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Injection and combustion modelling in hydrogen internal combustion engines

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Final dissertation

Injection and combustion modelling in hydrogen internal combustion engines

by
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Sommario

Questo lavoro di tesi è focalizzato sull'analisi numerica dei processi di iniezione, mixing, e combustione nei motori a combustione interna con iniezione diretta di idrogeno.

Con tutta probabilità, l'attuale transizione verso forme di mobilità sostenibile potrà essere attuata solo tramite una combinazione di diverse soluzioni tecnologiche. Per specifiche applicazioni come ad esempio il trasporto pesante su gomma, i motori a combustione interna alimentati a idrogeno, in particolare tramite iniezione diretta, potrebbero rappresentare una forma di powertrain competitiva in termini di prezzo e affidabilità rispetto a soluzioni più innovative come le celle a combustibile.

Per quanto i motori a combustione interna siano una tecnologia con più di cento anni di storia, le peculiarità chimico-fisiche dell'idrogeno rendono necessaria una nuova analisi dei processi alla base del funzionamento del motore, quali iniezione, miscelazione tra combustibile e aria, e combustione.

Per questo motivo, il primo step del presente lavoro di tesi è stato quello di caratterizzare la fluidodinamica del processo di iniezione ad alta pressione dell'idrogeno all'interno della camera di combustione. In particolare, sono state analizzate le strutture fluidodinamiche che caratterizzano l'iniezione diretta, ponendo attenzione al setup numerico necessario a risolvere tale tipologia di flussi.

Rispetto a quanto presente in letteratura, l'analisi è stata incentrata sull'effetto delle condizioni tipiche della camera di combustione sulla fenomenologia del getto. Più nello specifico, è stata condotta una analisi al variare della pressione del cilindro nel tempo, per determinare l'eventuale presenza di fenomeni dinamici che possano modificare la configurazione del flusso rispetto a quanto osservabile per rapporti di pressione costanti. Successivamente, è stata focalizzata l'attenzione sull'influenza della geometria della sezione di uscita dell'iniettore, allo scopo di determinare se specifiche configurazioni possano favorire la formazione di una carica idonea all'utilizzo nei motori a combustione interna. Sebbene le sezioni di uscita dell'iniettore siano principalmente circolari o anulari, sono state studiate nuove geometrie (triangolare, stella, rettangolare ed ellittica) per comprenderne l'effetto in termini di mixing tra getto e ambiente circostante. Nonostante alcune di queste configurazioni geometriche siano state già analizzate in ambito aeronautico, la loro utilità in ambito motoristico è stata testata nel presente lavoro di tesi. Sono anche emerse significative differenze nel sistema di shock ed espansioni che carat-

terizzano questi flussi, a cui è stata data puntuale spiegazione.

L'analisi è stata poi estesa al design space delle principali variabili che influenzano il processo di mixing, quali pressione di iniezione, timing di iniezione, geometria del nozzle. Il fine è stato quello di estendere l'operabilità del motore in condizioni di miscela sempre più magra rispetto allo stato attuale dell'arte. Più nello specifico, è stata focalizzata l'attenzione su miscele con rapporto di equivalenza pari a 0.25, che consentono di ridurre le perdite termiche a parete e di contenere le emissioni di ossidi di azoto. E' stato dimostrato che la stratificazione della miscela in tali condizioni è la via per incrementare la velocità del processo di combustione. In particolare, sono state testate strategie di multi-injection, che hanno dimostrato di poter ottimizzare la velocità del processo di combustione e le emissioni di NO_x .

In ultimo, nell'ottica di migliorare la modellistica dei motori a combustione interna, è stata sviluppata una procedura che consente di tenere conto dell'effetto delle instabilità termodiffusive delle fiamme di idrogeno nel contesto del modello di combustione basato sulla G-equation. I risultati preliminari mostrano la potenzialità di poter catturare efficacemente i trend di pressione a fronte di un unico processo di calibrazione preliminare relativo all'interazione fra la turbolenza in camera e il fronte di fiamma.

Abstract

This thesis focuses on the numerical analysis of the injection, mixing, and combustion in direct injection internal combustion engines fueled by hydrogen.

Most likely, the current transition towards a sustainable mobility will be achieved only through a combination of different technologies. For specific applications, such as heavy-duty road transport, hydrogen-powered internal combustion engines — particularly those based on direct injection — represent a competitive powertrain solution in terms of cost and reliability compared to more innovative alternatives like fuel cells.

Although internal combustion engines have been in use for over a century, the unique chemical and physical properties of hydrogen necessitate a renewed analysis of the fundamental processes governing engine operation, such as injection, fuel-air mixing, and combustion.

For this reason, the first step of this thesis is the characterization of the fluid dynamics of high-pressure hydrogen direct injection into the combustion chamber. The study analyzes the fluid-dynamic structures characterizing these flows, with particular attention to the numerical setup required to accurately resolve them. With respect to the state of art, the analysis focuses on the effect of the typical combustion chamber conditions on the jet phenomenology. More specifically, an analysis is proposed by varying the cylinder pressure over time to determine the possible presence of dynamic phenomena that could alter the flow configuration compared to what is observed under constant pressure ratios.

As a second step, focus has been posed on the influence of the injector exit section geometry, to determine whether specific configurations are more suitable for use in internal combustion engines. Although the injector outlet sections are primarily circular or annular, new geometries (triangular, star-shaped, rectangular, and elliptical) have been studied to understand their effect on the mixing between the jet and the surrounding environment. While some of these geometric configurations have already been analyzed in the aerospace field, their applicability in the automotive sector has been tested in this thesis work. Significant differences have been observed in the shock and expansion system characterizing these flows, for which a detailed explanation has been provided. Subsequently, the analysis has been extended to the design space of key variables affecting the mixing process, such as the injection pressure, timing, and nozzle geometry.

The goal has been to extend the engine operability under increasingly lean mixtures compared to the current state of the art. More specifically, focus has been placed on mixtures featured by an equivalence ratio of 0.25, which help to reduce wall heat losses while limiting nitrogen oxide emissions. It has been demonstrated that the mixture stratification under these conditions is the key to increasing the combustion process speed. In particular, multi-injection strategies have been tested, showing the potential to optimize the combustion speed and NO_x emissions.

Finally, in an effort to improve internal combustion engine modeling, a procedure has been developed to account for the effects of thermodiffusive instabilities in hydrogen flames within the framework of the G-equation combustion model. Preliminary results show the potential to effectively capture pressure trends with a single preliminary calibration process regarding the interaction between the flame front and the in-cylinder turbulence.

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Acronyms

aTDC	after Top Dead Center
AR	Aspect Ratio
bTDC	before Top Dead Center
BDC	Bottom Dead Center
BTE	Brake Thermal Efficiency
BMEP	Brake Mean Effective Pressure
CAD	Computer Aided Design
CMT	Clean Mobility & Thermofluids
DOI	Duration of the Injection
EOI	End of the Injection
EV	Electric Vehicle
FC	Fuel Cell
GHG	Greenhouse Gas
ICE	International Combustion Engine
IEA	International Energy Agency
IMEP	Indicated Mean Effective Pressure
IRENA	International Renewable Energy Agency
ITE	Indicated Thermal Efficiency
IVC	Inlet Valve Closing
NPR	Nozzle Pressure Ratio
RANS	Reynolds Average Navier-Stokes
SOI	Start of the Injection
SR	Swirl Ratio
TD	Thermodiffusive
TDC	Top Dead Center
TR	Tumble Ratio
UI	Uniformity Index

Chapter 1

Introduction

1.1 Context

The role of CO₂ as a greenhouse gas (GHG) was firstly recognized in the early XX century. In 1938, it was estimated that anthropogenic emissions totaled 150 billion tons of CO₂, much of which remained in the atmosphere, causing a temperature rise of 0.003 °C per year [1]. Nonetheless, the measurement was affected by uncertainties, particularly regarding the CO₂ concentration and the amount of CO₂ absorbed by oceans.

Starting from 1958, the Scripps Institution of Oceanography, systematically began to measure the atmospheric CO₂ at the Hawaii, to monitor the effects of burning fossil fuels. In 1965, the Institution reported an average CO₂ level rise of 0.7 ppm per year, a pattern known as the “Keeling Curve” [2]. In the same year, a new outlook significantly revised the earlier works: a possible 25% increase in atmospheric CO₂ by 2000 was forecast, with a corresponding dramatic climate impact [3]. By then, scientists recognized CO₂ induced warming as a serious issue to tackle [4].

Alongside scientific progress, an international effort arose to address climate change. A successful example was the response to the ozone hole, culminating in the 1985 Vienna Convention and the 1987 Montreal Protocol. However, the reduction of the GHG emissions is a more complex task, since the emissions are strictly related with power generation and the industrial and economical development of Nations. In 1972, the United Nations Conference on the Environment in Stockholm emphasized the need to balance environmental protection with development. In 1988, The United Nations Environmental Program (UNEP) and the World Meteorological Organization (WMO) established the Intergovernmental Panel on Climate Change (IPCC) to build scientific consensus. The IPCC first scientific report, in 1990, was the basis for the 1992 Rio Earth Summit, which led countries to sign the United Nations Framework Convention on Climate Change. In 1997, the Kyoto Protocol followed, aiming at reducing GHG emissions worldwide. Through these milestones — from early CO₂ measurements to international summits — scientists and policymakers gradually shaped the need to face the climate

change. Nowadays, the global consensus is that reducing GHG emissions is essential to mitigate the worst impacts of climate change.

1.2 Evolution of the strategies for the GHG reduction

The Kyoto Protocol (1997) was an initial step towards a global policy for reducing GHG emissions. However, subsequent events such as the withdrawal by Canada (2011) and United States (2001) highlighted the political challenges associated with the effort to define a worldwide shared policy.

In 2015, the Paris Agreement defined new ambitious goals. 196 nations agreed to achieve a zero emissions scenario by 2050. It was also introduced the ambitious goal of limiting the average global temperature increase to 1.5°C with respect to pre-industrial levels.

In support of these goals, in 2019 the International Energy Agency (IEA) delivered a study on hydrogen (H_2) as a possible pillar through which promoting the global energy transition. Subsequently, after the request of the 26th Conference of the Parties (COP26) in Glasgow, the IEA released a plan in 2021 to promote the H_2 adoption on a large scale. In the very same year, the International Renewable Energy Agency (IRENA) analyzed the geopolitical implications of a massive H_2 exploitation, further highlighting the potential to reach the decarbonization targets.

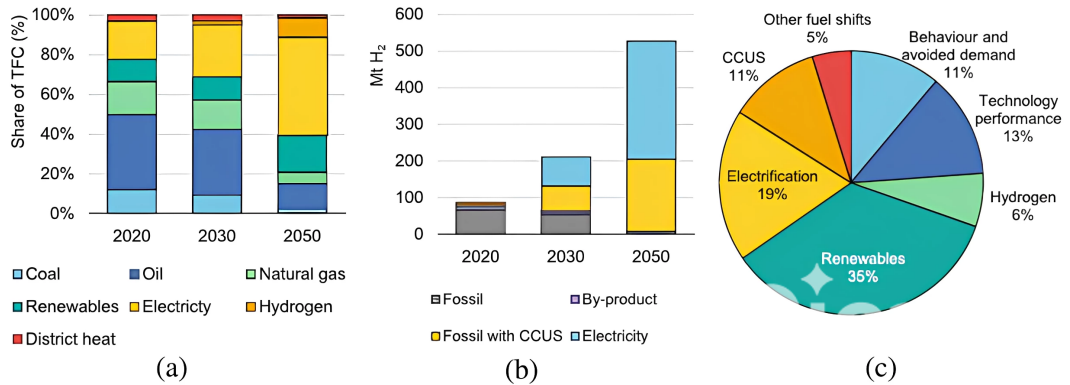


Figure 1.1: IEA report on: (a) the share of total fuel energy consumption (TFC) in 2020 along with the projections for 2030 and 2050; (b) the amount of H_2 production in 2020 and predictions for 2030 and 2050; (c) the expected impact on the reduction of GHG emissions by each of the green technologies deployed to reach the zero emission scenario.

In Figure 1.1(a), provided by IEA [5], the 2020 share of the total final energy consumption (TFC), along with the projections to 2030 and 2050, is reported. As it can be observed, a progressive increase of the renewable energy share is expected, with H_2 accounting for the 10% of total fuel consumption by 2050. Indeed, as shown in Figure 1.1(b), the worldwide amount of H_2 production is expected to increase from the less

than 100 Mt of 2020 to more than 500 Mt by 2050. Most of the H_2 produced in 2020 was derived from fossil fuels, whereas in 2050 it is envisaged that the production will be mainly derived from both electrolysis (powered by renewable sources), and Carbon-Capture Utilization and Storage (CCUS) technology.

Figure 1.1(c) shows the expected impact of the different technologies through which the fulfillment of the net-zero scenario is planned. In particular, renewables will play a major role in the drastic reduction of the GHG emissions, along with direct electrification and CCUS. H_2 will count for around the 6%.

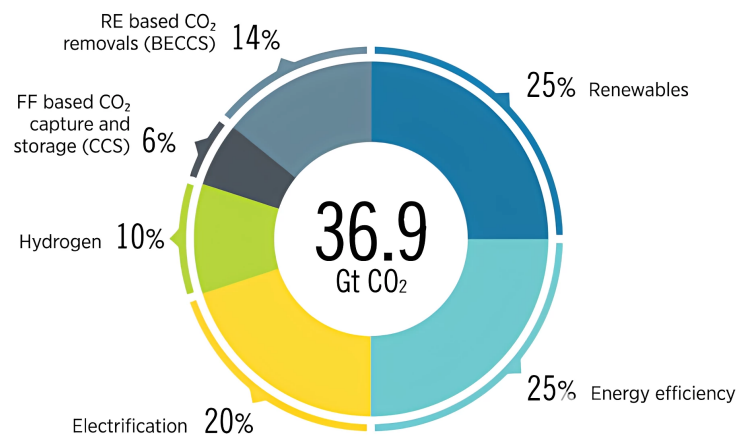


Figure 1.2: Impact of the several strategies to abate CO_2 emissions as estimated by IRENA.

Figure 1.2 reports the same kind of analysis by IRENA [6]. A strong contribution to the decarbonization will be provided by improvements in the efficiency of energy processes, which are expected to count for around the 25% of the GHG abatement. The renewables share is slightly below the forecast by IEA (33% vs 25%), whereas the impact of H_2 exploitation is a little higher, counting for around the 10%.

Concerning the usage of H_2 in the European Union up to 2030, two different scenarios, the “REPowerEU” and “Fit for 55”, have been hypothesized. There are marked differences between the two in terms of total H_2 consumption: according to the “REPowerEU” scenario, 20 Mt of H_2 will be used in 2030, whereas a significant lower amount (8 Mt) is forecast by the “Fit for 55” scenario.

Both the scenarios are reported in Figure 1.3. According to the “REPowerEU”, the highest demands of H_2 will come from ammonia production, the transportation sector, and heat generation for industry. In both the scenarios, H_2 for the transportation sector will count for around 10% of the overall production. To realize a H_2 based economy, massive investments need to be deployed. According to the IRENA forecast, 4 trillion USD must be invested by 2050 for the H_2 production and the build up of the related infrastructure. Figure 1.4 reports the breakdown of the total investment. The vast

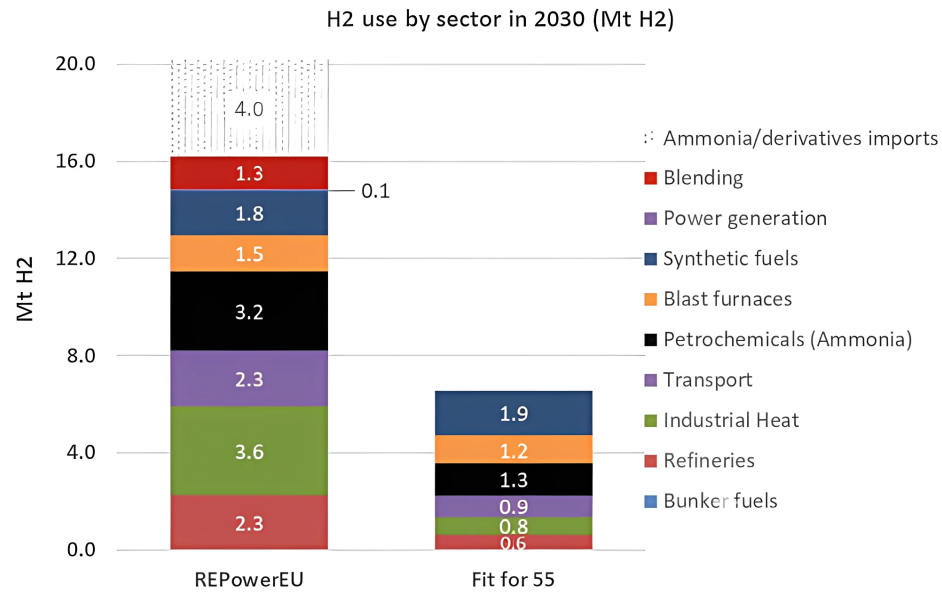


Figure 1.3: Forecast of H₂ usage in 2030, according to the *REPowerEU* scenario and *Fit for 55* program.

majority is due to power generation, followed by the cost of the electrolyzers. Other costs are related to the H₂ transportation, either by pipelines and ships, storage and conversion plants. Although the investment might look massive, it represents only the 8% of the global investment needed for the 1.5° scenario up to 2030 [7].

