple 3D and detailed 3D simulations. This is because, during the mesh independence tests, the model was not yet fully optimized, and several adjustments were introduced between the tests and the final version. In particular, the mesh independence tests employed a less refined Discrete Ordinates scheme, with a slightly reduced number of Divisions and Pixels. Also the Outlet Boundary Condition Radiation Type was set to opaque rather than transparent. Despite these changes, the mesh independence test remained valid, since conditions during the tests were the same for every mesh. Also, repeating the mesh independence tests would have high computational costs and would delay the overall work. It is important to emphasize that the settings listed in the tables of Chapter 3, defining the models and boundary conditions selected, are the refined and final version ones.

The temperature analysis will assess various measurements types, approaching both fuels and the three geometries, enabling a clear identification of the main similarities and differences observed across the simulations. Initially focusing on one of the most assessed temperature measurements in recent studies, this analysis will start by evaluating the adiabatic flame temperature obtained in each simulation. The values were obtained by calculating the maximum temperature in the combustion chamber, using CFD-Post. The results are presented in Table 5.15.

Table 5.15: Adiabatic flame temperature for the 11 kW simulations

Fuel	Detailed 3D Simulation [K]	Simple 3D Simulation [K]	2D Simulation [K]
100% CH ₄	2148.94	1872.28	1865.34
80% CH ₄ 20% H ₂	2184.74	1887.39	1881.70

As can be seen by the values presented in the table, the adiabatic flame temperature increased with the introduction of hydrogen into the fuel, as expected and as according to literature. Also, it is notorious that the 2D and simple 3D simulations' values were extremely similar, with the 2D simulation underestimating the simple 3D temperatures by around 6K, for both fuels. However, when comparing with the more-refined detailed 3D simulation, both these simulations underestimate the adiabatic flame temperature by, almost, 300K. When calculating the relative errors between the simpler simulations and the detailed 3D simulation, the error values fluctuate between 12.87% and 13.87%. This happens since in the simplified simulations the mixture is considered homogeneous, while, in the detailed 3D simulations, the influence of the injection system causes the formation of zones of fuel-rich and fuel-lean mixtures. The increase in adiabatic flame temperature happens due to the presence of locally stoichiometric zones, induced by the injection system, although the global operating conditions consider a 30% excess air ratio.

The average temperature in the combustion chamber was also calculated, since it is

another property whose behavior is influenced by the addition of hydrogen to the fuel. In the Table 5.16 are presented the results for the average temperature in the combustion chamber in each simulation.

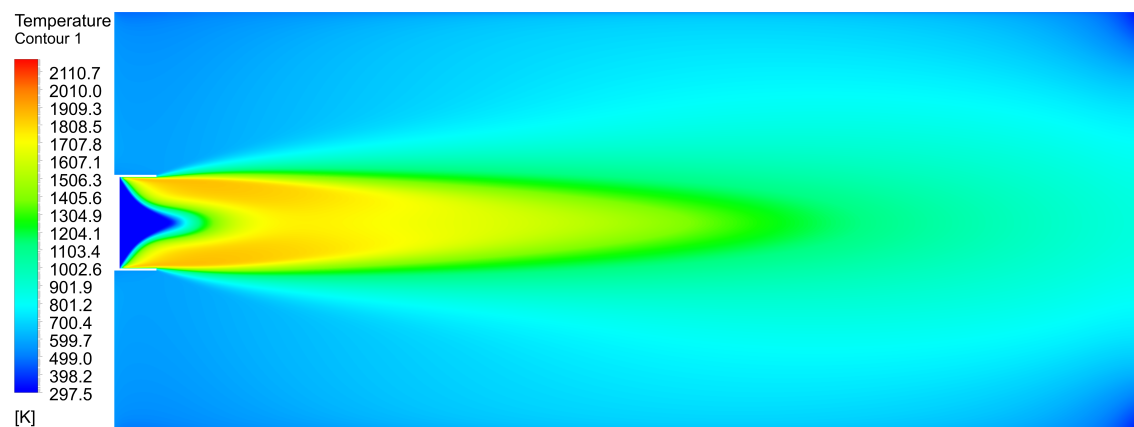
Table 5.16: Average temperature in the combustion chamber for the 11 kW simulations

Fuel	Detailed 3D Simulation [K]	Simple 3D Simulation [K]	2D Simulation [K]
100% CH ₄	508.87	470.56	732.27
80% CH ₄ 20% H ₂	510.32	472.35	756.32

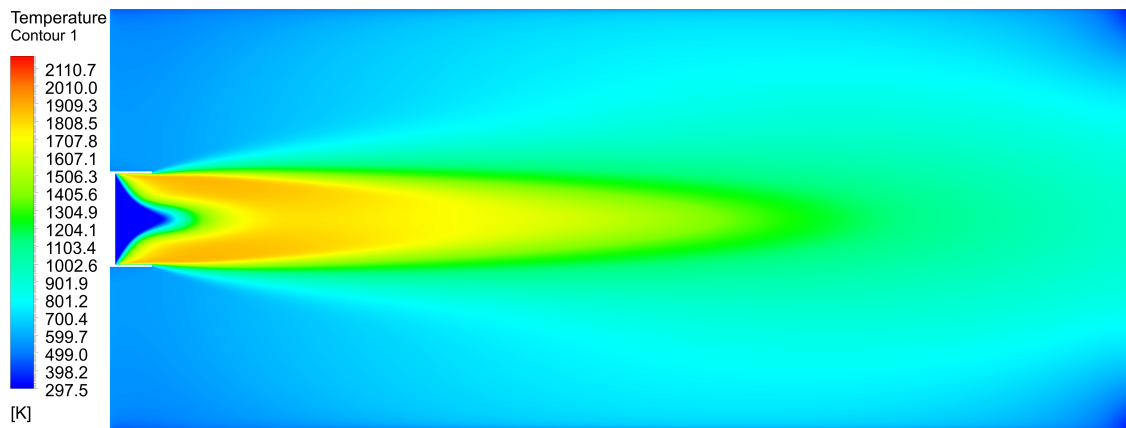
When analyzing the values in the table, it is noticeable that the 2D simulation presented unacceptably high values, with differences relatively to the detailed 3D simulation as high as 246K, representing a relative error of 48.21%. This factor can be explained by the unrealistic temperature field throughout the chamber presented by the 2D simulations, which will be further analyzed later in this chapter. On the other hand, the simple 3D simulations presented reasonable values, with differences below 40K and relative errors under 10%.

It is also important to note that the difference in the combustion chamber's average temperature between the two fuels decreased with the increase in mesh refinement, with the difference in the detailed 3D simulation being 1.45K, corresponding to less than 1% of the total temperature. According to literature, such as the works of Wang et al. [40], the average temperature in the combustion chamber does not increase significantly with the addition of hydrogen into the fuel, in contrast to the adiabatic flame temperature, which is in line with the temperatures displayed in Tables 5.15 and 5.16.

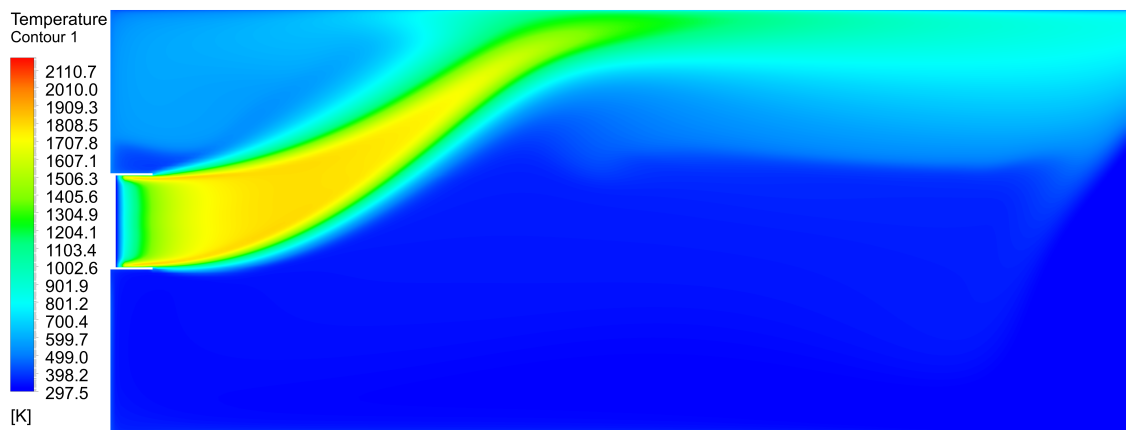
In order to visually represent the temperature fields throughout the chamber, for each geometry and fuel, in Figure 5.9 (a) to (f) are illustrated the temperature distributions in the vertical plane crossing the chamber's axis.