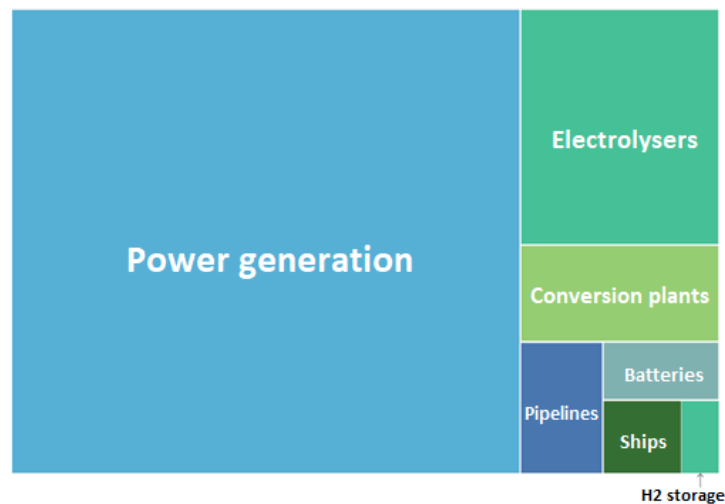


Figure 1.4: Graphical breakdown of the costs associated with the large scale usage of H₂ to achieve the 1.5°C scenario by 2030 [6].

1.3 Hydrogen cost and production capacity

According to IRENA, the cost of H_2 production has already substantially decreased (55%-85%) in the last ten years. This trend is expected to keep on in the near future, thanks to the progressive reduction of the cost of electricity from renewables and the improvements of the electrolyzers efficiency. Additionally, the economy of scale should lower the price of the electrolyzers from 1600-1800 USD/kW to around 400 USD/kW in 2030, followed by a further slight decrease below 400 USD/kW by 2050, as shown in Figure 1.5.

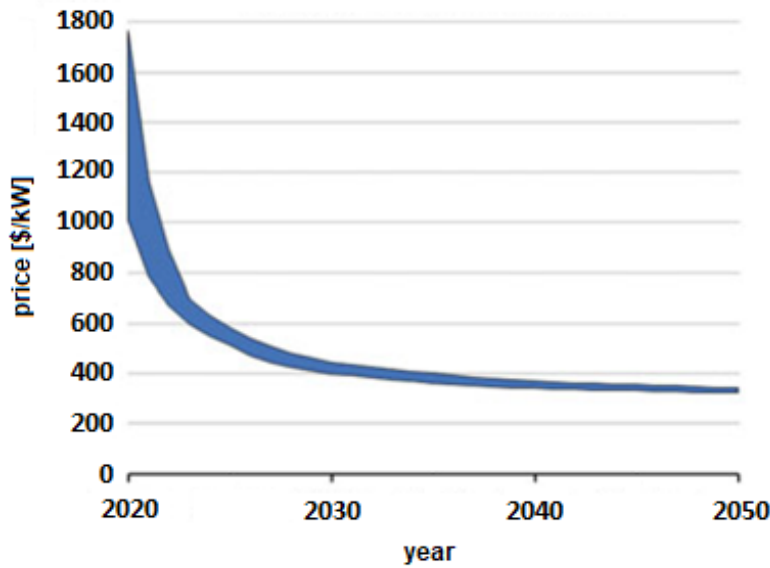


Figure 1.5: Forecast of the electrolyzers price drop (USD/kW) from 2020 to 2050.

Thanks to this trend, along with the improvements in the electrolyzers efficiency and the wider spread of renewables, green H_2 is expected to be cost-competitive with blue H_2 in 2030. As illustrated in Figure 1.6, the cost of H_2 produced by renewable energy is between 3 and 8 USD/kg, where the wide range of price is caused by the scatter in process efficiency and hours of operation of the electrolyzers.

For comparison, H_2 produced from natural gas by means of the steam reforming costs around 1 USD/kg, whereas the price increases by just 0.5 USD when exploiting the CCUS technology. More in detail, price of green H_2 strongly depends on the kind of renewable source exploited. To reach the same price of blue H_2 , cost electricity of renewables should be lower than 20 USD/MWh [5]. At the moment, this goal is considered achievable by 2030 using photovoltaic plants in specific regions in the Middle East. For instance, the price of photovoltaic electricity is currently 32 USD/MWh in Chile and 23 USD/MWh in Saudi Arabia.

Wind farms in the North Sea are a more expensive solution at the moment. According to [8], price of electricity from wind farms is in the range between 50-100 USD/MWh,

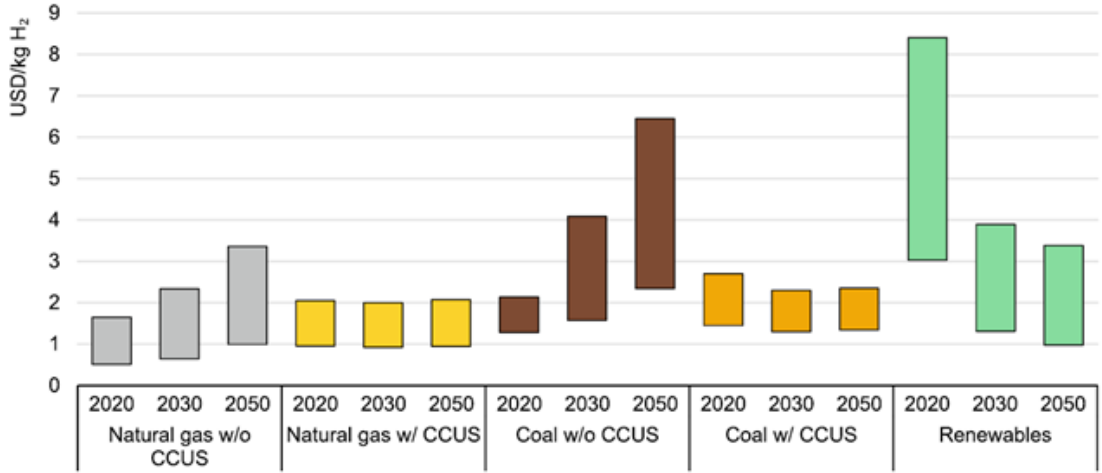


Figure 1.6: Cost of H_2 production by technology in 2020, and forecast for 2030 and 2050 [5].

with the most efficient plants that could reach 30 USD/MWh. If the price decrease to 25 USD/MWh in 2050, H_2 produced by wind would cost around 1.5 USD/kg, becoming competitive with blue H_2 . Although wind seems to be a more expensive solution, it represents the main way for green H_2 production in the north regions of the globe. Indeed, the projection by [9] estimates a future installed wind power capacity in the North Sea between 70-150 GW, which is the 20% of the overall European Union demand of electricity. [10] predicts that renewables will become the largest global electricity source in 2025. Wind and photovoltaic plants will supply nearly 20% of global power by 2027, and solar photovoltaic capacity alone will surpass coal by 2027.

Even if a huge increase in the exploitation of renewable energy is foreseen in the next 5-10 years, reports show that a limiting factor might be the capability to increase the electrolyzers capacity on time. In the IEA Net Zero Emissions Scenario, electrolysis capacity should be over 700 GW by 2030, while the installed capacity at the end of 2022 was just over 1 GW. The current manufacturing capacity is 8 GW per year though industry aims at a global manufacturing capacity of 65 GW per year by 2030. This gap highlights the need of a faster development in production capacity, especially considering that if all the announced projects actually came true, worldwide capacity in 2030 would still be limited at just 134–240 GW.

1.4 Hydrogen for the transportation sector

H_2 is surely considered one of the promising solutions to decarbonize the transportation sector. According to the IEA Net Zero Emissions Scenario, in 2030 around the 45% of H_2 and H_2 based fuels will be used to power road vehicles, either through Fuel Cells (FCs) or Internal Combustion Engines (ICEs). The former are considered an attractive

solution thanks to high conversion efficiency, which can be as high as 60%, while the peak efficiency for H_2 ICEs is estimated to slightly exceed the 40% [11]. Moreover, FCs do not produce any kind of NO_x emission, whereas this might happen for H_2 ICEs as will be later discussed. In spite of this, the widespread of FC vehicles is hindered by cost reasons. For instance, [5] estimates that the overall price of a FC based heavy-duty truck can be from 10% to 45% higher than a Diesel engine truck. Whatever the H_2 powertrain solution, several technological issues must be addressed to create a H_2 based transportation sector.

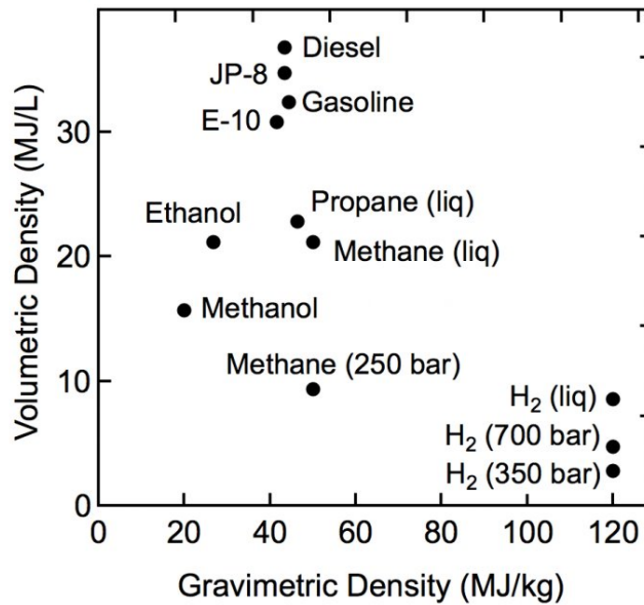


Figure 1.7: Gravimetric versus volumetric energy density of common and novel fuels for the transportation sector [12].

As shown in Figure 1.7, H_2 features the highest gravimetric energy density (around 120 MJ/kg) but the volumetric energy density is the lowest among the most common fuels. Cryogenic storage achieves a volumetric energy density comparable to compressed methane, but the shortcoming is the energy expense to liquefy and keep H_2 in a liquid state. Other solutions are currently under-development for the storage. State of art tanks are able to cope with an internal pressure as high as 700 bar, for which the volumetric energy density is roughly half that of compressed methane. Another solution is to exploit chemical bonds between H_2 and metal-hydrides or carbon-sorbents. Whatever the solution, the targets set by the U.S. Department of Energy (DOE) in terms of vehicles driving range are hardly achievable. These consist in ensuring a storage capacity between 4-10 kg to enable a driving range between 500 and 800 km.

High pressure storage leads to an increase of the vehicle weight due to the reinforced tank. For example, at 700 bar the H_2 to tank weight ratio is around 5%, which means that the tank weight is around 20 times higher than that of the stored fuel [12]. Under

this condition, the volumetric energy density is around 27 kg/m^3 , which is far below the U.S DOE target of 70 kg/m^3 .

Moreover, a non-negligible amount of energy must be provided to compress the fuel. Theoretically, compressing H_2 at ambient conditions up to 800 bar would require 8 MJ/kg through an ideal iso-thermal transformation. For an adiabatic process the figure would rise to 22 MJ/kg. A more realistic multi-staged and intercooled compression would require around the 12% of the energy content stored in the 800 bar fuel [13]. Further energy should be spent to deliver the gas. This amount strongly depends on the development of the distribution network. According to the *Fit for 55* program, the goal is to realize a distribution network with refueling stations every 150 km, able to deliver 2 tons of H_2 per day at 700 bar.

1.5 Thesis objectives

This work is devoted to the analysis of the direct injection (DI) and combustion processes in H_2 ICEs. As it will be discussed later, H_2 ICE can represent a bridge solution - based on the reliable technology developed throughout the last 150 years - as long as FCs and electric powertrains become economically affordable and allow for long driving ranges.

The DI technology is generally considered the way to reach a high power density and high efficiency, but many topics are still to be analyzed to optimize the engine performance, which markedly depends on the mixing process in the DI mode. Under this framework, numerical simulations are a valuable tool to study the injected flow features, the subsequent mixing, and the combustion. Commercial CFD codes, such as ANSYS Fluent and Converge CFD, have been extensively employed to analyze the main phenomena occurring throughout a complete engine cycle.

The current research aims at enabling leaner and leaner operation in an effective way, to reduce the thermal losses through the walls as well as to keep NO_x emissions as low as possible. Therefore, in this thesis work attention has been posed on the strategies to extend the engine operability at ultra-lean conditions. More in depth, strategies to burn a mixture featured by an equivalence ratio equal to 0.25 have been tested. To such an effort, the research has started by understanding the fundamentals of the mixing between air and fuel starting from the injection phase. Therefore, the study has started from the analysis of the peculiar characteristics of the under-expanded H_2 flow discharged by the injector. Focus has been posed on the understanding of the gas-dynamic phenomena caused by the high pressure injection which must be correctly solved for capturing the transport of the fuel.

Afterwards the effect of the nozzle exit section shaped has been thoroughly investigated either considering the influence on the structure of the shocks and the effect of the mixing between H_2 and air at the boundary of the jet. This kind of analysis has been carried

out to draw information about the possibility to increase the homogeneity level of the mixture or, in the opposite way, to stratify the charge distribution.

In addition, an analysis focused on performance and emissions has been carried out exploiting the SANDIA Optical Hydrogen Engine (SOpHy) engine geometry. For the same operating point, several combinations of the start of injection (SOI) and injection pressure have been numerically tested. Stark differences have been observed in the fuel distribution at spark timing which, in turns, lead to massive differences in the combustion velocity, combustion peak pressure and phasing, as well as in the NO_x production. Therefore, a new goal has been identified: to determine solutions to create an optimal stratification of the charge. To such a goal, both the enhanced mixing provided by the non-circular sections, as well as multi-injection strategies have been analyzed. The latter have show to enable a useful localized enrichment of the charge around the spark, which speeds up the combustion process while keeping NO_x at a low level. As a last goal, focus has been posed on the improvement of the existing combustion models to take into account the peculiarities of hydrogen lean flames. Specifically the increased laminar flame speed due to thermodiffusive instabilities has been considered in the context of the G-equation combustion model, to allow a better capture of the pressure trend in CFD simulations.

1.6 Thesis Structure

The thesis is organized in six chapters, as follows:

- **Chapter 1** introduces the research theme project with its motivations and objectives;
- **Chapter 2** provides recalls on internal combustion engines and describes the most interesting hydrogen features as a fuel;
- **Chapter 3** provides the initial analysis on under-expanded flows which arise during the in-cylinder injection;
- **Chapter 4** focuses on the influence of the nozzle cross section shape on the under-expanded flow, both in terms of the gas-dynamics and mixing fo the H_2 jet;
- **Chapter 5** analyzes the main parameters influencing the in-cylinder mixing. Ways to reach the charge stratification are also investigated, as well as the effect of the

fuel distribution on the combustion;

- **Chapter 6** provides a preliminary analysis regarding the inclusion of the thermodiffusive H_2 instabilities in the G-equation combustion model.

Chapter 2

Hydrogen for internal combustion engines

2.1 Potential and limitations of future technologies for sustainable mobility

Currently, ICEs account for around the 25% of the power generation in the world, producing the 17% of the GHG emissions along with other nocive gases such as carbon monoxide (CO), nitrogen oxides (NO_x), particulate matter (PM), and unburned hydrocarbons (HC) [11]. Most of the research is directed towards the development of electric vehicles, but ICEs fueled by novel fuels can still play a role in the energy transition scenario.

The large-scale adoption of electric vehicles (EV) in Europe has slowed down in 2024. With respect to August 2023, the reduction in the matriculation of EVs has been around the 44%, with the worst market drops in Germany (-69%), Italy (-41%), and France (-33%). The trend might be a joint result of the inflation raised in the European Union, together with a certain level of skepticism due to the need to overcome some limitations of the EVs.

Driving range is one of the main concerns for the customers [14]. Lithium-ion batteries (LIBs) can provide a higher energy density than other kind of batteries (0.1-0.27 kWh/kg), but the energy density of gasoline fuel (12.2 kWh/kg) is still markedly higher (100 times). As an example, one of of cheapest EV model on the EU market in 2024, the Dacia Spring, ensures a driving range of around 300 km.

In Table 2.1, some of the future requirements for EVs are reported. As LIBs approach their technological limits [15], new kind of batteries allowing for energy densities over 350 Wh/kg should be developed. Lithium-sulfur, Lithium-air, and Mg-ion batteries show the potential to increase the energy density, but they also represent a challenge for the safety and recyclability. Although batteries price has considerably lowered in the

last years, EVs still represent a costly technology, being the current price around 200 USD/kWh. To become economically competitive with ICEs, the price should further drop to 125 USD/kWh for the battery pack (i.e., including sensors, controllers, etc.) and 100 USD/kWh for the single battery cell [16].

Table 2.1: Desired features for a wider EV batteries spread [16].

Feature	Desired
Energy density	Higher than 350 Wh/kg
Cost	Lower than 100 USD/kWh per cell
Charging speed	80% of the total capacity in 15 min
Duration	15 years
Safety	No fire, mechanical failure, explosion

Part of the cost could be further reduced thanks to the expansion of the large-scale production, whereas increasing the energy density might decrease the need for raw material, contributing to lower the overall production cost. Cobalt is one of the most expensive materials in the batteries, because it is mined in unstable Nations. It is commonly employed to build the battery cathode because of its thermal stability. Avoiding cobalt usage might be one of the strategies to reduce the cost, but it is not easily replaceable because it is crucial for the battery safety and the capability to avoid over-heating. Along with the price and energy density, charging time is another crucial issue. Currently, a full recharge takes several hours, which is manageable when spread throughout the day but becomes inconvenient for long-haul trips due to the need for extended stops. As reported in Table 2.1, the current goal is to allow to recharge the 80% of the battery capacity in less than 15 minutes. This would require further development in the cell chemistry as well as in the electrodes materials and thermal management. Indeed, during the charge ions move from the cathode to the anode, with an associated heat production. Increasing the charging rate would increase the heat production, ultimately leading to a reduced battery life and safety. Attempts to improve the charging rate have been carried out either pre-warming the battery to increase its kinetics or using higher voltage to reduce the circulating current.

Battery life is another point to be addressed. Due to inner packaging, batteries are usually considered not-repairable. Hence, as stated by the U.S. Advanced Battery consortium [17] the target is 15 years life, which is considered over when the initial capacity reduces to the 80%.

Another concern is related to the environmental temperature at which battery is expected to operate. In general, batteries need to be optimized for a specific temperature range. High temperatures speed up the charging process, but also trigger the growth of a solid electrolyte interface (SEI), which is a phenomenon degrading the battery life. At lower temperature SEI is limited, but other phenomena influencing battery life, like lithium plating, can occur [18]. Therefore, a proper thermal management needs to be

developed to ensure the optimal performance of the device. From a safety perspective, battery failures can be catastrophic events. They can be caused by improper use, crashes, or internal mechanisms such as lithium dendrite growth. This last might trigger short-circuits, or strong exothermal reactions leading to thermal runaway. The thermal runaway might be mitigated by new materials [19], but at the current state of the art novel materials for the electrodes can affect the cell performance, therefore setting the need to find a trade-off.

Fuel cells are another pillar through which abating GHG emissions. This kind of device directly transforms the chemical energy of the fuel into electricity, skipping the intermediate conversion into thermal energy needed by ICEs. This results in generally higher efficiencies than those of ICEs, as shown for instance in Figure 2.1, where peak efficiency is over 54%.

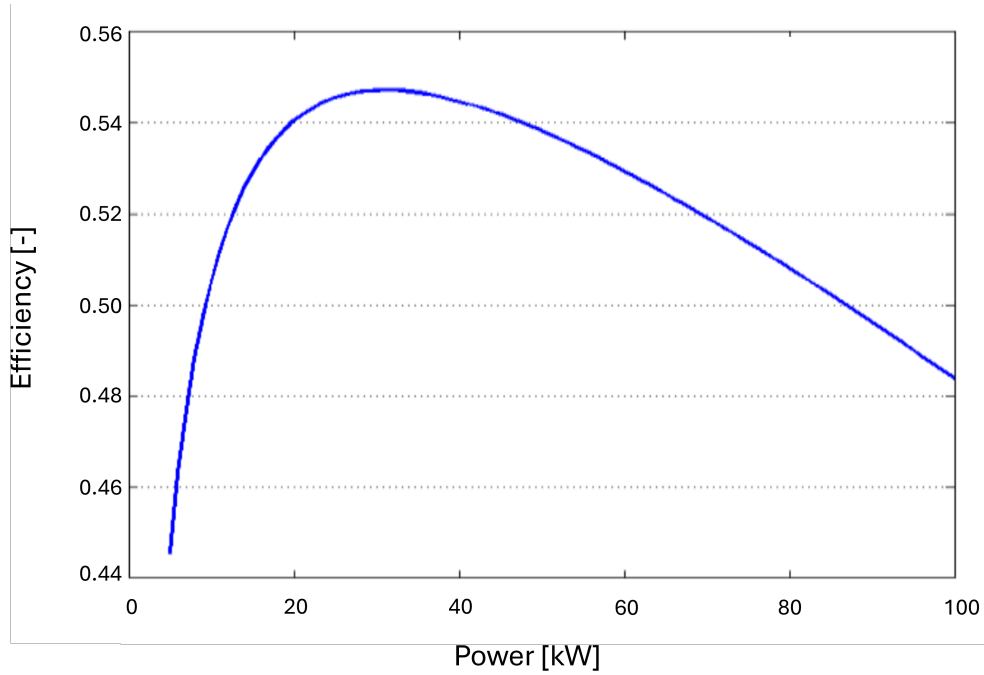


Figure 2.1: Typical trend of fuel cell efficiency curve [20].

Nonetheless, FCs spread is mainly hindered by cost reasons, because rare materials such as platinum are usually employed to catalyze the electrochemical reaction. Additionally, the tolerance to fuel impurities, such as carbon-monoxide (CO), is low, causing the deactivation of the catalyst due to the adsorption of CO into the electrodes.

For all of these reasons, ICEs fueled by H_2 are an open field of research, since H_2 ICEs can be considered a bridge-solution while waiting for improvements for both batteries and FCs. Therefore, in the next paragraph some basic concepts about ICEs are recalled.

2.2 Recalls on internal combustion engines

ICEs are mechanical devices converting the chemical energy of a fuel into mechanical work applied to a shaft. A combustion process turns the fuel chemical energy into heat supplied to the working fluid, whose expansion is exploited by a connection rod-crank mechanism to apply mechanical work to the shaft. The device is schematically made up of a cylinder, inside which a piston slides alternatively, the connection rod-crank mechanism, and the shaft as illustrated by Figure 2.2. The volume swept by the piston is defined displacement volume V_d . The Top Dead Center (TDC) is the axial position where the piston is closest to the cylinder head. The specular position, the furthest from the cylinder head, is defined Bottom Dead Center (BDC).

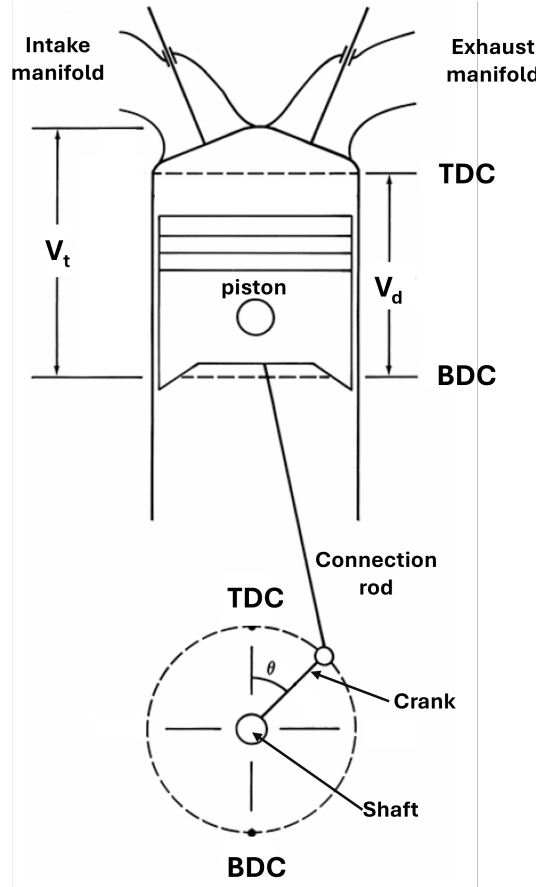


Figure 2.2: Sketch of the main components of an ICE [21].

The minimum volume, or clearance volume V_c is reached when piston is at the TDC, while the maximum volume, or total volume V_t is obtained at the BDC. The compression ratio CR is defined as follows:

$$CR = \frac{V_t}{V_c} \quad (2.1)$$

The following relations there exist between V_d , V_t , and V_c :

$$V_d = V_t - V_c \quad (2.2)$$

$$V_t = \frac{CR}{CR - 1} V_d \quad (2.3)$$

$$V_c = \frac{1}{CR - 1} V_d \quad (2.4)$$

The operation is cyclic. Every cycle starts with the intake of fresh air or fresh air/fuel mixture and finishes with the discharge of burnt gases. Depending on the number of shaft rotations, ICEs are classified either as 4-stroke or 2-stroke engines. In a 4-stroke engine, the thermodynamic cycle can be divided into:

- an intake stroke: piston moves from the TDC to the BDC. The intake valves are open allowing the depression caused by the piston motion draw fresh air or fresh air/fuel mixture from the intake runners into the cylinder;
- a compression stroke: all the valves are closed. Piston moves from the BDC to the TDC compressing the gas trapped in the cylinder;
- a power stroke: the air-fuel mixture burns, with an increase of both pressure and temperature. The expansion of the gas pushes the piston from the TDC to the BDC, providing useful mechanical work to the shaft.
- an exhaust stroke: the exhaust valves are open while the piston moves back from the BDC to the TDC, allowing to discharge the burnt gases from the cylinder to the exhaust runners. A new cycle can start.

Another distinction depends on how the mixture is ignited. In spark ignition (SI) engines, mixture is ignited by means of the energy provided by a spark. Conversely, in compression ignition (CI) engines, the in-cylinder thermodynamic conditions reached towards the end of the compression stroke are sufficient to ensure the auto-ignition of the mixture.

Figure 2.3 shows an experimental pressure trend inside the cylinder of a 4-stroke SI engine. Such kind of measurement is useful to compute the work extracted by each cycle, defined "indicated work", W_i , as follows:

$$W_i = \oint F_{piston} dx = \oint p S_{piston} dx = \oint p dV \quad (2.5)$$

being F_{piston} the net force applied by the gas to the piston surface, S_{piston} , by means of the in-cylinder pressure, p . Accordingly, the indicate power P_i is defined as:

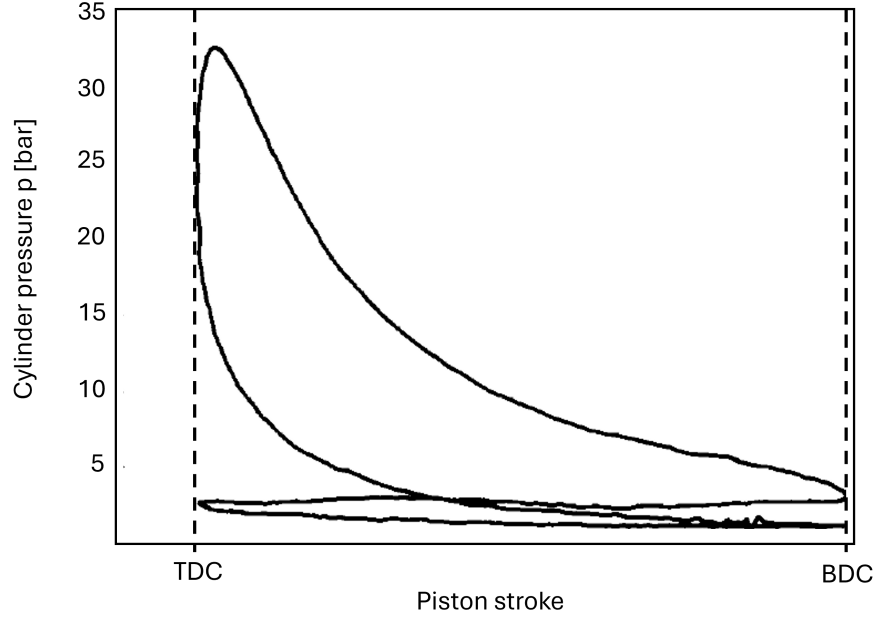


Figure 2.3: Pressure traces in a spark ignition engine [21].

$$P_i = W_i \frac{n_{shaft}}{m} \quad (2.6)$$

being n_{shaft} the number of shaft revolutions per second and m a constant equal to 1 for 2-stroke engines and equal to 2 in 4-stroke engines. The effective power P_e provided to the shaft is lower than P_i because of the mechanical losses and the power needed by the auxiliary systems. These two contributes can be gathered into a lost power P_w such that:

$$P_e = P_i - P_w = C\omega \quad (2.7)$$

being C the momentum applied to the shaft and ω its rotational speed in rad/s. Dividing Equation (2.7) by n_{shaft}/m we get a similar expressions for the effective work:

$$W_e = W_i - W_w \quad (2.8)$$

Dividing W_e by the displacement volume V_d we get:

$$BMEP = \frac{W_e}{V_d} \quad (2.9)$$

being BMEP the brake mean effective pressure, i.e., a quantity expressing the effectiveness in extracting useful work from the cylinder. It has the dimension of a pressure quantity. Different levels with growing complexity can be used to model the thermodynamics of ICEs. The simplest approach relies on *ideal* cycles, based on the following

assumptions:

1. the working fluid is a perfect gas;
2. fluid-dynamic and thermal losses are negligible;
3. changes of the chemical and physical properties of the working fluid are not taken into account;
4. the working fluid is neither drawn into the cylinder nor discharged, i.e., phases in which mass exchange takes place are neglected.

Under such assumptions, compression and expansion strokes are considered isentropic processes. Therefore, the Otto cycle generally used to model SI engines, illustrated in Figure 2.4 in pressure-volume diagram, is made up of the following transformations:

1. isentropic compression (1-2)
2. heat supply at constant volume (2-3)
3. isentropic expansion (3-4)
4. heat release at constant volume (4-1)

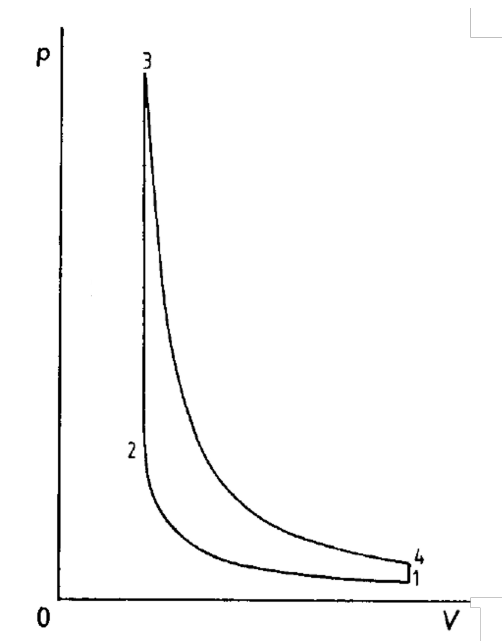


Figure 2.4: Otto cycle in the pressure-volume diagram.

In a CI engine, combustion is usually split into a premixed phase followed by a diffusive stage. Consequently, the best ideal approximation is provided by a Sabathè cycle, reported on the same pressure-volume diagram in Figure 2.5. The Sabathè cycle comprises:

1. an isentropic compression (1-2)
2. a heat supply at constant volume (2-3)
3. a heat supply at constant pressure (3-3')
4. an isentropic expansion (3'-4)
5. a heat release at constant volume (4-1)

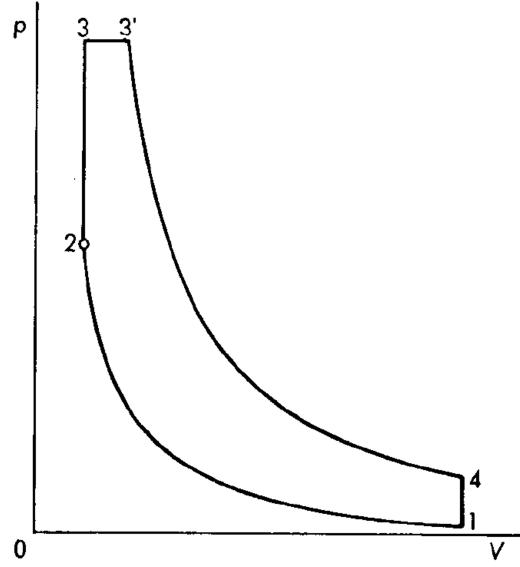


Figure 2.5: Sabathè cycle in the pressure-volume diagram.

For the sake of the following analyses about H_2 internal combustion engines, it is worth discussing about the heat supply phase. In an ideal cycle, the first law of thermodynamics reads:

$$W_{id} = Q_1 - Q_2 \quad (2.10)$$

being W_{id} the ideal work extracted by the cycle and Q_1 and Q_2 the heat supplied and heat released, respectively. On a temperature-entropy diagram, the area under a generic reversible transformation represents the heat exchanged throughout the process. Let us compare three cycles, starting from the same conditions (point 1), with the same compression ratio, and the same amount Q_1 of heat supplied, as shown in Figure 2.6. The three cycles differ in the way the heat is supplied. Cycle 1234 is characterized by a constant volume heat supply (Otto cycle), cycle 123'4' by a constant pressure heat supply (Diesel cycle), and cycle 123''4'' by a first constant volume heat supply followed by a constant pressure heat supply. From Figure 2.6, reader can notice that constant volume heat supply transformation has a higher slope than that of the constant pressure transformation. Therefore, when comparing a constant volume against a constant

pressure transformation for a fixed Q_1 , the entropy of point 3 results to be lower than the entropy of point 3'. The same can be stated for points 4 and 4' at the end of the expansion strokes. As a main consequence, the heat released Q_2 in the transformation 41 is lower than Q_2 of the transformation 4'1. This means that higher work is extracted by the cycle 1234 according to Equation 2.10, i.e., the efficiency is higher than that of cycle 123'4'.

The split constant-volume/constant-pressure heat supply of the cycle 123''4'' results in an intermediate efficiency between the two former cases. The main consideration drawn by this comparison is that, as a general rule, the higher the combustion process the higher the thermodynamic efficiency of the cycle. As it will be shown in the following section, H_2 features a laminar flame speed (s_L) generally higher than what observed burning carbon-based fuels, enabling the possibility to reach high engine efficiencies.