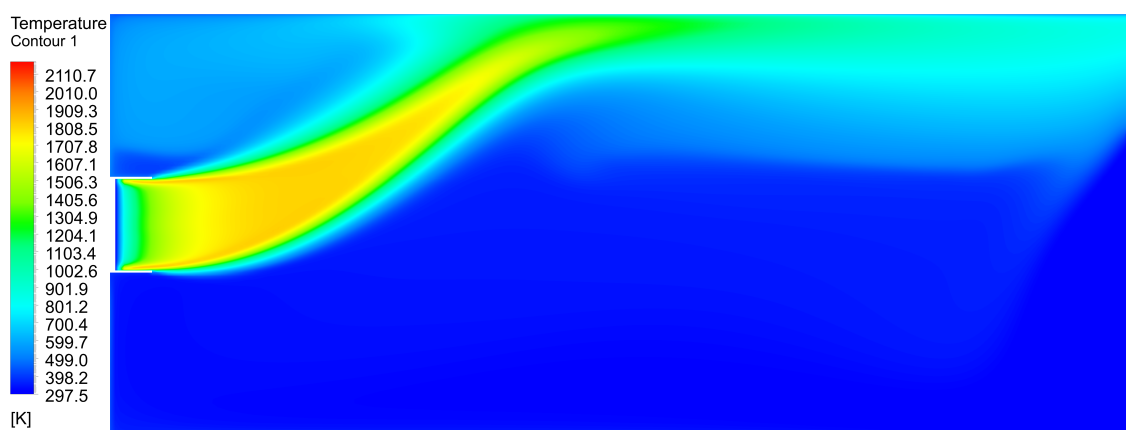
(a) 2D simulation of 100% CH₄ fuel at 11 kW



(b) 2D simulation of 80% CH₄ + 20% H₂ fuel at 11 kW



(c) Simple 3D simulation of 100% CH₄ fuel at 11 kW



(d) Simple 3D simulation of 80% CH₄ + 20% H₂ fuel at 11 kW

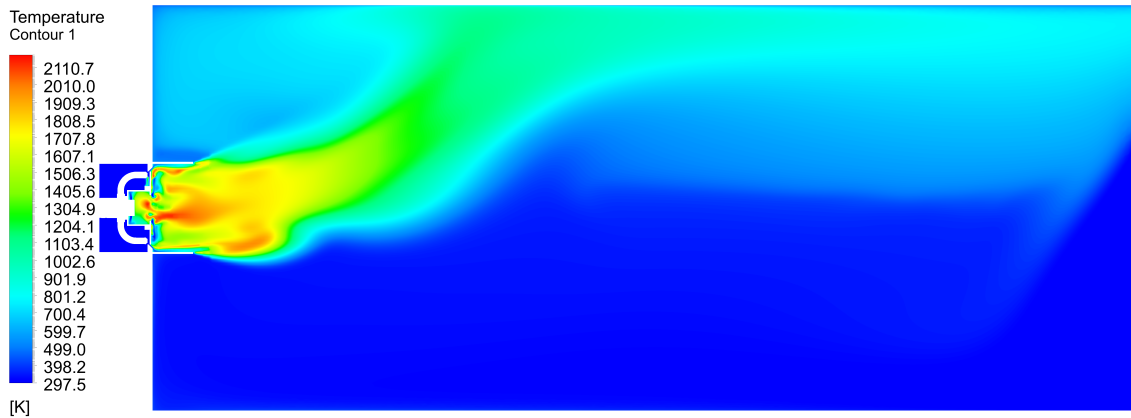
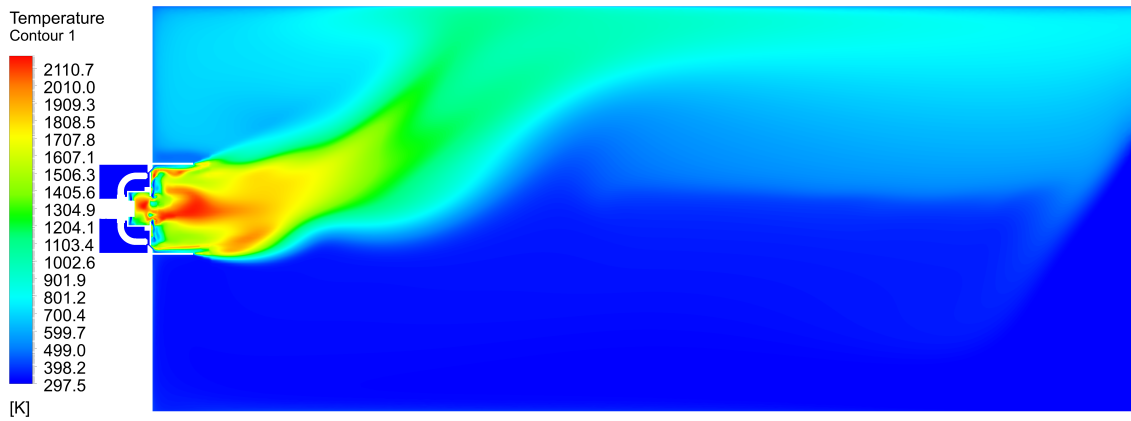
(e) Detailed 3D simulation of 100% CH₄ fuel at 11 kW(f) Detailed 3D simulation of 80% CH₄ + 20% H₂ at 11 kW

Figure 5.9: Vertical axial plane's temperature profiles for the 100% CH₄ and 80% CH₄ + 20% H₂ fuels at 11kW

As can be seen throughout the figures, the 2D simulations do not accurately capture the temperature profile throughout the chamber, one of the main reasons being the absence of an option to account for gravity in the Y axis. With this limitation it becomes impossible to model buoyancy effects originated by thermal gradients and density variation. This justifies the lack of ability calculating the average temperature in the combustion chamber, preventing the model from accurately reproducing the key physical phenomena occurring in reality. As can be observed, neither the backflow nor the temperature stratification at the top of the combustion chamber are being correctly represented.

When analyzing the temperature profiles of both the simple 3D and the detailed 3D simulations, the differences introduced by the injection system modeling become evident, particularly in the temperature distribution. Moreover, the movement of the thermal

plume resulting from the addition of hydrogen to the fuel is more apparent in the detailed 3D simulations, as not only is a larger area affected by higher temperatures, but also a larger thermal plume can be observed in the 80% CH₄ + 20% H₂ case.

Although the errors introduced by the simple 3D simulation in predicting both the adiabatic flame temperature and the average combustion chamber temperature are not notably significant, a temperature profile along the combustion chamber axis was generated in order to assess the differences in the temperature distribution in a more technical and analytical manner. In Figures 5.10 and 5.11 are exhibited the profiles obtained for the simple 3D and detailed 3D simulations, respectively.