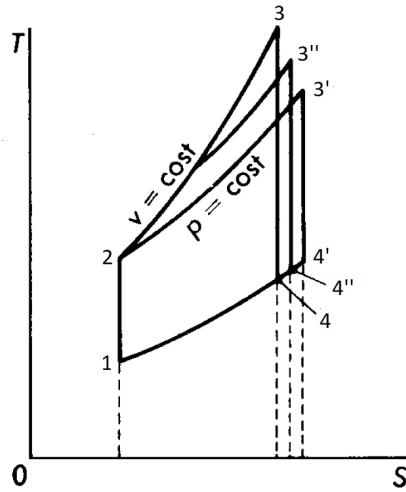


Figure 2.6: Comparison among the different ideal engine cycles.

While a preliminary analysis based on ideal cycles can be useful to compute rough data about trends of pressure and temperature, the approach results too simplified to catch the real operation of the engine, which includes various and complex chemical and physical phenomena. In particular:

1. the working fluid is not a perfect gas: specific heats c_p (at constant pressure) and c_v (at constant volume) vary with temperature, and so does the elastic constant R ;
2. Heat is not supplied externally as modeled by ideal cycles. Rather, it is provided by a combustion process whose reactions are generally not in equilibrium. Therefore, the chemical kinetics has a huge effect of the engine operation;
3. to start a new cycle, burnt gases must be discharged at the end of the expansion

stroke and new fresh mixture must be blown into the cylinder. Such a process constitutes the bottom cycle in Figure 2.3, requiring work from the shaft;

4. heat losses through the walls are not negligible, especially during the combustion and expansion strokes. This results in a lower pressure throughout the expansion stroke and ultimately in a lower efficiency. Heat losses are proportional to the time by which the working fluid is in contact with the walls. Consequently, heat losses are more relevant for lower rotational speed regimes. They also depend on the geometry of the chamber, specifically on the ratio between the overall wall surface and the displacement volume. To minimize the losses, the ratio between the piston stroke and piston bore should be close to 1.
5. the amount of air drawn from the intake runners into the cylinder is lower than the theoretical amount equal to $\rho_a V_d$. The reduction is caused by either the losses through the runners and the intake valves and the density drop caused by the heat provided by hot walls. A further reduction is due to the presence of residual burnt gases at higher pressure inside the cylinder, which must expand during the first stages of the intake stroke to allow for the introduction of the fresh gas. A volumetric efficiency λ_v can be then defined as the ratio between the effective drawn mass m_a and the theoretical one:

$$\lambda_v = \frac{m_a}{\rho_a V_d} \quad (2.11)$$

Due to the complexity of such phenomena and their mutual interaction, the full understanding and optimization of the engine operation is a challenging task. In most of the cases, 0D/1D models - once properly calibrated - can quickly and cheaply provide maps of the engine. Nonetheless, further phenomena linked to the injection process and mixing between fuel and oxidizer can be better investigated by means of 3D RANS/LES simulations. Numerical simulations provide the possibility to test different geometries for the chamber, the injectors, spark position, revealing more thoroughly how the physical phenomena occurring throughout the engine operation interact.

Lastly, it is worth recalling that for a fixed amount of fuel m_{fuel} to be burnt, there exists an exact amount, or stoichiometric amount of air, $m_{air,st}$, required for the combustion. The ratio between air and fuel masses is the air/fuel ratio, α . When the minimum mass of air for a complete oxidation of the fuel is considered, we are under stoichiometric conditions:

$$\alpha_{st} = \frac{m_{air,st}}{m_{fuel}} \quad (2.12)$$

α_{st} depends on the kind of fuel. The equivalence ratio, ϕ , defined as:

$$\phi = \frac{\alpha_{st}}{(m_{air}/m_{fuel})} \quad (2.13)$$

indicates whether the combustion is led with excess of air (lean mixture, $\phi < 1$) or with excess of fuel (rich mixture, $\phi > 1$). For engine applications, it is common practice to use the parameter λ , defined as the reciprocal of ϕ . Therefore, lean mixtures are characterized by $\lambda > 1$ and rich mixtures by $\lambda < 1$.

2.3 Hydrogen as a fuel

H₂ as a fuel for ICEs has both favorable and negative features. A comparison of the chemical and physical properties of H₂ against standard hydrocarbon fuels (methane CH₄, iso-octane C₈H₁₈) at ambient conditions (pressure = 1 atm, temperature = 293.15 K) is reported in Table 2.2.

Table 2.2: Properties of H₂ against methane and iso-octane at ambient conditions.

Property	H ₂	Methane	Iso-octane
Lower Heating Value [MJ/kg]	120	50	44.3
Lower Heating Value [MJ/Nm ³]	10	33	30656
Density [kg/m ³]	0.08	0.67	692
Flammability limits (λ)	0.14-10	0.6-2	0.26-1.51
Stoichiometric ratio	34.2	17.1	15
Minimum ignition energy [mJ]	0.02	0.28	0.28
Minimum quenching distance [mm]	0.64	2.03	3.5

Trivially, the most significant feature is the absence of carbon atoms in the molecule, allowing for a combustion without CO₂ emissions. Nonetheless, particulate emissions cannot be considered fully negligible. For instance, in [22], an experimental analysis was run to compare particulate emissions from a Diesel engine, modified to also operate with compressed natural gas (CNG), gasoline, a CNG/H₂ blend, and pure H₂. The results showed that burning H₂ resulted in the lowest emissions, still not negligible, as shown in Figure 2.7. As for the other fuels, particulate increased at higher loads. The PM emissions were attributed to the incomplete combustion and pyrolysis of lubricating oil. Similar conclusions can be also found in [23] and [24].

Comparing the energy content reported in Table 2.2, a huge difference exists between the H₂ gravimetric and volumetric Lower Heating Values (LHVs). On a mass basis, H₂ has the highest LHV. Nonetheless, due to the extremely low density at ambient conditions, the volumetric LHV is around one third that of methane, and three orders magnitude lower than iso-octane. To address this issue, research is focused on high-pressure storage solutions for gaseous H₂. Currently, tanks able to store H₂ up to 700

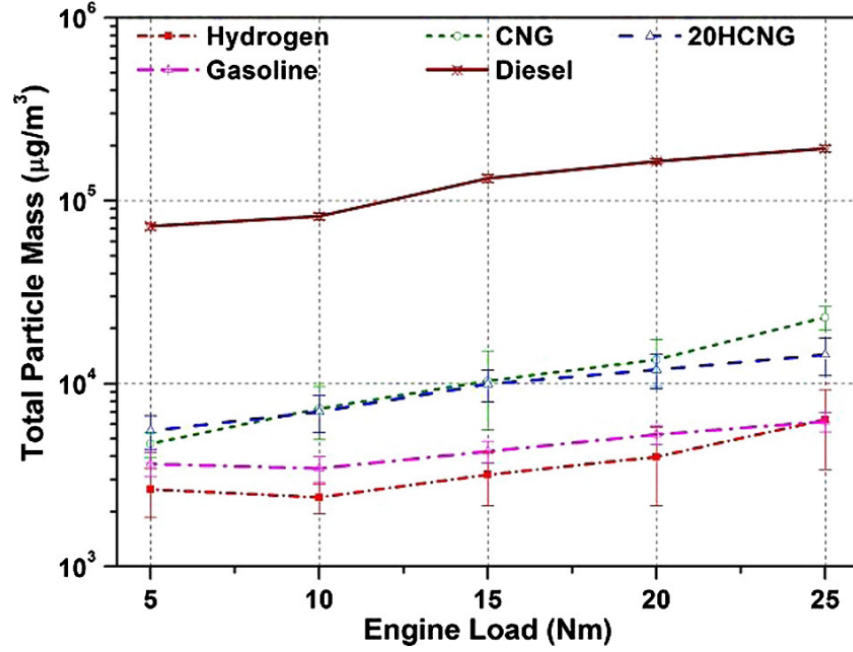


Figure 2.7: Particulate emissions burning different fuels. H_2 emissions are due to traces of lubricant oil in the combustion chamber. [22]

bar at ambient temperature are under-development [25]. At such a pressure level, the volumetric LHV would rise to 5000 MJ/Nm^3 , allowing for longer missions between two consecutive refuels. Fuel properties reported in Table 2.2 refer to ambient pressure and temperature, but significantly change under ICE conditions.

In ICEs applications, mixture properties, which depend on the excess of air, λ , should be taken into account. An example is reported in Table 2.3 for H_2 -air, methane/air, and iso-octane/air mixtures. For H_2 , two mixtures are considered, either at $\lambda=1$ and $\lambda=4$.

Table 2.3: Properties of H_2 /air mixtures at $\lambda=1$ and $\lambda=4$ versus methane/air and iso-octane/air at $\lambda=1$.

Property	H_2 /air $\lambda=1$	H_2 /air $\lambda=4$	Methane/air $\lambda=1$	Iso-octane/air $\lambda=1$
Fuel volume fraction [%]	29.5	9.5	9.5	1.65
Autoignition temperature [K]	858	>858	813	690
Adiabatic flame temperature [K]	2390	1061	2226	2276
Specific heat ratio [-]	1.4	1.4	1.354	1.389
Laminar flame speed at 360 K [cm/s]	290	12	48	45

Due to the already discussed low molecular weight, the volume fraction of H_2 in a

stoichiometric mixture at ambient conditions is almost 30%, while at $\lambda=4$ it is close to the stoichiometric volume fraction of methane, but more than five times higher than iso-octane. Even though pressure and temperature are far from ambient conditions in ICE applications, the problem of the low H_2 density still stands and can hinder the achievement of high power-density in specific ICE architectures.

One of the most interesting and useful properties of H_2 as a fuel is the possibility to reach a fast flame propagation, which better approximates a constant volume combustion. As previously demonstrated, the constant volume combustion provides the highest ideal efficiency.

As shown in Table 2.3, at ambient pressure and for a temperature of 360 K, the H_2 laminar flame speed (s_L) of a stoichiometric mixture is 290 cm/s, around 6 times the s_L of methane and iso-octane at the same conditions. However, when diluting the H_2 mixture, s_L can significantly drop especially under ultra-lean conditions. Such a problem has been addressed in the context of this doctoral work, and will be discussed in the next Chapters. The generally higher H_2 laminar flame speed can be explained by several physical and chemical features. The high diffusivity of H_2 molecule has surely a role, as well as the high adiabatic temperature. Further, the flame speed can be also explained in terms of chemical kinetics, specifically looking at the production of chemical radicals. Table 2.4 reports the H_2 - O_2 reactions of the San Diego chemical mechanism, each with the coefficients of the kinetics expressed by the following Arrhenius law:

$$k_i = AT^n e^{\frac{-T}{T_a}} \quad (2.14)$$

being k_i the reaction rate of the i – th reaction, A the pre-exponential factor, T the reaction temperature, and T_a the activation temperature.

The mechanism is organized into groups of reactions. Shuffle reactions describe the rapid interconversion of H, OH, O atoms/molecules composing the radical pool of the flame. Summing the reactions, it results that the shuffle group converts three H_2 molecules into two highly reactive H radicals.

In presence of a third-body molecule M, the H radical can be converted into HO_2 , which combines with H, O, and OH radicals by means of the strongly exothermal hydroperoxyl reactions.

Radicals can also recombine by means of the radical-radical reactions R1-R4 which are relevant for stoichiometric and rich deflagrations as well as for rich diffusion flames. Besides, the reaction R2 is also significant for the auto-ignition process of rich mixtures [12]. Combustion scenarios characterized by high pressures and low temperatures tend to facilitate the formation of substantial quantities of hydrogen peroxide H_2O_2 by means of the hydrogen peroxide reactions, the last group of the chemical mechanism. This occurs because elevated concentrations of HO_2 radicals enhance the production of H_2O_2 , primarily through the reaction HP2. In the presence of hydrogen peroxide, the regeneration of

Table 2.4: Reactions of the H₂-O₂ San Diego Mechanism. Coefficients are provided by [26] [27] [28] [29] [30] [31] [32].

Reaction	A	n	T _a	Name
Shuffle reactions				
H + O ₂ ⇌ OH + O	3.42e+16	-0.7	8590	S1
H ₂ + O ⇌ OH + H	5.06e+04	2.67	3165	S2
H ₂ + OH ⇌ H ₂ O + H	1.17e+09	1.3	1825	S3
H ₂ O + O ⇌ OH + OH	7.00e+05	2.33	7321	S4
Hydroperoxyl reactions				
H + O ₂ + M ⇌ HO ₂ + M	k ₀ 5.75e+19 k _∞ 4.65e+12	-1.44 0.44	0 0	H1
HO ₂ + H ⇌ OH + OH	7.08e+13	0	148	H2
HO ₂ + H ⇌ H ₂ + O ₂	1.66e+13	0	414	H3
HO ₂ + H ⇌ H ₂ O + O	3.10e+13	0	866	H4
HO ₂ + O ⇌ OH + O ₂	2.00e+13	0	0	H5
HO ₂ + OH ⇌ H ₂ O + O ₂	k ₀ 2.89e+13 k _∞ 4.50e+14	0	-250 5500	H6
Radical - radical recombination reactions				
H + OH + M ⇌ H ₂ O + M	4.00e+22	-2.0	0	R1
H + H + M ⇌ H ₂ + M	1.30e+18	-1.0	0	R2
O + O + M ⇌ O ₂ + M	6.17e+15	-0.5	0	R3
H + O + M ⇌ OH + M	4.71e+18	-1.0	0	R4
Hydrogen peroxide reactions				
OH + OH + M ⇌ H ₂ O ₂ + M	k ₀ 2.76e+25 k _∞ 9.55e+13	-3.22 -0.27	0 0	HP1
HO ₂ + HO ₂ ⇌ H ₂ O ₂ + O ₂	k ₀ 1.03e+14 k _∞ 1.94e+11	0 0	5556 -709	HP2
H ₂ O ₂ + H ⇌ HO ₂ + H ₂	2.30e+13	0	4000	HP3
H ₂ O ₂ + H ⇌ H ₂ O + OH	1.00e+13	0	1804	HP4
H ₂ O ₂ + OH ⇌ H ₂ O + HO ₂	k ₀ 1.74e+12 k _∞ 7.59e+13	0 0	160 3660	HP5
H ₂ O ₂ + O ⇌ HO ₂ + OH	9.63e+06	2.0	2009	HP6

radicals through the reverse reaction HP1 creates an alternative chain-branching mechanism. This mechanism becomes crucial for high-pressure deflagrations near flammability limits, detonations near detonability limits, and for the autoignition of the mixture.

As previously stated, the higher laminar flame speed of H₂ mixtures with respect to hydrocarbon fuels is determined - among the others - by the production of radicals. Specifically, shuffle reaction S1 consumes one H radical producing two radicals, OH and O. This reaction is in competition with the reaction H1 for the consumption of H. It has been observed that the combustion kinetics is strongly influenced by S1 over a crossover temperature around 1050 K, whereas S4 is predominant below this threshold.

Over the crossover temperature, the O and OH radicals produced by reaction S1 enable the fuel consumption reactions S2 and S3, which in turn release two new H

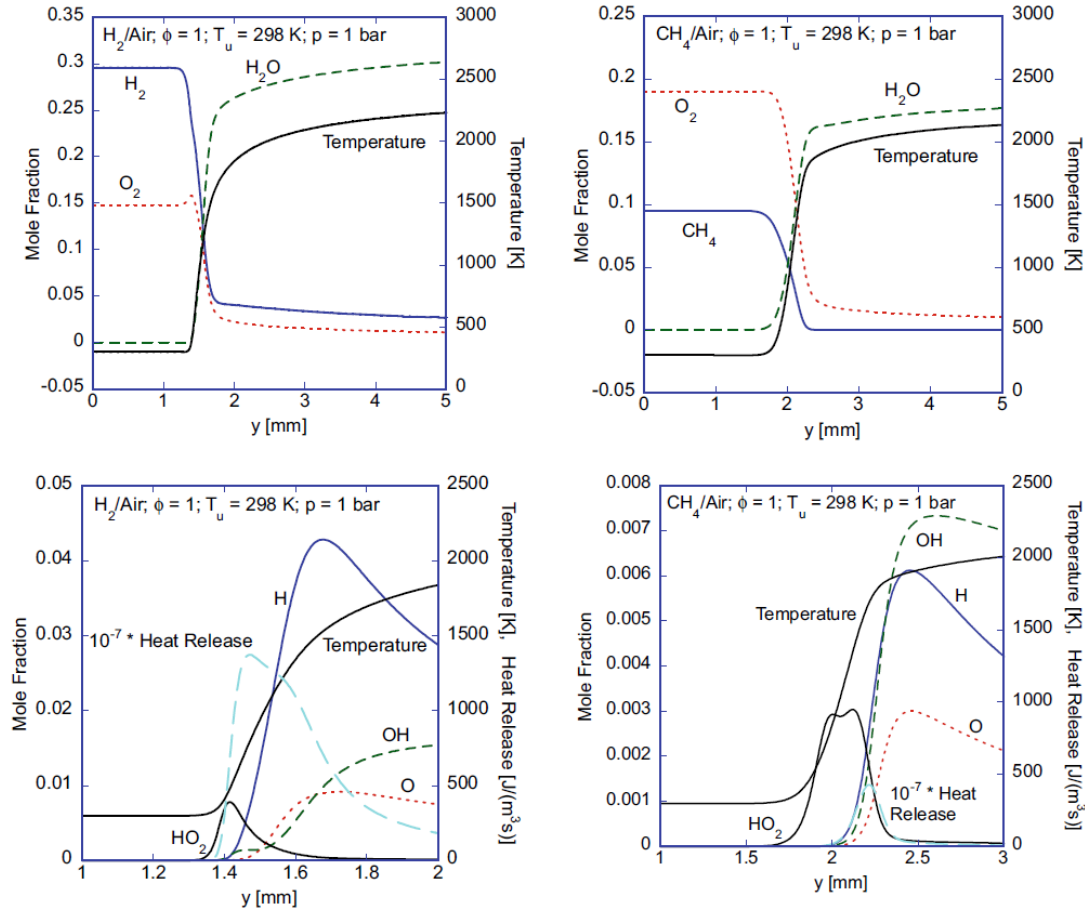


Figure 2.8: Left plots: structure of a stoichiometric H_2 flame. Right plots: structure of a stoichiometric CH_4 flame.

radicals. These three reactions influence the flame characteristics, as illustrated by Figure 2.8 which reports, on the left plots, the structure of a stoichiometric H_2 flame. The sum of S1-S2-S3 gives the following chain starting reaction:



which creates a layer of intense H production, roughly spanning between 1.5 and 1.8 mm. The H radical can then diffuse towards a second layer whose temperature is below the crossover temperature. In this layer, the chain breaking reactions H1, H3, H6 are activated. In this region, also the chain-propagating reaction H_2 is enabled, but it is generally seen that the sum of H1, H3, H6 and H_2 is still a chain-breaking. These reactions are strongly exothermal, and the layer can be identified by the extension of heat release curve in Figure 2.8.

Thus, the efficiently propagation of the flame then stems in high production of H radicals by reactions S1-S3 and the following diffusion in the radicals consumption layer.

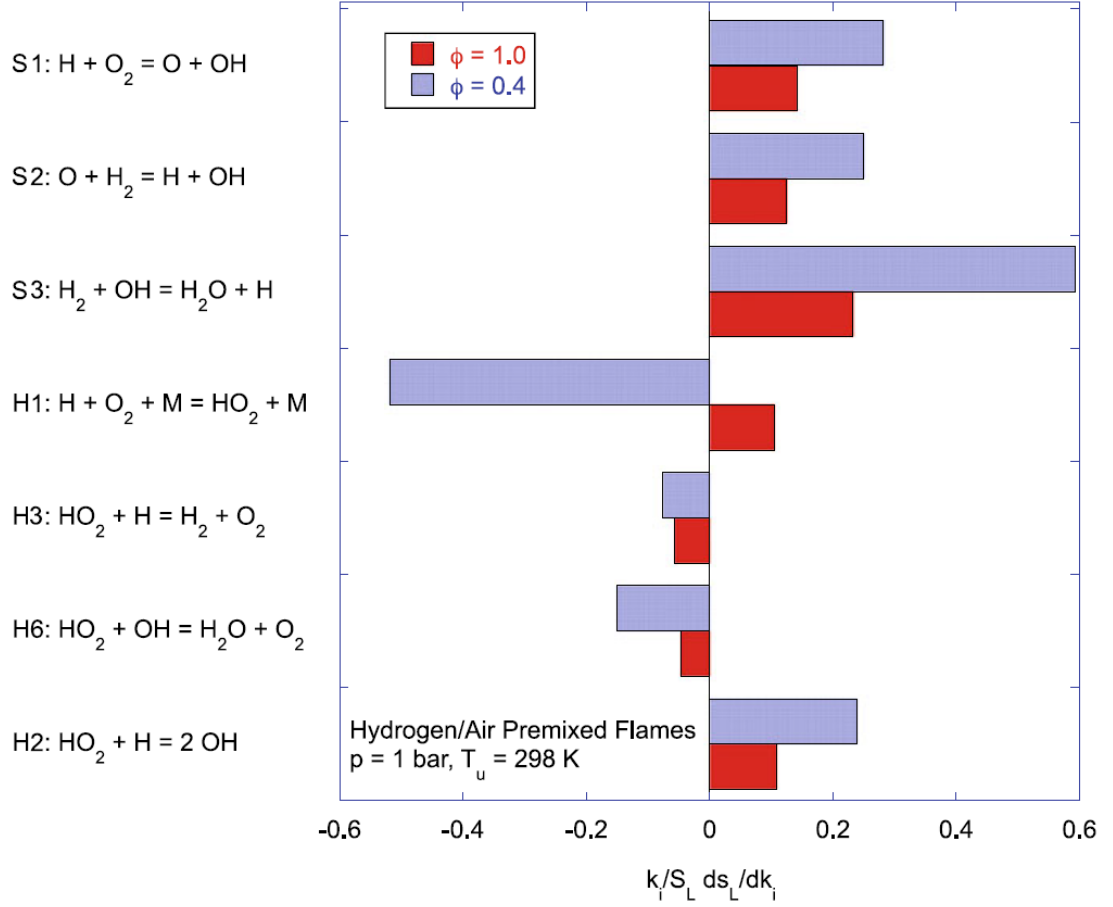


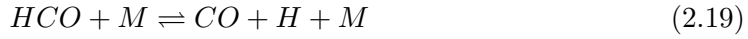
Figure 2.9: Sensitivity analysis for the H_2 laminar flame speed [12].

A typical sensitivity analysis for s_L is reported in Figure 2.9 for both stoichiometric and lean H_2 flames at ambient conditions. The reader can observe that the laminar flame speed is positively influenced by S1-S2-S3 which enrich the radical pool, also competing with the radical consuming reactions H1-H3-H6 whose kinetics reduces s_L in lean flames. Also the reaction H2 is seen to act positively on the propagation of the flame, since it competes with the radical consuming reactions H1-H3-H6 subtracting them hydroperoxyde molecule HO_2 while releasing two OH radicals. For the stoichiometric case, a specular effect of H1 can be observed, even though H1 starts the chain-braking sequence. The behavior stems in the strongly exothermic nature of the reaction near stoichiometric conditions, and the consequent enhanced diffusion of the H from the production layer to the radical consumption layer. This increases the heat release rate with additional preheating at very low temperatures, ultimately accelerating the flame.

For the lean case, a lower number of radicals is available, and the radical consuming nature of H1 is preponderant with respect to exothermicity, thus leading to a negative effect of the reaction rate on the laminar flame speed.

For hydrocarbon fuels, additional reactions hinder the production of radicals, resulting in

lower flame speeds. For instance, taking into account methane, the following reactions:



along with the previous S2-S3 reactions globally consume two H radicals for each methane molecule according to:



Therefore, the creation of the H radical pool results slowed down, and radicals cannot diffuse since they are rapidly consumed for the oxidation of the fuel, ultimately resulting in a lower laminar flame speed. As previously stated, physical properties such as the H_2 high diffusivity, together with the high adiabatic flame temperature, do contribute to the final laminar flame speed. The enhanced H_2 molecular diffusivity is usually taken into account in chemical and CFD computations by setting the Lewis number (Le) below one. The Lewis number is defined as follows:

$$Le = \frac{\text{thermal diffusivity}}{\text{molecular diffusivity}} \quad (2.21)$$

For hydrocarbon fuels, Le is generally seen to be close to one, whereas for H_2 is around 0.3. To roughly assess the impact of the higher molecular diffusivity, one can compute the laminar flame speed by setting the Le to one. The results of this approach are reported in Figure 2.10.

As the reader can observe, for a Lewis number equal to one the peak velocity decreases for about the 30%. Conversely, the effect of unity Lewis number in methane premixed flames is less relevant. Moreover, the H_2 laminar flame speed is markedly higher than methane both considered at unity Lewis number, which is a further confirmation of the highly reactive kinetics of the H_2 flames.

H_2 is also characterized by wider flammability limits than those of conventional fuels. As reported in Table 2.2, the flammability limits for a stoichiometric mixture at ambient conditions span from $\lambda = 0.14$ to $\lambda = 10$. Such a property is relevant for ICEs operation because enables the possibility to employ lean mixtures. Lean combustion reduces the risk of pre-ignition events, lowers the cycle temperatures and the related NO_x production, and results beneficial in reducing the wall heat losses [11]. Additionally, flammability limits are widened when temperature increases, as shown in Figure 2.11. Therefore, under ICE relevant conditions even leaner mixture could be theoretically employed, but this might result detrimental to the combustion rapidity, as discussed in the next

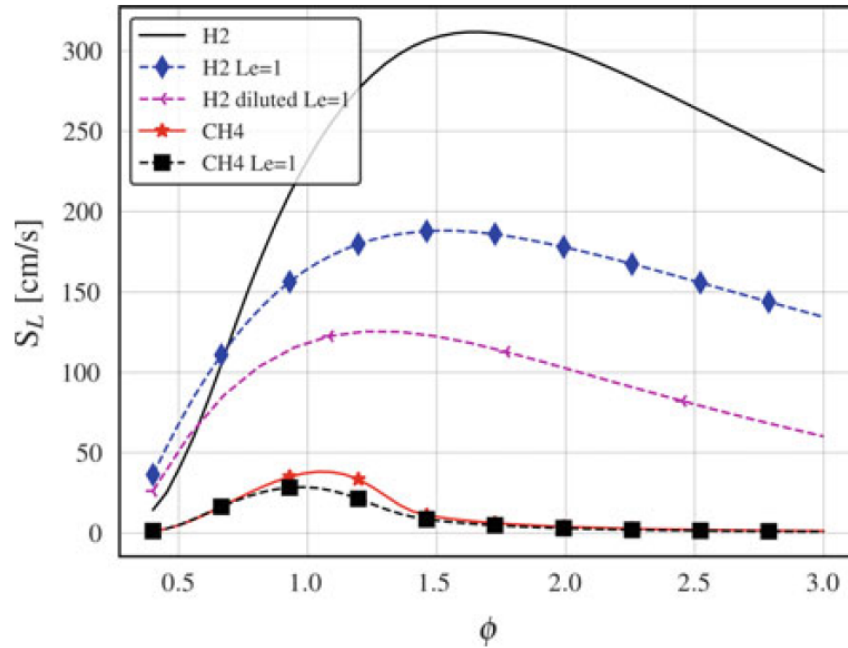


Figure 2.10: Influence of the Lewis number on the laminar flame speed in H_2 and CH_4 flames.

Chapters.

The low H_2 ignition energy is one of the characteristics which must be carefully taken into account when design the combustion chamber. At atmospheric conditions, the H_2 ignition energy is one-order magnitude lower than that of hydrocarbon fuels [34]. Consequently, attention must be paid to avoid the presence of hot-spots in the engine cylinder. Spark might require proper cooling, leakage of lubricant oil must be minimize, as well as the design of the chamber must minimize the presence of residual hot gases at the end of the exhaust stroke.

2.4 Highlights on hydrogen fueled internal combustion engines

First attempts to exploit H_2 in internal combustion engines date back to the beginning of the XIX century [35]. Nonetheless, the research on H_2 ICEs has gained momentum only in the last fifteen years, due the the increased awareness regarding the climate-change consequences. Most of the research is focused on the fuel supply architecture, the related injection strategies, and combustion anomalies such as pre-ignition and knock.

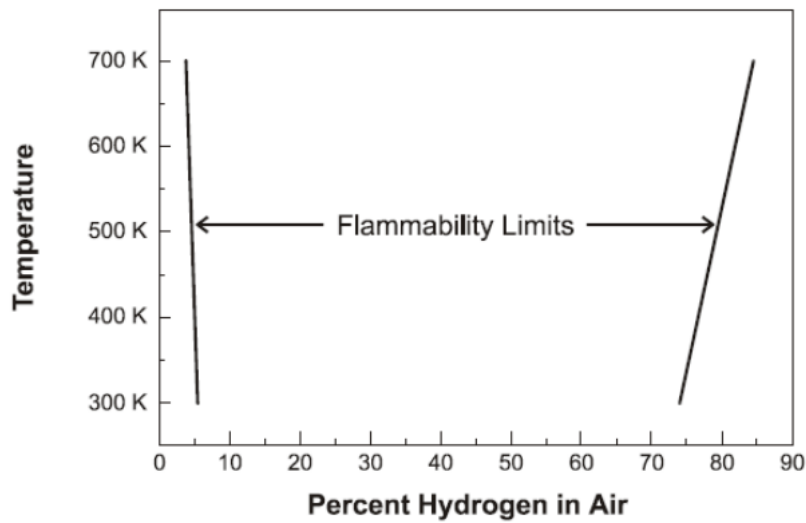


Figure 2.11: H_2 flammability limits as a function of the mixture temperature [33].

2.4.1 Fuel supply architectures

One of the key distinctions for H_2 ICEs is the way by which fuel is delivered. Indeed, the H_2 peculiarities previously discussed, along with fuel supply architecture, have a major impact on the final engine performance and stability.

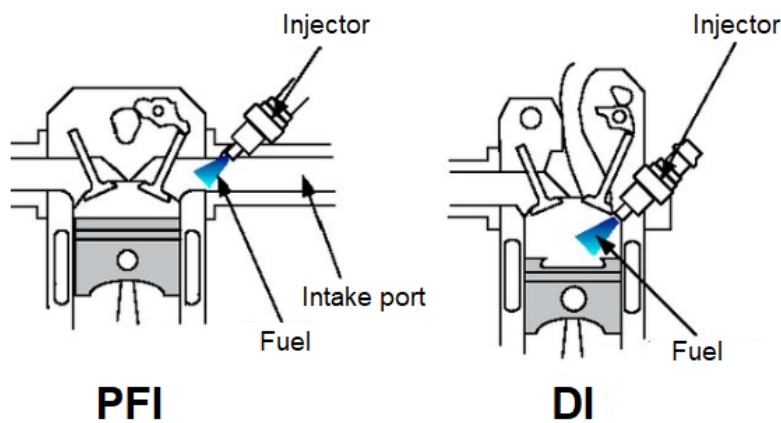


Figure 2.12: Schemes of the PFI and DI architectures [36].

Figure 2.12 shows sketches of the two principal fuel supply modes. In the Port Fuel Injection (PFI) system, H_2 is injected into the intake manifold allowing for an prolonged mixing with the oxidizer, which ultimately produces a homogeneous charge. Conversely, in the Direct Injection (DI) approach, fuel is directly delivered by the injector into the combustion chamber. This introduces the start of the injection (SOI) as a new degree of freedom influencing the uniformity of the mixture.

In the development of H_2 ICEs, the PFI solution has been widely tested due to the ease of implementation [37], especially when retrofitting gasoline engines [38]. As a drawback, the volumetric efficiency is usually not sufficient to reach a good power density due to the low H_2 density, and the maximum brake thermal efficiencies are generally between 35-40% [39]. Moreover, abnormal combustion events such as pre-ignitions and backfiring are easily triggered by the low H_2 ignition energy, as shown for instance in [40]. Here, an investigation regarding the injection timing in the PFI mode was run, highlighting the onset of backfiring for early injections due to the presence of fully ignitable mixture inside the intake runner. Late injections - almost at the intake valve closing - reduced the risk of backfiring but the possibility to inject the entire amount of fuel was compromised.

As a consequence, both industry [41] and academia are currently committed to the development of the DI technology, which increases the engine volumetric efficiency and avoids back-firing events [42]. Comparisons between the PFI and DI modes have been conducted both experimentally and numerically. For instance, in [43] experimental tests run on single-cylinder H_2 engine highlighted a superior performance of the DI approach in terms of indicated thermal efficiency (2% higher than PFI) and increased power output. In [44], the comparison has been carried out by a numerical investigation at two different λ , namely 1.5 and 2. In both the cases, the adoption of the DI architecture has proven to increase the volumetric efficiency up to the 35%, leading to constantly higher BMEPs as shown in Figure 2.13.

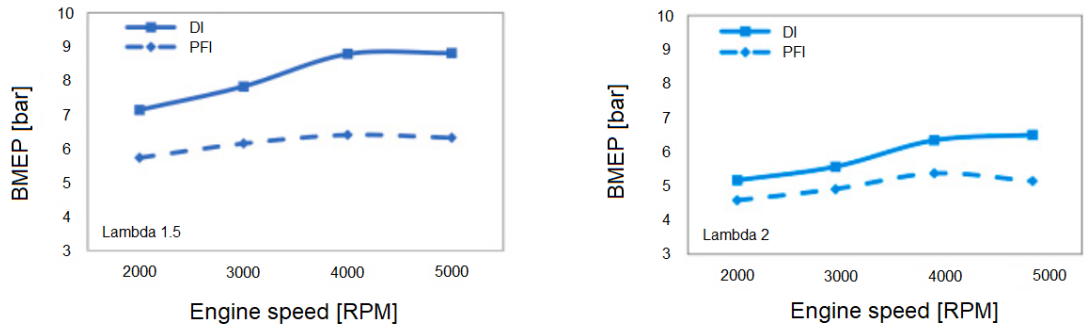


Figure 2.13: Influence of the fuel supply system on the brake mean effective pressure (BMEP) as reported in [44] at $\lambda = 1.5$ (left) and $\lambda = 2.0$ (right).