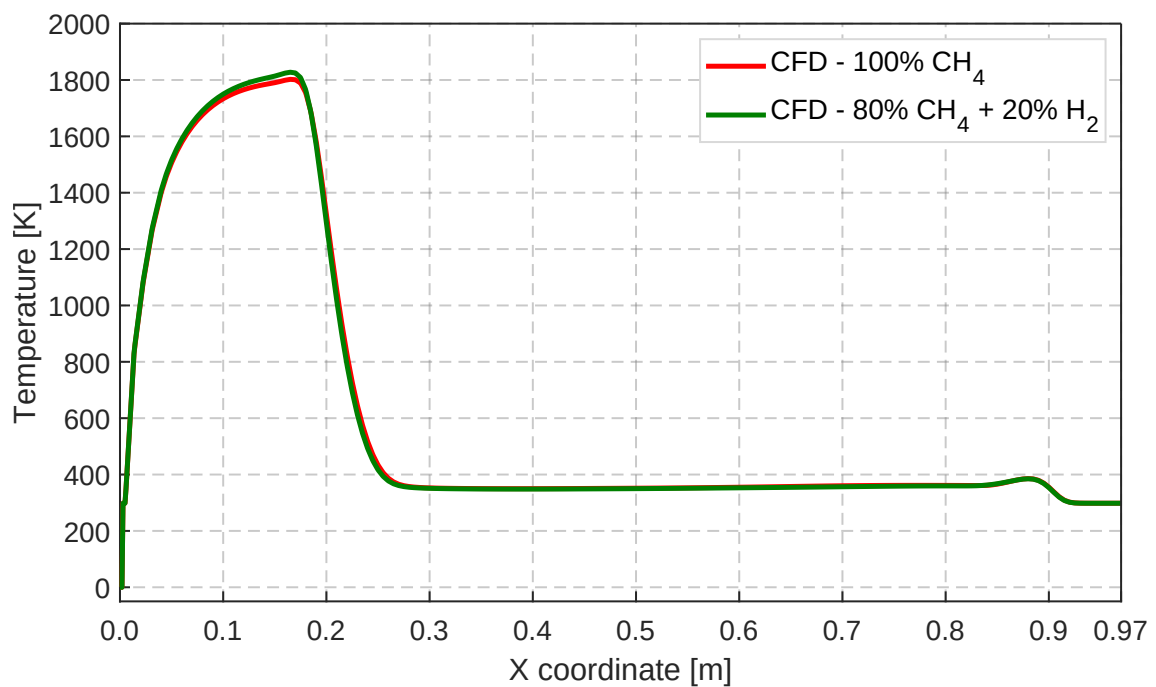


Figure 5.10: Simple 3D simulations temperature profiles at 11kW

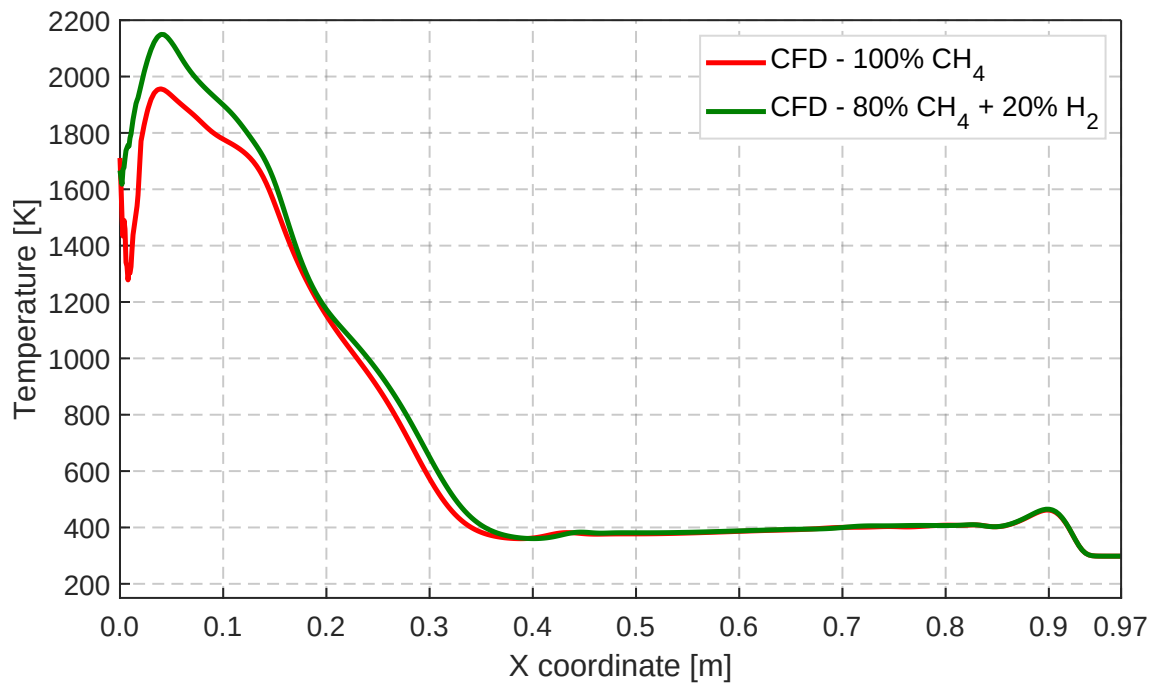


Figure 5.11: Detailed 3D simulations temperature profiles at 11kW

From these figures, the main differences become easily identifiable, particularly near the flame core. It is visible that, in the detailed 3D simulations, the temperature profiles start at an high temperature, unlike the simple 3D simulations, which begin at 0 K. Also, the difference in adiabatic flame temperatures resulting from the addition of hydrogen to the fuel is considerably more pronounced in the detailed 3D simulations and reach higher temperatures. Furthermore, it is noticeable that the corresponding temperature peak occurs at an earlier position along the x-axis in the detailed 3D simulations, with the subsequent temperature drop being considerably smoother than in the simple 3D simulations. Near the end of the chamber, both simulations exhibit similar behavior, particularly because the flame no longer directly influences the temperature and the backflow plays a major role in affecting the temperature distribution. The 2D simulation temperature profile were not generated, since the previous figures already make it clear that the results are highly inaccurate. Producing a temperature curve would therefore deviate so significantly from reality that it would not provide a meaningful insight.

5.2.2 Species Analysis

The species analysis in this section will not focus on the mole fraction measurement on a specific point in the chamber, like the analysis made in the model validation. Instead, since there is not the need to measure on the location of the gas analyzer probe, a more practical analysis will be made, by measuring the species' mass flows through the chamber's outlet. This approach provides a more industry-relevant perspective, as the pollutant mass flow rates at the outlet are the quantities directly used in emissions assessments

and regulatory compliance, thereby offering a more realistic measure of the combustion system's environmental impact.

Since the backflow phenomena takes place in all three geometries, a data processing was made, in order to filter out its influence on the accurate calculation of pollutant species mass flow rates. The data processing consisted of obtaining the velocity value for each outlet cell, in order to easily identify whether the species mass flow in those cells was entering or exiting the combustion chamber. This process was based on the following equation,

$$\dot{m}_i = u_i A_i \rho_i Y_i \quad (5.6)$$

with i being a cell face in the outlet, $\dot{m}_i$ the respective mass flow, u_i the velocity value perpendicular to the face, A_i the cell face area, ρ_i the density and Y_i the mass fraction for the species in study. With the mass flow for each individual cell face obtained, a sum was made, selecting only the faces with a positive u_i value.

The results obtained for the CO₂ and NO_x mass flow rates are displayed in Table 5.17. It is important to note that a CO mass flow rate evaluation was not made, due to the lack of validation of CO values.

Table 5.17: Mass flow rates of CO₂ and NO_x exiting the combustion chamber at 11 kW

Fuel	Detailed 3D Simulation		Simple 3D Simulation		2D Simulation	
	CO ₂ [kg/h]	NO _x [kg/h]	CO ₂ [kg/h]	NO _x [kg/h]	CO ₂ [kg/h]	NO _x [kg/h]
100% CH ₄	4.189	1.097 · 10 ⁻³	2.153	6.145 · 10 ⁻³	0.692	3.435 · 10 ⁻³
80% CH ₄ 20% H ₂	3.891	4.676 · 10 ⁻⁴	2.001	4.228 · 10 ⁻³	0.643	6.137 · 10 ⁻³

As shown in the table, the three geometries produced different values in every case, revealing inconsistencies between them. It can be observed that the simplified simulations with homogeneous inlet mixtures predicted lower CO₂ formation than the detailed 3D simulations. This may be explained by the presence of the locally fuel-rich zones, where higher CO₂ production is expected. Nevertheless, a common trend across all geometries is the decrease in CO₂ values when hydrogen is added to the fuel, as expected. In both 3D geometries, a decrease in NO_x values can also be observed when hydrogen is introduced, which at first sight appears counterintuitive, since an increase in NO_x would normally be anticipated. However, when assessing the NO_x mole fractions near the flame core, the detailed 3D simulations show an increase from 3667ppm to 3782ppm with the addition of hydrogen to the fuel, corresponding to a 3.12% rise, as expected. This confirms that, even though a larger amount of NO_x is produced in the 80% CH₄ + 20% H₂ case, most of it does not reach the outlet, in contrast to the 100% CH₄ case. Moreover, when analyzing the NO mass fraction distribution throughout the chamber, in the detailed 3D simulations, through a 3D volume render, it becomes evident that higher mass fractions extend further downstream in the 100% CH₄ case, as seen in Figures 5.12 (a) and (b).

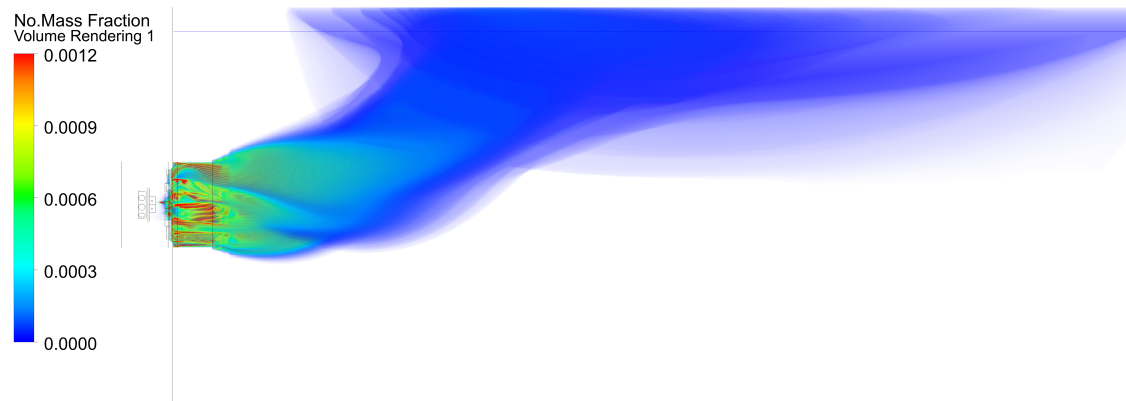
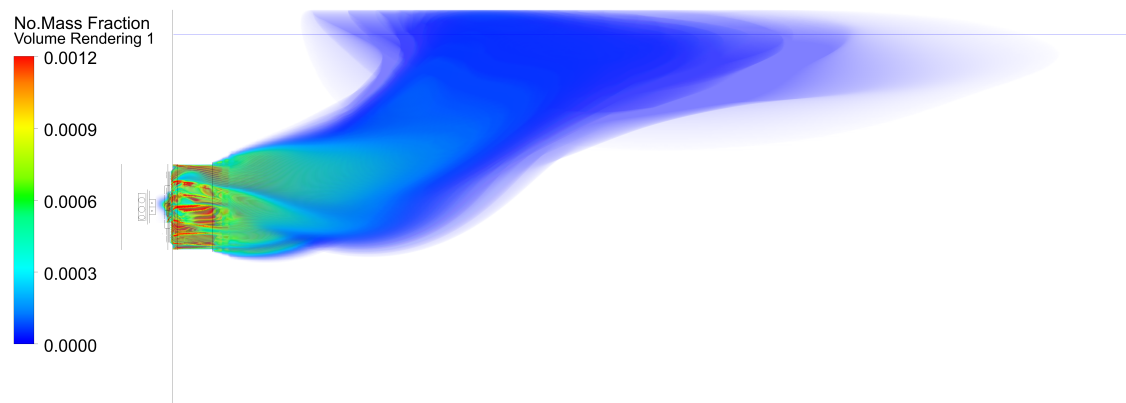
(a) 100% CH₄ fuel(b) 80% CH₄ + 20% H₂ fuel

Figure 5.12: Comparison between NO mass fraction distribution, in the detailed 3D simulations, for the 100% CH₄ and 80% CH₄ + 20% H₂ fuels at 11kW

This phenomenon can be explained by the different axis-aligned velocity profiles exhibited in each case. Figures 5.13 (a) and (b) show the velocity contours for the 100% CH₄ and 80% CH₄ + 20% H₂ fuels, respectively, on the horizontal plane intersecting the region where the difference in the extent of the NO_x mass fractions is most evident. This plane, indicated by the thin blue line near the upper boundary of Figures 5.12(a) and (b), is located 17.5 cm above the combustion chamber axis.

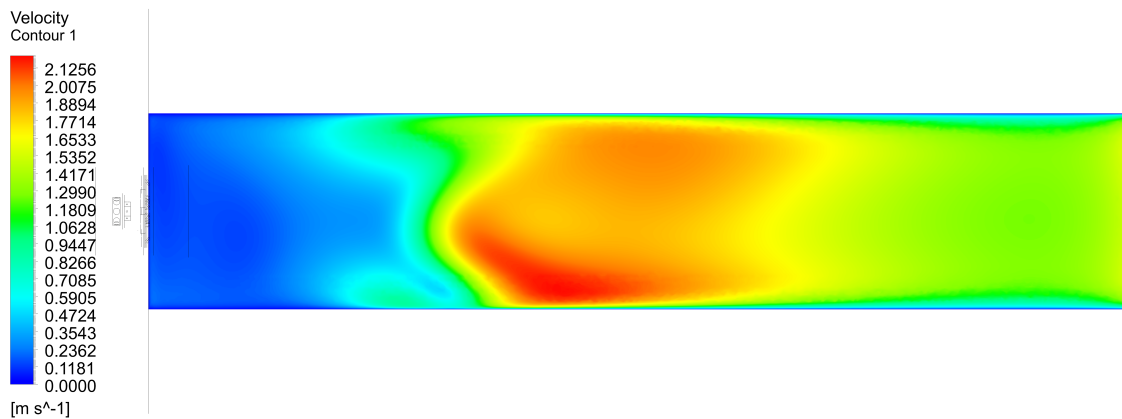
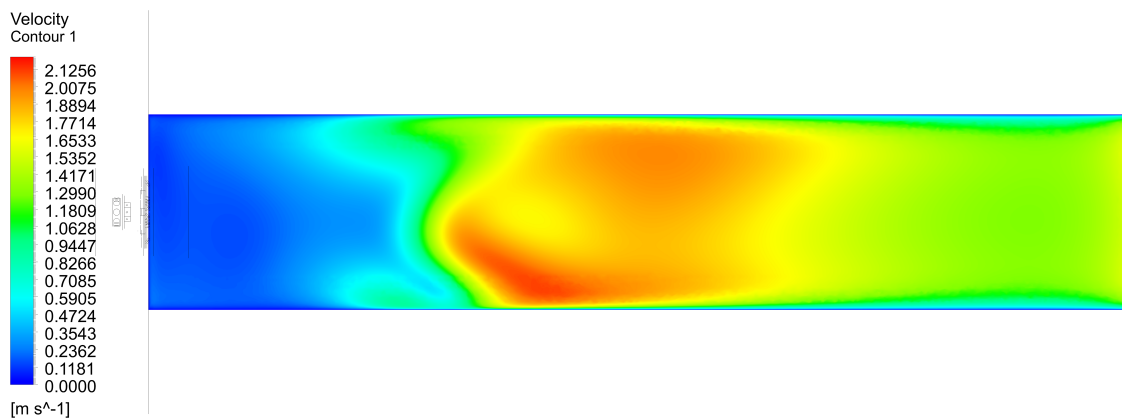
(a) 100% CH₄ fuel(b) 80% CH₄ + 20% H₂ fuel

Figure 5.13: Comparison between the axis-aligned velocity profile near the NO_x mass fraction gradient, in the detailed 3D simulations, for the 100% CH₄ and 80% CH₄ + 20% H₂ fuels at 11kW

As noticed in the figure, a bigger axis-aligned velocity is noticed for the 100% CH₄ case, near the chamber top, which may be transporting the NO_x mass fraction values downstream. This may also indicate a limitation of the model, more specifically of the relax to chemical equilibrium approach, in excess-air conditions, where species governed by slow kinetics and that remain far from equilibrium, such as NO_x, are not correctly predicted. Since these variations occur for the 11kW simulations, where there is an high excess air ratio, and not for the close-to-stoichiometric experimental simulations, the excess air ratio seems to be a key factor in this circumstance.