In [45], a research funded by the US Department of Energy (DOE) demonstrated that H_2 DI engines can reach significantly high efficiencies. More specifically, an average BTE over 35% was measured over the 80% of the engine map, with a peak value equal to 45.5% at an operating point characterized by 2000 RPM and a BMEP of 13.5 bar. The adoption of the DI architecture extends the design space of the engine. Mixing between fuel and oxidizer massively depends on the injector position and geometry, as well as on the injection pressure and start of the injection. The effect of such design variables can be assessed by mean of CFD analyses, which can be a valuable tool to

test the effect of different injector exit sections [45] or to analyze the fuel distribution at spark timing [46] [47]. Depending on the SOI, different levels of the charge stratification can be obtained, allowing to optimize the engine operation. As a general rule, early injections lead to a homogeneous mixture, while retarding the SOI is beneficial when a stratification of the charge is desired [48] [49]. Moreover, the chance of pre-ignition is reduced as a consequence of the shorter time in which the mixture can be ignited by hot-spots [50] [42].

Part of the research is currently devoted to the development of injectors able to operate with higher and higher feeding pressures (over 100 bar [42] [51]), which can be used to increase the engine compression ratio as well as to enable multi-injection strategies for an optimized distribution of the fuel [52].

2.4.2 Combustion Modes

A number of combustion modes has been tested in the literature, depending on the fuel supply architecture employed. For PFI configurations, ignitions by a spark device, pilot diesel jets, or auto-ignition have been tested. For DI H₂ engines, most of the works employ a spark or a glow-plug. Spark assisted PFI engines have been widely analyzed in the literature [39] [53]. Abnormal combustion events are well known issues under such a configuration, which can hinder acceptable performance [54], since the maximum global equivalence ratio strongly depends on the compression ratio, the rotational speed, and the engine cooling. To reduce the chance of pre-ignitions and knocking, the equivalence ratio must be reduced: when gasoline engines are retrofitted to operate with H₂, the reduction of the power can reach the 50% [55]. In terms of NO_x production, operating with equivalence ratios below 0.5 allows to limit the emissions to less than 100 ppm, which can be further reduced by the adoption of a three-way catalytic converter [56].

The homogeneous charge provided by the PFI system has pushed towards the analysis of the homogeneous charge compression ignition (HCCI) mode. In [57], a single cylinder Diesel engine has been retrofitted to operate with hydrogen under the HCCI modality. NO_x resulted three-orders of magnitude lower than Diesel operation, under a compression ratio equal to 18. Nonetheless, the adoption of ultra-lean mixtures in HCCI is strongly limited by the high H₂ auto-ignition temperature. For instance, [58] reports that an unfeasible compression ratio equal to 42 would be required to auto-ignite a uniform mixture with an equivalence ratio of 0.1. Moreover, the control of the combustion process and the related peak pressure is challenging. In [59], it is reported that the combustion of an ultra-lean mixture (equivalence ratio equal to 0.25) can release the 90% of the total heat release in around 3° crank angles under a compression ratio of 17 and intake temperature of 390 K.

In the context of retrofitting Diesel engines, several studies have been carried out to in-

investigate the ignition of PFI H_2 mixtures by means of pilot Diesel jets. Such an approach provides high flexibility in terms of H_2 /Diesel energy share, even though abnormal combustion is once again an issue. The H_2 energy share is usually limited to around 30% - 40% at low loads conditions and 25% for high loads [60] [61]. In this combustion mode, CO_2 emissions reduce proportionally to the H_2 energy share whereas literature reports some controversy regarding the NO_x production. In [62] a massive reduction of the NO_x has been experimentally observed by H_2 enrichment, from 2700 to 500 ppm at 70% of the load. This has been mainly attributed to the lowered peak temperature of the engine cycle. Conversely, H_2 enrichment in [63] has constantly led to increased NO_x emissions, which have been explained by the conversion of H_2 unburnt molecules into HO_2 , a NO_x promoter.

For pure H_2 DI engines, ignition can be operated either by a glow plug or spark plug. The former, schematically illustrated in Figure 2.14, is an electrically heated hot-surface. It is a historically tested solution, derived by Diesel engines in which glow-plugs are usually employed to help with cold starting.

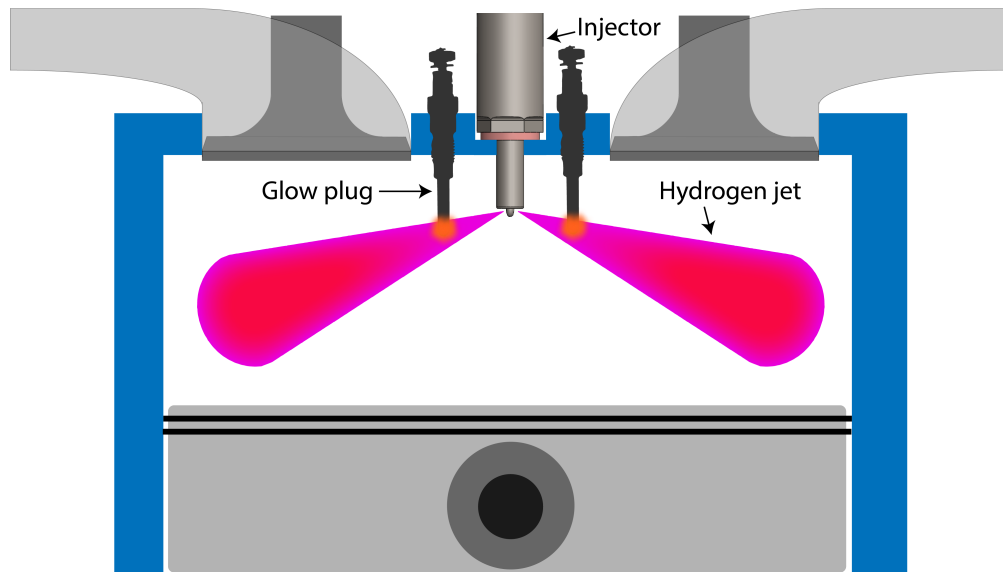


Figure 2.14: Sketch of a glow-plug protruded into the combustion chamber.

When used for H_2 ignition, the surface temperature must be between 1200-1400 K [64]. In the retrofitting a Diesel engine, this kind of solution also leads to an increase of the specific fuel consumption, as reported in [65] where a 10% increase was measured with respect to Diesel operation. The high surface temperature of the glow plug raises concerns about its durability in commercial applications, making this technology rarely used in recent engine development [66].

Nowadays, spark assisted DI H_2 are probably the most common solution of H_2 engines [67]. The arrangement of both the injector and the spark can be exploited to realize a fast combustion speed. For instance, in [68] two ignition strategies, defined as *plume-*

head and *plume-tail* have been tested in combination with delayed SOIs. In the *plume-head* solution, ignition is started just after the SOI, whereas in the *plume-tail* spark is activated just after the end of the injection. Both the strategies aim at igniting the H_2 jet to promote a fast combustion process. Specifically, the plume-tail ignition provides higher indicated thermal efficiency (48% vs 37%) and lower cycle-to-cycle variability [69]. This highlights the need to ensure a rich equivalence ratio around the spark, ideally reducing closer to the walls. When dealing with lean mixtures which have achieved a uniform distribution of the charge, novel spark concepts could be useful, such as the brake discharge igniter. This device creates a non-equilibrium low temperature plasma, which ignites a higher volume of the charge with respect to traditional sparks, allowing for a reduction of the cycle-to-cycle variability as demonstrated in a PFI configuration in [70].

All the considerations extracted by the literature constitute the motivation of this thesis, which is mainly focused on H_2 direct injection engines by delving into injection and mixing analyses and the consequences in terms of combustion speed and emissions.

Chapter 3

Under-expanded phenomena in hydrogen direct injection

The adoption of H_2 as a fuel in ICEs requires specific focus to mitigate some drawbacks. For instance, the low ignition energy can lead to pre-ignition events, knocking, and back-firing, and the volumetric efficiency is not sufficient when the Port Fuel Injection (PFI) architecture is employed [42]. All of these complications can be overcome by adopting the Direct Injection (DI) technology to deliver fuel into the combustion chamber.

Due to the short time available to inject the fuel, DI requires a high feeding pressure (between 100 and 250 bar) [71] at the nozzle inlet, leading to the onset of an under-expanded H_2 jet. The main features of such flows are the subject of the analysis reported in this chapter. Because of the vast number of engineering applications in which underexpanded jets can be found, literature is rich in both experimental and numerical studies.

Historically, the first analyses have focused on the *nearfield* zone of the jet, where the most intense gas-dynamics phenomena occur [72] [73]. Thanks to the increasing computational power available for research, numerical simulations have become a reliable tool to study the main properties of these jets. Banholzer [74] numerically characterized underexpanded methane jets at various Nozzle Pressure Ratios (NPRs), reporting the different structures observed. Jet-tip penetration was studied for several ambient pressures and the effect of fuel and ambient temperatures on the phases separation was analyzed. Regarding fossil fuel powered ICEs, DI of natural gas has been studied in [75]. Here, a CFD code has been validated against the experimental data regarding the flow discharged at ambient conditions. Vuorinen et al. [76] were the first to propose a systematic evaluation of the NPR influence on the jet structure by means of LES simulations. More recently, as research has shifted towards the development of climate-neutral solutions, focus has been placed on H_2 underexpanded jets. A LES analysis is reported in [77] for a fixed NPR equal to 10 and several ambient pressures. For higher ambient pressures, a slightly quicker formation of the Mach disk has been reported and correlations have been proposed for the timewise jet-tip penetration.

The promise of a H_2 based economy poses relevant concerns about safety [78]. Since H_2 is stored at high pressure and the flammability range is wide, a tank failure can easily lead to the formation of ignitable jets. Most of the hazards are related to the farfield zone, namely the region downstream of the shock structures where an intense H_2 -air mixing takes place. The need of quick tools for the risk assessment cannot be satisfied by time-expensive simulations run on detailed meshes of the whole jet. Thus, several strategies have been tested and reported in the literature. In [79], RANS simulations have been employed on a reduced domain to solve the nearfield structure, which has been subsequently imposed as initial condition to run LES computations of the farfield zone. Another common approach is the replacement of the nearfield structure with a *notional nozzle* [80], according to a pseudo-source approach. Among the several models to describe the notional nozzle, the *Mach disk approach* places the notional nozzle just after the Mach disk, a jet feature later described in this paper.

Literature regarding the complex phenomena of H_2 jets under the specific conditions found in ICEs is scarce, even though the high pressure injection is the starting point of the fuel-air mixing markedly influencing the thermodynamic cycle. Therefore, the goals of this investigation reported in this chapter have been:

- to determine the correct numerical setup for computing the main features of the underexpanded jets. Attention has been paid to the optimum grid size to minimize the computational effort required for ICE simulations;
- to improve literature models regarding the Mach disk characteristics. Such data can be useful in the context of the leakage risk assessment too;
- to determine the influence of the ICE conditions on the jet. Focus has been posed to the variable in-cylinder pressure, to determine the change of observing hysteretic phenomena;
- to analyze the fundamentals of the jet-jet interaction. This topic has received little focus in the context of H_2 jets. Nonetheless, it can have a serious influence on the mixture formation process when multi-hole nozzles are employed.

3.1 Underexpanded jet structure

Depending on the NPR, literature distinguishes among moderate (Figure 3.1a), highly (Figure 3.1b) [81] and very highly underexpanded jets (Figure 3.1c) [80]. All the three configurations exhibit a supersonic field just downstream of the nozzle exit section, where pressure quickly drops as a result of the flow acceleration. The expansion waves of the Prandtl - Mayer fan, originating from the nozzle lips, are reflected by the constant pressure line and turned into compression waves. These waves then coalesce into a single

oblique shock (the intercepting shock) pointing to the jet centerline.

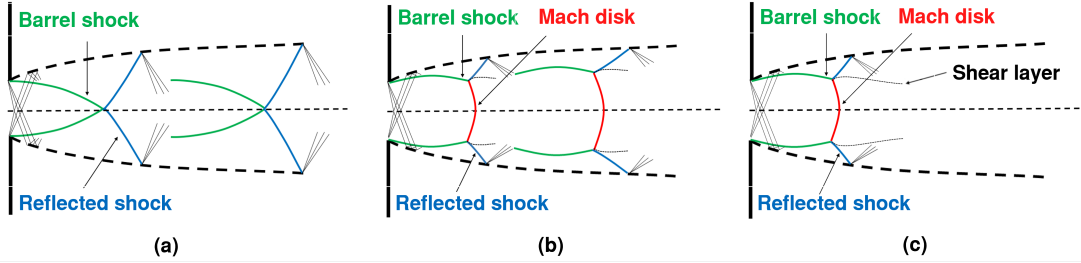


Figure 3.1: Graphical representation of the main under-expanded jet structures: (a) moderately underexpanded jet ($2 < \text{NPR} < 4$), (b) highly underexpanded jet ($4 < \text{NPR} < 7$), (c) Very highly (or extremely) underexpanded jet ($\text{NPR} > 7$).

From a kinematic point of view, the axis behaves as a wall, requiring the flow not have a radial velocity component along the centerline. In order to meet this constraint, in the moderately underexpanded case ($2 < \text{NPR} < 4$), a reflected shock originates from the axis to fix the flow deviation imposed by the intercepting shock. This new shock will be once again reflected by the external boundary and turned into a new expansion fan, allowing the pattern to be replicated further downstream. As it can be observed in Figure 3.2, for a given Mach number there exists a maximum value of the deflection that can be imposed through the formation of an oblique shock. For $4 < \text{NPR} < 7$, the turning angle through the intercepting shock exceeds the maximum deflection which can be imposed by the reflected shock. In such a situation, the kinematic constraint can be met through the formation of the Mach disk shock, which is locally normal to the axis location [82]. The point where the intercepting shock, the reflected shock, and Mach disk meet each other is defined as the triple point. An embedded shear layer propagates from this point, dividing the subsonic flow downstream of the Mach disk and the supersonic flow behind the reflected shock. The $\text{NPR} > 7$ jet is considered extremely underexpanded and it is characterized by a single shock cell downstream of the nozzle exit.

The distance between the Mach disk and the nozzle exit section (namely the Mach disk height, H_{disk}) is mainly determined by the pressure ratio [83] [84] [85] and seems to be independent of the fluid nature [86] [87] and the nozzle exit angle. Thus, its location is usually computed using the following equation:

$$H_{\text{disk}}/D_{\text{nozzle}} = C_H \sqrt{\text{NPR}} \quad (3.1)$$

where D_{nozzle} is the nozzle exit diameter and C_H is a constant. Various authors have proposed different values for C_H [76] [88] [89] either numerically or experimentally assessed. A high level of uncertainty is present in the literature concerning the Mach

disk diameter. It seems to be dependent on the pressure ratio and the nature of the fluid, showing an inverse proportionality to the ratio of specific heats ($k = C_p/C_v$) [84]. Moreover, it seems to be influenced by the shape of the duct [90] [91]. For a contoured nozzle, the following expression is proposed in [80]:

$$D_{disk}/D_{nozzle} = 0.36\sqrt{NPR - 3.9} \quad (3.2)$$

being D_{disk} the Mach disk diameter.

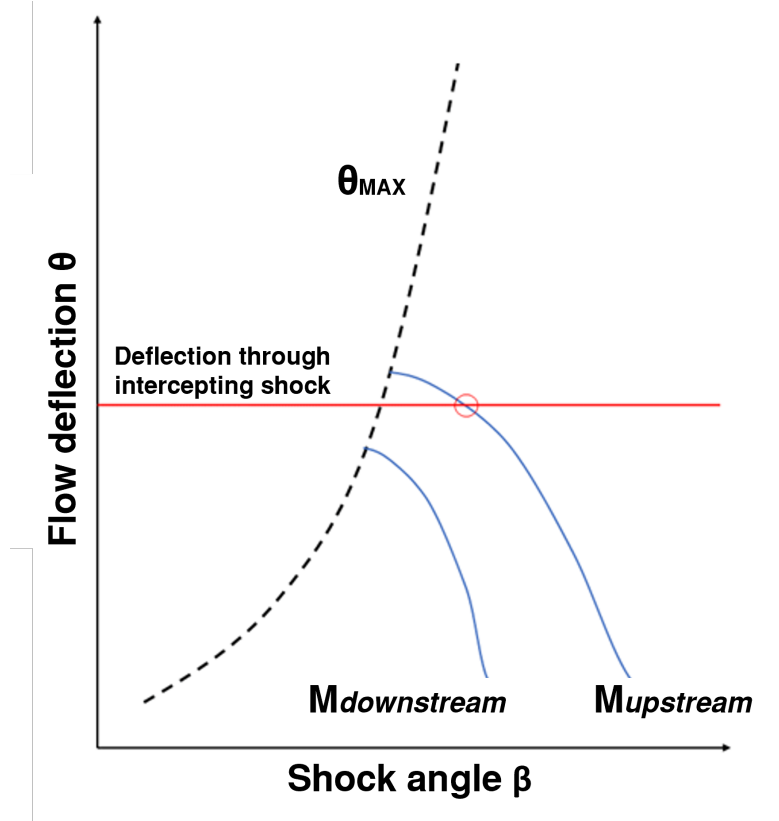


Figure 3.2: Representation of the Mach reflection on the shock angle β - flow deflection θ plane. For a fixed Mach number upstream of a shock, a maximum value of the flow deflection exists. If the maximum deflection relative the Mach number downstream of the incident shock is lower than the imposed deflection, a Mach reflection occurs.