In order to better analyze the predictions, made by the three simulations, on the species variations when introducing hydrogen into the fuel, in Table 5.18 are represented the relative variations of pollutant mass flow rates.

Table 5.18: Mass flow rates variations of CO₂ and NO_x, when adding hydrogen, exiting the combustion chamber at 11 kW

Fuel	Detailed 3D Simulation	Simple 3D Simulation	2D Simulation
CO ₂	-7.115%	-7.039%	-6.993%
NO _x	-57.39%	-31.20%	+78.67%

Although some differences were observed between the simulations in predicting the CO₂ mass fraction values, the analysis of the mass flow rate variations reveals more consistent results, with CO₂ reductions in all cases being close to 7%. In contrast, NO_x once again proved challenging to characterize accurately, as its variations differed significantly between models. To provide a clearer comparison of the different simulations capacity to predict species formation, in Table 5.19 are presented the relative errors of the 2D and simple 3D simulations, benchmarked against the detailed 3D simulation, for both the species mass flow rates and their variations.

Table 5.19: Relative errors of the 2D and simple 3D simulations, compared with the detailed 3D simulation, when predicting CO₂ and NO_x mass flow rates and their variations

Parameter	Fuel	Simple 3D Simulation	2D Simulation
CO ₂ Mass Flow Rate	100% CH ₄	-48.61%	-83.49%
	80% CH ₄	-48.57%	-83.47%
	20% H ₂		
CO ₂ Mass Flow Rate Variation		-1.073%	-1.713%
NO _x Mass Flow Rate	100% CH ₄	-44.01%	-96.87%
	80% CH ₄	-9.59%	-86.88%
	20% H ₂		
NO _x Mass Flow Rate Variation		-45.63%	-237.1%

As presented by the table values, both simplified geometries exhibited limited accuracy in predicting the species mass flow rates. The only acceptable error corresponds to the simple 3D simulation when predicting the NO_x mass flow rate for the methane–hydrogen mixture. These results emphasizes the importance of geometric and mesh refinement when coupling mass transport with species formation, revealing a requirement for greater detail.

5.3 Experimental Simulations vs 11kW Simulations

This section will focus on comparing the differences between the two burner powers tested, and the respective excess air percentages, in order to study the influence of increased power on temperature distribution and species formation. As in the two previous sections, the discussion will be divided into temperature and species analyses. Since the previous sections focused on different properties in each analysis, this chapter addresses the remaining ones, providing a more comprehensive understanding and enabling a complete comparison of the results. Certain results are intentionally repeated to ensure a clearer and more fluent comparison between them. Also, since a 2D simulation was not developed for the experimental simulations, in this section only the detailed 3D and simple 3D simulations results will be compared.

5.3.1 Temperature Analysis

Starting through the same order as in the last section, both the adiabatic flame and average combustion chamber temperatures were obtained for the experimental simulations. The results are in Table 5.20, along with the values for the 11kW simulations.

Table 5.20: Adiabatic flame and average combustion chamber temperatures for the experimental and 11kW simulations

Parameter	Simulation Type	Fuel	Experimental Simulation	11 kW Simulation
Adiabatic Flame Temperature [K]	Detailed 3D Simulation	100% CH ₄	2173.45	2148.94
		80% CH ₄ 20% H ₂	2198.20	2184.74
		100% CH ₄	2118.12	1872.28
	Simple 3D Simulation	80% CH ₄ 20% H ₂	2146.15	1887.39
		100% CH ₄	570.53	508.87
		80% CH ₄ 20% H ₂	567.90	510.32
Average Combustion Chamber Temperature [K]	Detailed 3D Simulation	100% CH ₄	531.68	470.56
		80% CH ₄ 20% H ₂	528.54	472.35
	Simple 3D Simulation	100% CH ₄		
		80% CH ₄ 20% H ₂		

As can be seen by the values presented on the table, the temperatures increased for the experimental simulations, as expected due to the higher burner power. Also, on the experimental simulations, the adiabatic flame temperature remained consistent with the literature, by presenting higher values for the methane-hydrogen mixed fuel. On the other hand, the average combustion chamber temperature had the opposite outcome, with temperatures being higher for the 100% CH₄ fuel, in the experimental simulations, as opposed

to the 11kW simulations, revealing a bigger effect of hydrogen's laminar burning speed for a higher power along a lower excess air ratio.

The temperature profiles along the combustion chamber's axis and the thermocouples height were also generated for both simulations. From Figure 5.14 to Figure 5.17 are represented the respective temperature profiles for the detailed 3D simulations. Since the temperature profiles for the simple 3D simulations were already proved as unreliable they were not analyzed.

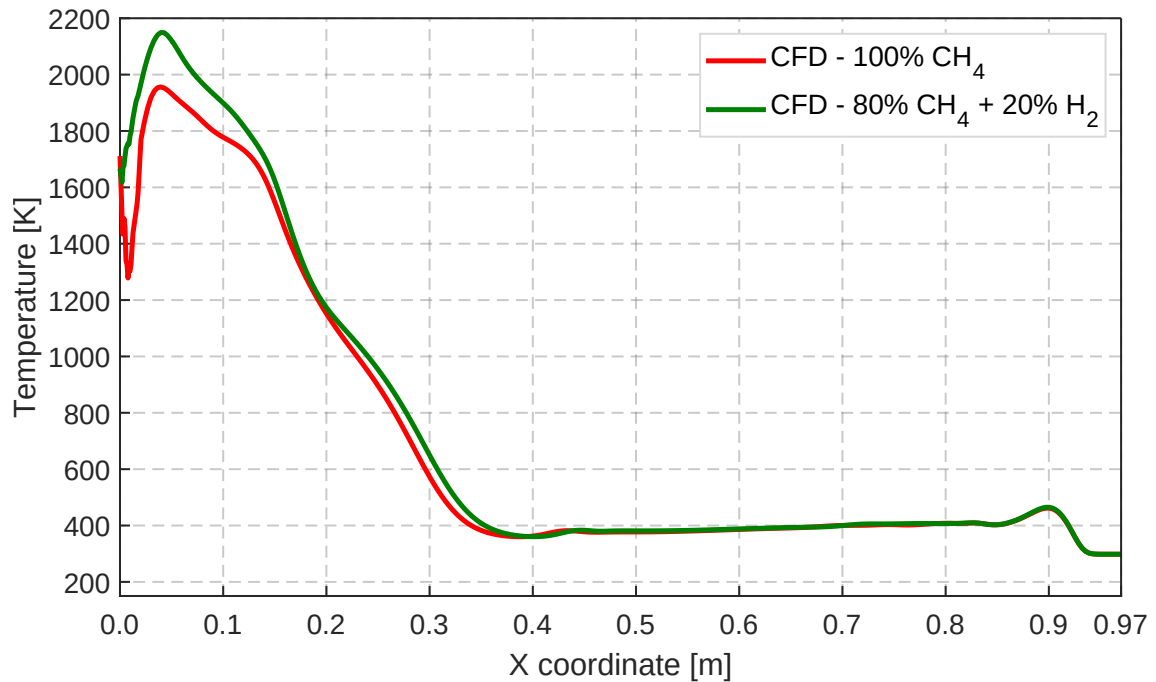


Figure 5.14: Temperature profile along the combustion chamber axis, for the detailed 3D simulations, at 11kW

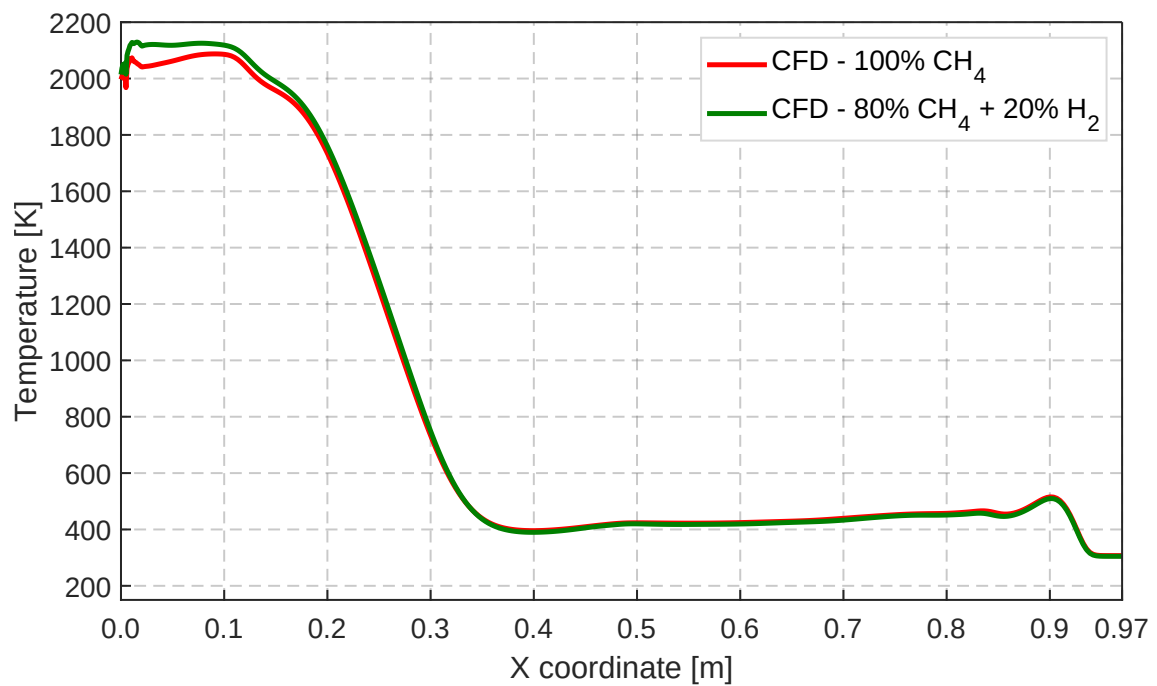


Figure 5.15: Temperature profile along the combustion chamber axis for the experimental detailed 3D simulations

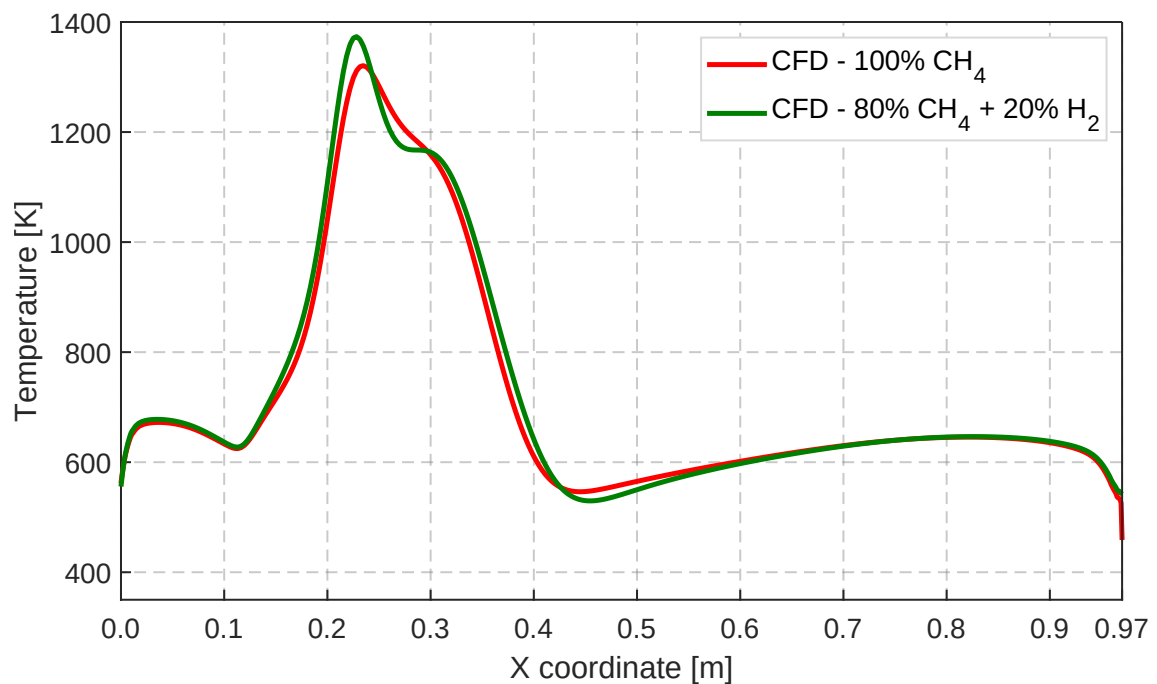


Figure 5.16: Temperature profile along the thermocouples height, for the detailed 3D simulations, at 11kW

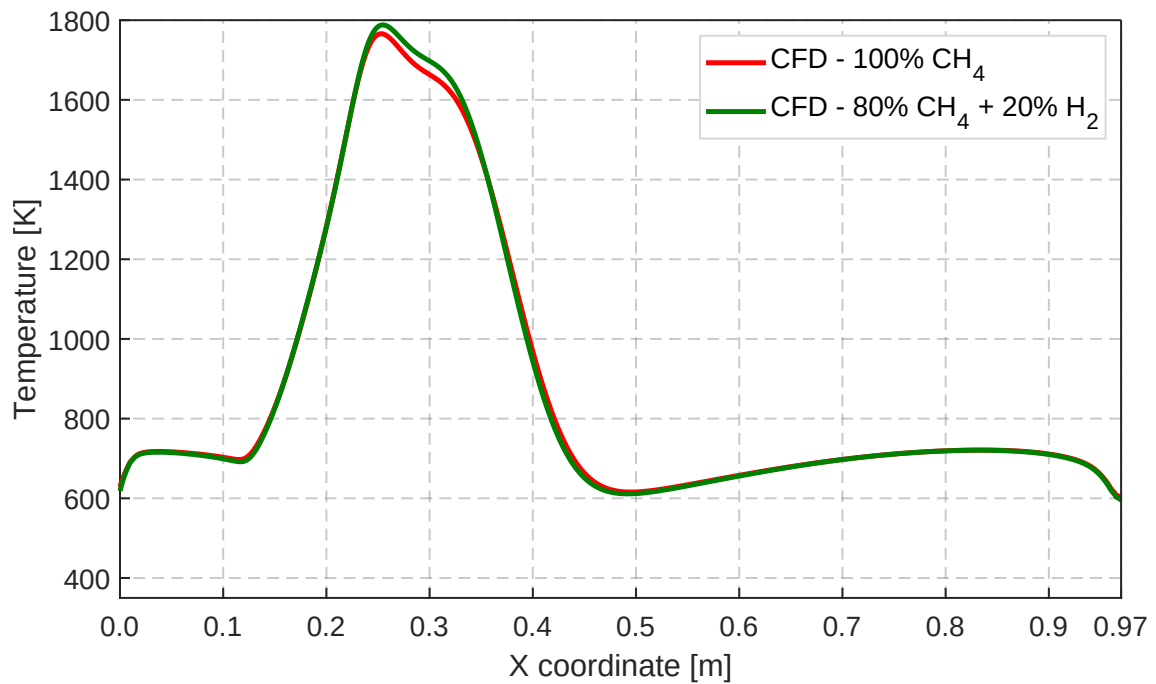


Figure 5.17: Temperature profile along the thermocouples height for the experimental detailed 3D simulations