3.2 Numerical methods

Steady and unsteady RANS simulations have been carried out by means of the commercial CFD code ANSYS Fluent[®]. For ICE analyses, the RANS approach is still a valuable way to get insights of the mixture formation process in a short time. Indeed, Hamzehloo and Aleiferis [92] compared RANS and LES simulations for a direct-injection test case, showing that the bulk motion of the injected flow was reliably captured by the

RANS approach.

To find the correct numerical setup, a preliminary numerical assessment has been performed. Figure 3.3(a) shows the 2D axisymmetric computational domain employed for the simulations, together with the imposed boundary conditions. At the inlet of the plenum (on the left side), a total pressure of 10 bar and a total temperature of 300 K are imposed. To fill the plenum with pure H_2 , the inlet mass fractions of O_2 and N_2 are set to zero. A convergent nozzle, sketched following the ASME MFC-3M-2004, has been placed between the plenum and the following discharging chamber. The convergent nozzle has been preferred to convergent-divergent configurations in order to analyze flows at sonic condition (Mach equal to 1) in the nozzle exit section. The nozzle exit diameter has been chosen equal to 1 mm, in order to validate the numerical model against the experimental data reported in [93]. Keeping the inlet total pressure constant, the desired NPR is defined by changing the uniform static pressure at the outlet. Inside the discharging chamber, the mass fractions of O_2 and N_2 are 0.23 and 0.77, respectively. A hybrid mesh has been employed, featuring structured blocks in the jet zone, as shown in Figure 3.3(b). Here the cell size has been varied from 6 to 300 μm , in order to carry out a mesh sensitivity analysis. The length of the first refinement block just downstream the exit plane has been set to $15D_{nozzle}$, while the second (with a slightly higher cell dimension) has been set to $10D_{nozzle}$. A structured mesh has been applied to the nozzle region as well, with the average cell size equal to 5 times the dimension chosen for the nearfield zone. For the boundary layer treatment, wall functions have been employed ensuring a $y^+ > 30$.

Steady RANS equations have been solved using a coupled-pressure based scheme, and a second order accurate upwind scheme has been adopted for the spatial derivatives discretization. H_2 - air mixing has been assessed solving the species transport equations provided by ANSYS Fluent[®] and here reported for the i -th chemical species:

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i \quad (3.3)$$

where Y_i is the local mass fraction for the i -th species, R_i the rate of production by chemical reactions and S_i a source term. $\vec{J}_i$ is the diffusion flux of species i due to both concentration and thermal gradients. For a turbulent flow, ANSYS Fluent computes $\vec{J}_i$ as:

$$\vec{J}_i = -\left(\rho D_{i,m} + \frac{\mu_t}{Sc}\right) \nabla Y_i - D_{T,i} \frac{\nabla T}{T} \quad (3.4)$$

where $D_{i,m}$ is the mass diffusion coefficient, μ_t the turbulent viscosity, Sc the Schmidt number (depending on the turbulent diffusivity D_t) and $D_{T,i}$ is the thermal diffusion coefficient, accounting for the Soret effect [94]. To close the RANS equations, the $k-\omega$ SST turbulence model has been adopted, being able to efficiently capture shocks and expansions, as referred by the literature [74] [95]. Turbulence equations have been

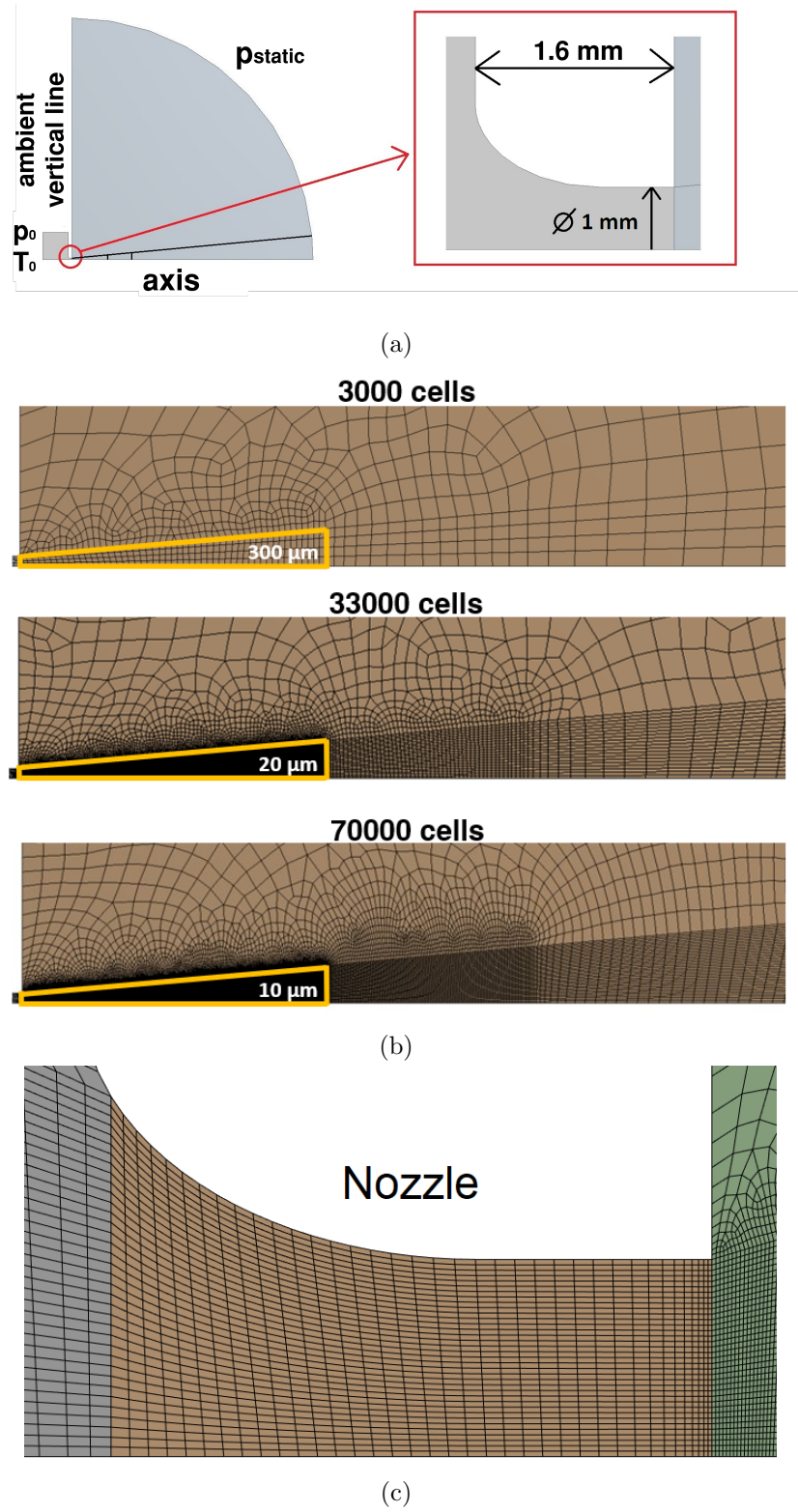


Figure 3.3: (a) View of the computational domain with blocks partition and details of the nozzle geometry; (b) Comparison of three different mesh refinements in the jet zone. (c) Structured mesh inside the nozzle.

discretized by means of a second-order accurate upwind scheme. In addition to the ideal gas law, real gas assumptions have been tested using the Redlich - Kwong and Peng - Robinson models for the Equation of State (EoS). These are both cubic models, whose general form is:

$$p = \frac{RT}{v - b + c} - \frac{a}{v^2 + v\delta + \epsilon} \quad (3.5)$$

being a , b , c , δ and ϵ constants related to the fluid critical pressure p_c , critical temperature T_c , and acentric factor ω . In the Redlich - Kwong model these constants are computed as follows:

$$\begin{aligned} a(T) &= \frac{a_0}{(T/T_c)^{0.5}} \\ a_0 &= \frac{0.42747R^2T_c^2}{p_c} \\ b &= \frac{0.08664RT_c}{p_c} \end{aligned}$$

while δ is equal to b and both c and ϵ are set to zero. For the Peng-Robinson model, the following equations are solved:

$$\begin{aligned} a(T) &= a_0[1 + n(1 - (T/T_c)^{0.5})^2] \\ n &= 0.48 + 1.574\omega - 0.176\omega^2 \\ a_0 &= \frac{0.45724R^2T_c^2}{p_c} \\ \omega &= -\log_{10} \frac{p_v}{p_c} - 1 \\ b &= \frac{0.07780RT_c}{p_c} \end{aligned}$$

In the definition of the acentric factor ω , computed for $T = 0.7T_c$, p_v is the saturation vapor pressure. When dealing with real-gas mixtures, ANSYS Fluent uses the pseudo-critical method, by which the generic critical constant of the mixture C_{cm} is computed on the basis of the mass fractions and the critical constants of each i -th component:

$$C_{cm} = \sum_{i=1}^N x_i C_{ci} \quad (3.6)$$

A mass-weighted mixing law has been enabled to compute the local viscosity, where the i -th component viscosity has been modeled by the Sutherland's law with three parameters.

3.3 Validation

The validation of the numerical setup has been carried out imposing a total pressure of 10 bar in the plenum and 1 bar in the ambient. In this way, the capability to reconstruct the underexpanded structure has been tested against the experimental results reported in [93]. At such a level of underexpansion, the Mach disk height has been considered a valuable benchmark for validation.

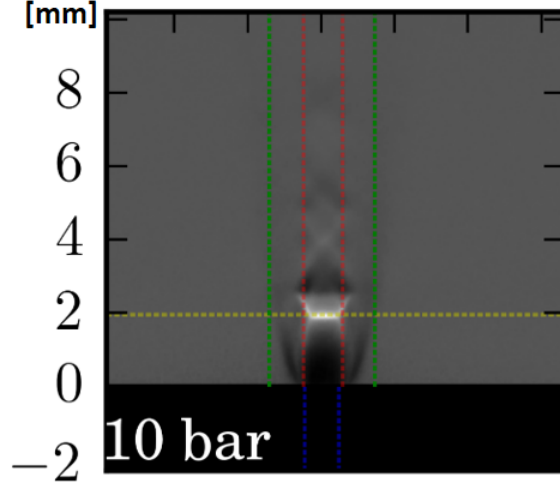


Figure 3.4: Schlieren picture of the H_2 underexpanded jet for $NPR = 10$ and nozzle exit diameter of 1 mm [93]. The Mach disk is placed at 2 mm from the nozzle exit section.

As it can be seen in the Schlieren picture reported in Figure 3.4, for a NPR of 10 and a nozzle exit diameter of 1 mm, the Mach disk height is about 2 mm. A mesh sensitivity analysis has been carried out by varying the cell size in the nearfield zone of the jet according to the values reported in Table 3.1.

Table 3.1: Mesh sensitivity data

Cell dimension [μm]	Number of cells
300	3000
100	5000
30	18000
20	33000
10	70000
6	130000

The numerical Mach disk height is plotted in Figure 3.5 as a function of the number of cells. It is interesting to note that when the coarsest mesh has been employed, it has not been possible to identify the Mach disk. Therefore, this can be seen as a threshold under which the computed jet structure is not physically correct. As expected, an asymptotic behaviour can be observed when the mesh density increases. Considering ~ 2 mm as the

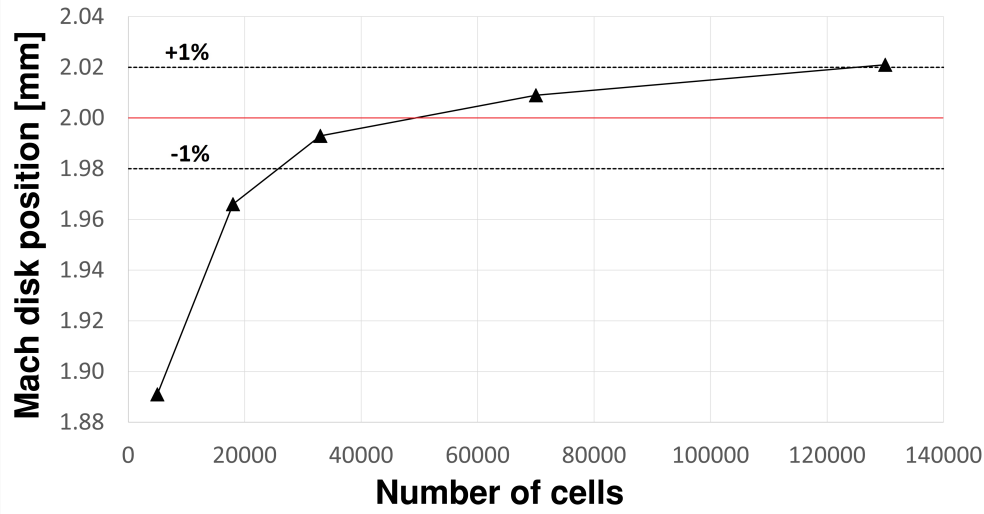


Figure 3.5: Numerical Mach disk position as a function of the number of cells, $NPR = 10$. The red straight line represents the experimental disk position (2 mm) [93]. An error band of $\pm 1\%$ is delimited by the dashed lines. Meshes between ~ 30000 and ~ 130000 cells provide results inside the error band.

experimental value of the disk height, an error band of 1% has been applied to Figure 3.5 in order to evaluate the acceptable mesh sizing. The reader can observe that, starting from a grid size of 33000 cells, all the solutions fall within the error band.

Figure 3.6 shows the Mach number contours varying the mesh density. The occurrence of the Mach disk starts when imposing a cell size of 0.1 mm near the nozzle exit plane, as visible in Figure 3.6(b). Nonetheless, the reflected shock, the shear layer and the region downstream of the Mach disk are not clearly defined. Meshes from 18000 to 130000 cells are instead fully able to reconstruct the underexpanded jet according to the structures previously described and reported in the literature. For ICEs analysis, another key feature to consider is the H_2 -air mixing along the jet. The numerical H_2 axial distribution is reported in Figure 3.7. The coarser the mesh, the quicker the mass fraction drops along the axis: at 15 mm from the exit plane, the difference in the H_2 mass fraction is almost 100% between the coarsest and the finest mesh. A good agreement in the resolution of the mass fraction is found for the meshes from 33000 to 130000 cells. For all the reasons mentioned above, the grid with 70000 cells has been considered a good candidate to achieve a reliable solution of the underexpanded jet in acceptable computational time. In Figure 3.8 the results obtained by using the three different equations of state are compared in terms of Mach number evolution along the axis. The shock position is fully comparable, while shock intensity is slightly higher for the real-gas models, as also reported by Bonelli [96]. The Redlich-Kwong model has been adopted for the subsequent simulations, in which the general higher nozzle pressure can require a more realistic equation of state.

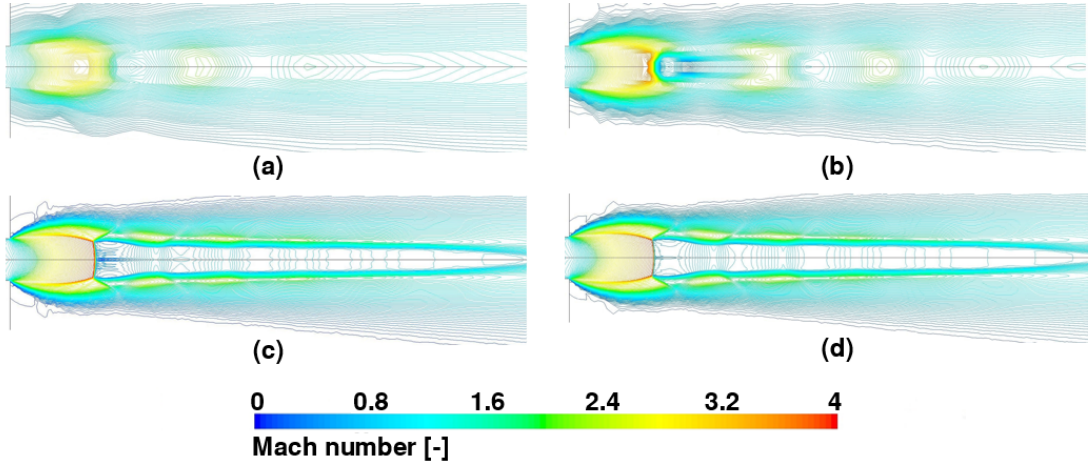


Figure 3.6: Mesh sensitivity analysis: contours of the Mach number, NPR 10. (a) Mesh with 3000 cells: jet structure is not well solved, since flow is still supersonic after the Mach disk. (b) Mesh with 5000 cells: a better reconstruction of the Mach disk can be observed, but the other major jet features are not well defined. (c) Mesh with 70000 cells and (d) mesh with 130000 cells: the barrel shock, Mach disk and reflected shocks are properly resolved.