As seen in the figures and in the previous table, the experimental simulations adiabatic flame temperature increased only slightly when compared with the 11kW simulations, despite the increased burner power and lower excess air ratio. The big differences were felt throughout the chamber, with the average chamber temperature having a bigger difference between both power cases than the adiabatic flame temperature. This can also be confirmed by Figures 5.16 and 5.17, which show that at the thermocouples height the temperatures were considerably higher for the experimental case, especially in the peak temperature where differences were as high as 400K. The increase in heat proliferation throughout the chamber can also be noticed when comparing the vertical axial plane's temperature profiles for both cases, represented in Figures 5.5 (a) and (b) for the experimental simulations and in Figures 5.9 (e) and (f) for the 11kW simulations. By comparing these figures it is possible to notice a more consistent and better defined thermal plume for the experimental case, while maintaining higher temperatures further downstream. This effect can also be seen through the more smooth decreasing slope, after the peak temperature in Figure 5.15 compared to the more abrupt slope presented in figure 5.14.

As shown in the figures and the previous table, the adiabatic flame temperature in the experimental simulations increased only slightly compared to the 11kW cases, despite the higher burner power and lower excess air ratio. The most significant differences were observed throughout the combustion chamber, where the average chamber temperature exhibited a larger variation between the two power settings than the adiabatic flame temperature itself. This trend is confirmed by Figures 5.16 and 5.17, which demonstrate

that, at thermocouple height, the temperatures in the experimental case were considerably higher, with peak temperature differences reaching up to 400K. The enhanced heat propagation within the chamber, at a higher burner power, is also evident when comparing the temperature profiles along the vertical axial plane for both cases, shown in Figures 5.5 (a) and (b) for the experimental simulations and in Figures 5.9 (e) and (f) for the 11kW simulations. From these comparisons, a more consistent and well-defined thermal plume can be observed in the experimental case, which also maintain higher temperatures further downstream. This effect is further illustrated by the smoother temperature decay after the peak in Figure 5.15, compared to the sharper decline observed in Figure 5.14.

5.3.2 Species Analysis

To enable a fair comparison of pollutant species formation between the experimental and 11kW simulations, the mole fractions at the gas analyzer probe position were calculated and are presented in Table 5.21.

Table 5.21: Comparison between CO₂ and NO_x mole fractions at the gas analyzer probe location for the experimental and 11kW simulations

Parameter	Simulation Type	Fuel	Experimental Simulation	11 kW Simulation
CO ₂ Mole Fraction [%]	Detailed 3D Simulation	100% CH ₄	3.542	2.547
		80% CH ₄ 20% H ₂	3.274	2.321
		Variation	-7.576%	-8.850%
	Simple 3D Simulation	100% CH ₄	3.715	2.752
		80% CH ₄ 20% H ₂	3.438	2.614
		Variation	-7.444%	-4.985%
NO _x Mole Fraction [ppm]	Detailed 3D Simulation	100% CH ₄	16.150	15.480
		80% CH ₄ 20% H ₂	18.08	8.732
		Variation	+11.97%	-43.57%
	Simple 3D Simulation	100% CH ₄	51.77	23.39
		80% CH ₄ 20% H ₂	48.20	22.03
		Variation	-6.905%	-5.840%

As shown in the table, the CO₂ mole fractions reveal a similar behavior between the experimental and 11kW simulations, with the 11kW values being slightly lower than those of the experimental case, as expected due to the reduced burner power and higher excess

air ratio. The relative variations in CO₂ when hydrogen is added to the fuel are consistent across all simulations, with the exception of the 11kW simple 3D simulations, which slightly underestimate the variation, although still within an acceptable range.

When analyzing the NO_x mole fractions, clear differences can be identified between the various simulations. In the experimental detailed 3D simulations, the introduction of hydrogen into the fuel resulted in an increase in NO_x formation, which is in line with the expected behavior. However, the 11kW simulations exhibited an opposite trend, with NO_x values decreasing when hydrogen was added. In particular, the 100% CH₄ case presented considerably high values, while the 80% CH₄ + 20% H₂ simulation revealed considerably low values, in the detailed 3D simulation. This behavior reinforces the model difficulties in accurately predicting NO_x formation under high excess air operating conditions. On the other hand, the simple 3D simulations systematically overestimated the concentrations for both cases and fuels, confirming that this geometry is not adequate for reliable predictions of NO_x emissions.

On another note, the CO₂ and NO_x mass flow rates at the outlet were also calculated for the experimental simulations. The result for the latter and the 11kW simulations are presented in Table 5.22.

Table 5.22: Comparison between CO₂ and NO_x mass flow rates at the outlet for the experimental and 11kW simulations

Parameter	Simulation Type	Fuel	Experimental Simulation	11 kW Simulation
CO ₂ Mass Flow Rate [kg/h]	Detailed 3D Simulation	100% CH ₄	5.635	4.189
		80% CH ₄ 20% H ₂	5.240	3.891
		Variation	-7.006%	-7.115%
	Simple 3D Simulation	100% CH ₄	2.898	2.153
		80% CH ₄ 20% H ₂	2.696	2.001
		Variation	-6.958%	-7.039%
	Detailed 3D Simulation	100% CH ₄	$4.819 \cdot 10^{-4}$	$1.097 \cdot 10^{-3}$
		80% CH ₄ 20% H ₂	$5.252 \cdot 10^{-4}$	$4.676 \cdot 10^{-4}$
		Variation	+8.982%	-57.39%
NO _x Mass Flow Rate [kg/h]	Simple 3D Simulation	100% CH ₄	$5.340 \cdot 10^{-4}$	$6.145 \cdot 10^{-4}$
		80% CH ₄ 20% H ₂	$4.268 \cdot 10^{-4}$	$4.228 \cdot 10^{-4}$
		Variation	-20.07%	-31.20%
	Detailed 3D Simulation	Variation	-20.07%	-31.20%

These values reveal, once again, the limitations of the model in capturing NO_x formation. In the 11kW simulations, the mass flow rates were higher than the experimental

values for the 100% CH₄ fuel and lower for the 80% CH₄ + 20% H₂ fuel, both in the detailed 3D and simple 3D cases. For the experimental condition, the simple 3D simulations produced values reasonably close to those of the detailed 3D simulations, however, the predicted trend was incorrect, as the higher NO_x concentration was obtained for the methane–hydrogen fuel.

When it comes to CO₂ values, the panorama is different, with both geometries for both power cases predicting really similar variation values. However, when it comes to mass flow rate predictions, it is visible that the simplified geometries underestimate the values in both power cases, in about 50%. When comparing CO₂ mass flows between the experimental and the 11kW simulations it is easy to observe that, as expected, the 11kW simulations present lower values, for both the detailed 3D and simple 3D simulations.

As for the CO₂ mass flows rates, the values calculated reveal an underestimation by the simple 3D simulations, with values being approximately 50% lower in both power cases, when compared to the detailed 3D simulations. In contrast, analyzing CO₂ mass flow rates between the experimental and the 11kW simulations, it is noticeable that the latter predicted lower values, as expected, for both the detailed 3D and simple 3D cases. In terms of CO₂ mass flow rate variations, the simulations were in good agreement, revealing extremely similar values in all of the four cases, with reductions in CO₂ formation surrounding the 7%. These values are also in good agreement with most of the bibliography, where CO₂ reduction values are typically reported between 5% and 10%, as shown in the works of AIChE – Chemical Engineering Progress [41], Zhang et al. [42] and Liu et al. [43].

Since the reduction of CO₂ emissions is one of the main concerns of the industry today, reinforced by European guidelines aiming at decarbonization and also a key motivation for investigating hydrogen introduction into fuels, estimating the annual CO₂ output becomes essential to assess the potential impact of introducing hydrogen. In Table 5.23 are presented the values obtained for CO₂ emissions over a full year of operation, for the detailed 3D simulations of both the experimental and 11kW cases.

Table 5.23: CO₂ emissions over an full year of operation for the experimental and 11kW simulations

Parameter	Experimental Simulation		11 kW Simulation	
	100% CH ₄	80% CH ₄ 20% H ₂	100% CH ₄	80% CH ₄ 20% H ₂
Fuel				
Power [kW]	14.80	14.81	11.00	11.00
Mass Flow Rate [kg/h]	5.635	5.240	4.189	3.891
Emissions per year [tonCO ₂ /yr]	49.36	45.90	36.70	34.09
GigaJoule per year [GJ/yr]	466.73	467.05	346.90	346.90
Emissions per GJ [kgCO ₂ /GJ]	105.76	98.28	105.79	98.26

As shown in the table, the use of 80% CH₄ + 20% H₂ fuel results in a reduction of 3.46 tons of CO₂ per year under the experimental operating conditions, a reduction of 2.61 tons of CO₂ per year under the 11kW simulation conditions and a reduction of around 7.5 kgCO₂/GJ for both scenarios. These reductions are considerably modest in scale, but demonstrate that hydrogen blending can contribute to lowering emissions under the studied conditions. Even if limited, it provides an additional option for decarbonization, which is valuable given the need for multiple approaches.

Chapter 6

Conclusions and Future Works

6.1 Conclusions

This work combined experimental tests and numerical simulations in order to evaluate the effect of hydrogen enrichment in a natural gas burner. The experiments were carried out with two fuel compositions, pure methane and a blend of 80% CH₄ + 20% H₂, while numerical simulations were developed progressively, from simplified two-dimensional cases to detailed three-dimensional geometries including the full injection system.

The experimental campaign demonstrated that stable combustion could not be achieved at the initial target of 11 kW with 30% excess air, which led to the adoption of higher power and conditions closer to stoichiometry. The temperature measurements did not allow firm conclusions regarding the adiabatic flame temperature, since the thermocouple positions did not coincide with the flame core. When considering average values across the probes, slightly higher temperatures were in fact observed with hydrogen addition, although the magnitude of this variation must be interpreted carefully given the measurement uncertainty and the spatial limitations of the probes. Gas analysis confirmed reductions in CO₂ mole fractions when hydrogen was added, consistent with the lower carbon content of the mixture, although NO_x levels showed high variability due to measurement uncertainties, a consequence of the wide range of thermal powers considered in order to obtain averaged values consistent between both fuels. The carbon monoxide results, both in the experiments and in the CFD, also displayed some unpredictability, underlining the difficulty of consistently quantifying this pollutant and the need for more robust measurement and modeling approaches. Despite these experimental limitations, the CFD analysis provided complementary insight into the flame structure and species formation, helping to interpret the observed trends and to separate the limitations imposed by the measurement setup from the actual physical behavior of the flame.

The CFD analysis was in reasonable agreement with the experimental results, providing confidence in the selected turbulence and combustion models. The validation exercise

confirmed that the numerical model captured the main trends in temperature fields and species concentrations, within the limits imposed by the experimental uncertainty.

Once corroborated, the model was extended to assess the conditions not accessible in the laboratory. At the planned 11kW operation, the simulations reproduced the expected increase in adiabatic flame temperature with hydrogen enrichment, with maximum values of about 2149K for pure CH₄ and 2185K for the 80/20 CH₄ + H₂ mixture. The average chamber temperature remained close to 509.5K for both fuels, showing little influence of hydrogen at this power level. In terms of species, the CO₂ mole fraction at the probe position decreased from 2.55% for methane to 2.32% with hydrogen, while the predicted NO_x mole fractions were approximately 16ppm for CH₄ and 9ppm for the hydrogen-enriched case. For comparison, the experimental simulations predicted peak flame temperatures of about 2173K for pure methane and 2198K with hydrogen, with average chamber temperatures around 569K. The corresponding CO₂ mole fractions decreased from 3.54% to 3.27%, while NO_x increased from 16ppm to 18ppm. The model also revealed a modest but consistent reduction of yearly CO₂ emissions, of about 2.6 tons per year at 11kW and approximately 3.5 tons per year at the experimental operating conditions, when introducing 20% H₂. Although limited in scale, these reductions illustrate the potential of hydrogen enrichment as one of several measures contributing to decarbonization. The results also highlighted the sensitivity of NO_x prediction to the chemical model used, reinforcing the importance of careful model selection and validation.

An additional outcome of the numerical study was the comparison between different computational geometries. The 2D simulations were able to reproduce reasonably well the adiabatic flame temperature, but they failed to capture the overall flame structure and the local gradients of temperature and species, which limited their usefulness beyond that specific parameter. The 3D cases provided a more detailed representation of the burner, although their predictive capability varied significantly with the level of geometric detail. In the simple 3D geometry the flame was poorly represented, with shape and position differing markedly from the experimental observations, as illustrated in the figures of Chapter 5. By contrast, the 3D geometry including the full injection system reproduced the flow distribution, the thermal field and the plume structure with much greater accuracy, leading to results in closer agreement with the measurements. These findings confirmed that simplified geometries can support preliminary analysis, but only detailed three-dimensional models are capable of reliably describing the behavior of the flame in practical burners.

Overall, this dissertation demonstrated the feasibility of enriching natural gas with hydrogen in a low power burner, quantified the impact on temperature distribution and emissions, and validated a CFD model that can be further extended to other conditions. The integration of experimental and numerical approaches proved essential, as each compensated the limitations of the other and together provided a comprehensive understanding of the system.

6.2 Future Works

Several developments can be pursued to extend the present study. One possible improvement is to refine the CFD methodology by explicitly modeling the thermocouples' geometry and material, enabling a direct comparison between the experimental tests and CFD thermocouples' bead temperature, therefore eliminating the need to correct and transform the experimental thermocouples' temperature readings into the actual gas temperature. Another important step is the testing of alternative turbulence–combustion interaction models, for instance replacing the finite-rate/eddy-dissipation approach with the Eddy Dissipation Concept, to investigate their effect on the prediction of temperature and chemical species formation. In addition, it would be valuable to implement different chemical kinetic schemes, both reduced and more detailed, in order to assess the sensitivity of the results to the reaction mechanism. Another promising line of research is the use of transient simulations to study the dynamic behavior of the flame, which would allow a better understanding of ignition, extinction and oscillatory phenomena that cannot be captured in steady-state conditions.

On the experimental side, more tests with a wider range of hydrogen fractions, both below and above 20%, would provide a more complete validation of the numerical model and offer additional insight into stability limits and emission trends. Finally, particular attention should be given to the prediction and measurement of carbon monoxide. The inconsistencies observed in this work suggest that improved measuring techniques and more detailed kinetic models are required in order to achieve reliable results for this pollutant, which remains a critical indicator of incomplete combustion. Long-term material effects and possible issues of flashback or flame stability in practical appliances fueled with $\text{CH}_4\text{--H}_2$ mixtures should also be investigated, since these aspects are essential for the safe integration of hydrogen into real domestic and industrial systems.

These future works would not only refine the current findings but also contribute to a deeper understanding of the challenges and opportunities associated with hydrogen enrichment in combustion technologies.

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