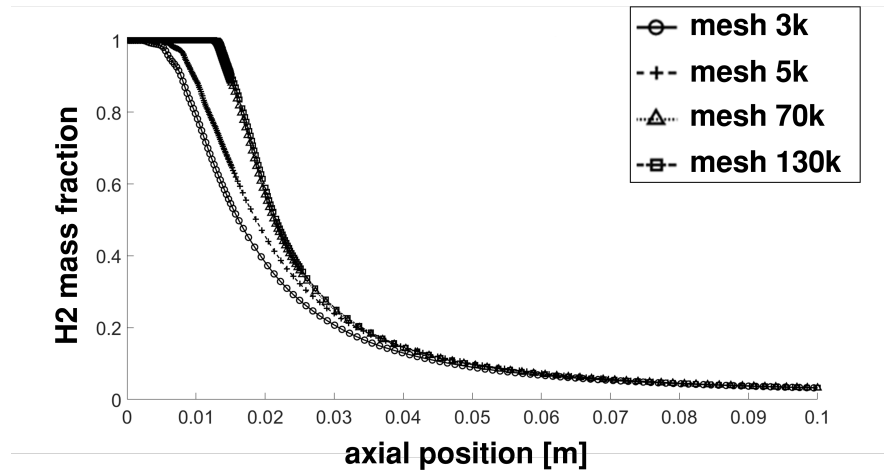


Figure 3.7: Mesh sensitivity analysis: axial distribution of the H_2 mass fraction for different mesh densities, NPR 10. Coarser meshes result in a quicker drop of the mass fraction.

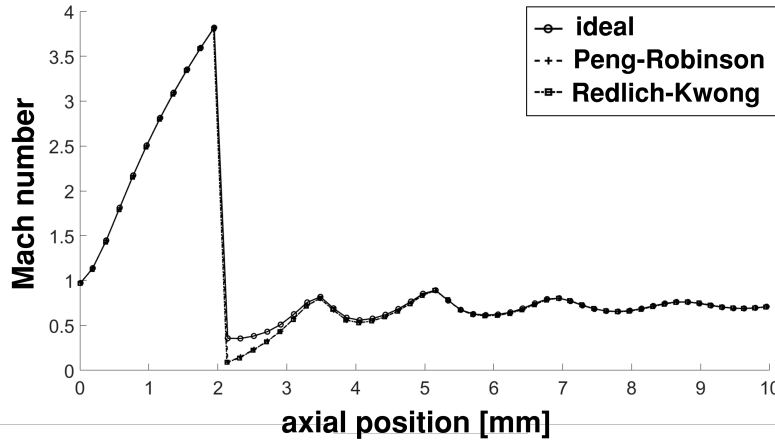


Figure 3.8: Comparison among different equations of state: ideal gas, Peng-Robinson, and Redlich-Kwong. This plot shows the evolution of the Mach number along the jet axis, NPR 10. The Mach disk position is the same for all the three models (~ 2 mm), whereas shock intensity is higher for the real gas models, according to the results presented in the literature [96].

3.4 Influence of the Nozzle Pressure Ratio

Once the correct numerical setup and the mesh resolution have been determined, steady RANS simulations have been performed by keeping the inlet conditions constant while varying the pressure outlet. In such a way, differences in the jet structure have been analyzed for NPR values ranging from 2.5 to 60. As it will be discussed later, for ICE analyses RANS and URANS are able to capture the main jet features at a specific NPR with good accordance.

A shock diamond structure occurs when the $NPR < 4$, since the regular reflection of the incident shock can take place along the axis. An example of the diamond structure is reported in Figure 3.9(a), which shows the Mach numbers contours for a $NPR = 3$. For a $4 < NPR < 7$, the Mach disk forms and multiple shock cells appear, as visible in Figure 3.9(b) for a $NPR = 5$. When $NPR > 7$, the underexpanded jet is characterized by a singular shock cell as discussed in the previous paragraphs (see Figure 3.6). The axial position of the first reflecting point (L_{RR}) in the diamond structure is reported as a function of NPR in Figure 3.10. This trend can be accurately approximated by the linear function the authors propose here, being the coefficient of determination (R^2) equal to 0.997:

$$L_{RR} = 0.4549 NPR - 0.6347 \quad (3.7)$$

The Mach disk diameter and height have been assessed in the NPR range 5-60. These results are reported in Tables 3.2 and 3.3. Mach disk diameters measured from the numerical results have been compared to the values determined by using Equation

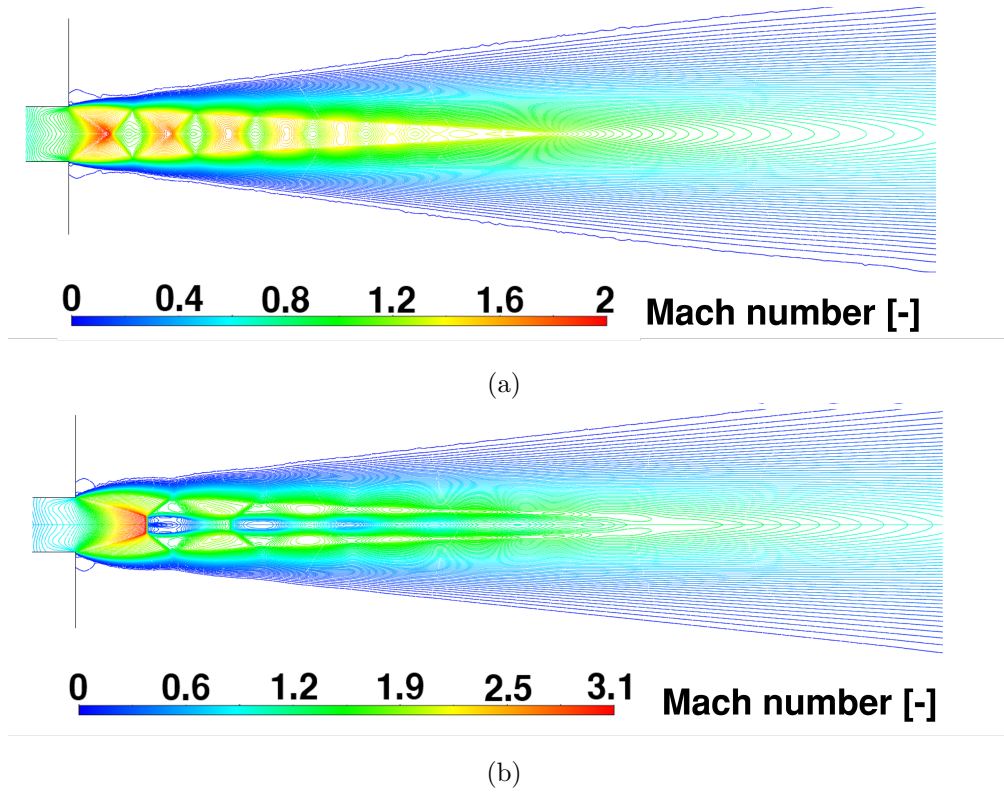


Figure 3.9: Contours of the Mach number for two different levels of jet under-expansion conditions: (a) shock diamond structure, NPR 3; (b) multiple shock cells structure, NPR 5.

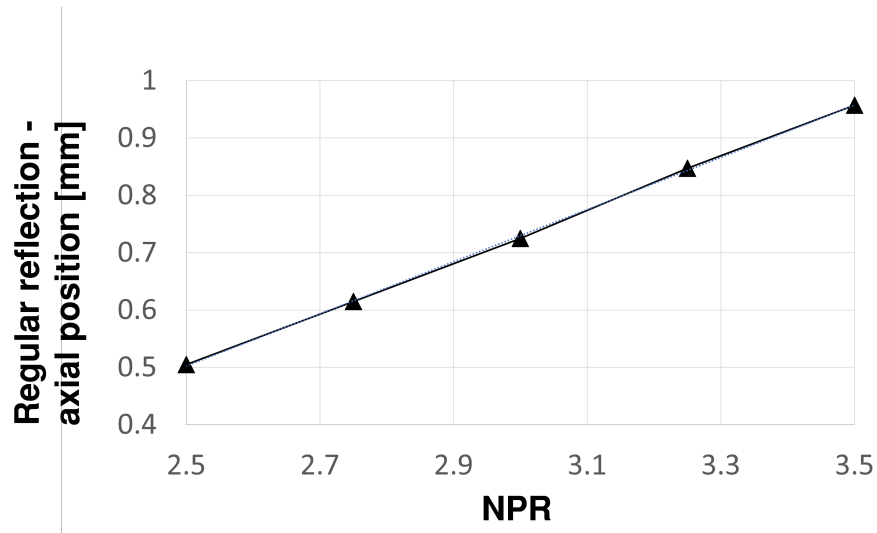


Figure 3.10: Axial position of the regular reflection as a function of the NPR in the range of moderately underexpanded jets. Numerical data are well approximated by a linear regression.

3.2, resulting in a maximum difference of about 21% at NPR 60. This can be considered a satisfactory result when the high level of uncertainty affecting the model for the disk diameter is taken into account. Exploiting the numerical results, a better agreement is found replacing the constant value 0.36 in Equation 3.2 with a function of NPR:

$$D_{disk}/D_{nozzle} = [3 \cdot 10^{-6}NPR^3 - 3 \cdot 10^{-4}NPR^2 + 0.0112NPR + 0.2734] \sqrt{NPR - 3.9} \quad (3.8)$$

By this tuning, a maximum error of about 12% is found at NPR 60. In Table 3.3, the Mach disk height resulting from the CFD simulations is compared against the values computed using eq. 3.1, for $C_H = 0.62$. A good agreement is found at the medium-low NPRs, worsening at the higher NPRs. An opposite trend, not reported for the sake of brevity, is found for $C_H = 0.67$. This suggests that defining C_H as a function of the NPR, as shown in Figure 3.11, can be a better approach. Results reported in Paragraph 7 will confirm the validity of this idea. Moreover, the C_H trend shown in Figure 3.11 suggests the presence of an asymptotic value of about 0.69. This result is coherent with the value of 0.67 suggested by [88] in the range $15 < NPR < 17000$.

Table 3.2: Mach disk diameter (D_{disk}) resulting from RANS simulations and comparison with the correlation provided by the literature (Equation 3.2)

NPR	Disk diameter CFD [mm]	Disk diameter from Equation 3.2 [mm]	Difference %
5	0.337	0.377	12.04
10	0.886	0.889	0.35
15	1.258	1.199	-4.65
20	1.586	1.444	-8.92
40	2.434	2.163	-11.13
60	3.425	2.696	-21.27

Table 3.3: Mach disk height (H_{disk}) resulting from RANS simulations and comparison with the correlation provided by the literature (Equation 3.1, $C_H = 0.62$)

NPR	Disk height CFD [mm]	Disk height from Equation 3.1 [mm] ($C_H = 0.62$)	Difference %
5	1.299	1.389	6.30
10	2.009	1.961	-2.47
15	2.522	2.401	-5.02
20	2.981	2.772	-7.51
40	4.350	3.921	-10.93
60	5.362	4.802	-11.65

In Figure 3.12, the H_2 mass fraction and the turbulent kinetic energy can be observed

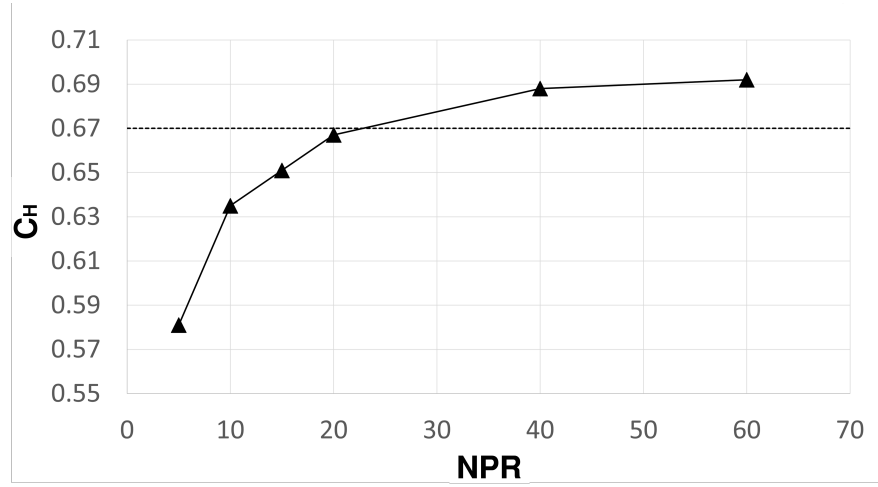


Figure 3.11: Evolution of the parameter C_H which links the Mach disk height and the exit nozzle diameter to the NPR (see Equation 3.1).

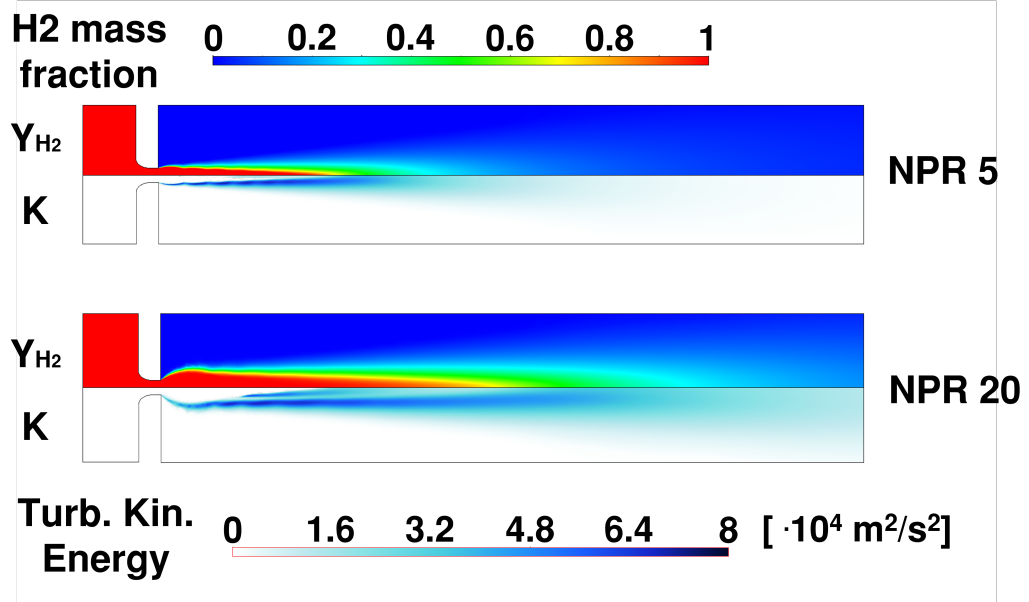


Figure 3.12: Contours of the H_2 mass fraction, Y_{H_2} , and turbulent kinetic energy, K , for two underexpanded flow conditions: NPR 5 (top) and NPR 20 (bottom). The inner core of the jet, where mixing does not occur, is characterized by negligible levels of turbulent kinetic energy. Conversely, high values of the turbulent kinetic energy are observed in the external mixing layer.

for NPRs equal to 5 and 20. Since the total conditions at the inlet are equal in both cases, the H_2 jets are characterized by the same choked mass flow and the same momentum at the nozzle exit section. Consequently, the higher jet penetration observed when $NPR = 20$ can be attributed to the higher rarefaction of the air in the discharging chamber. Looking at the H_2 mass fraction distribution, two zones are clearly distinguishable: the inner core, dominated by the gas-dynamics phenomena, where the flow is isolated from the ambient fluid, and the external mixing layer, characterized by an intense mixing promoted by turbulence, as confirmed by the turbulent kinetic energy contours in Figure 3.12. The axial and radial extents of both the zones increase with NPR. This is shown in Figure 3.13 where $L_{0.3}$ is plotted against NPR. $L_{0.3}$ is defined as the axial position where the H_2 mass fraction drops to 30%, which is roughly the ending point of the mixing layer. Beyond this point, the farfield zone of the jet starts. In this last zone of the jet, the radial distribution of the major variables of the flow (pressure, velocity) can be described by gaussian profiles, and self-similarity hypothesis is expected to be valid [80] [97].

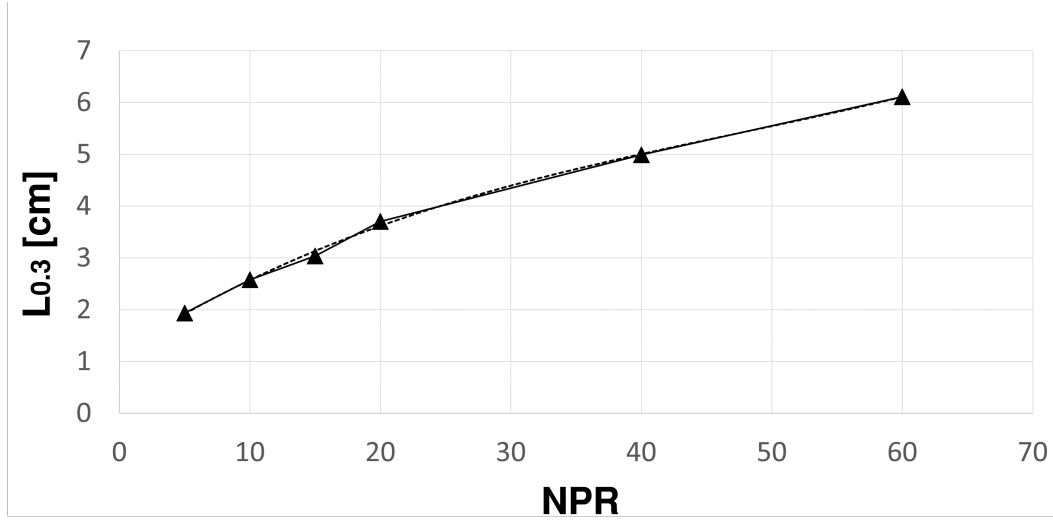


Figure 3.13: Evolution of $L_{0.3}$, i.e., the axial distance where the H_2 mass fraction is equal to 0.3, as a function of the NPR.

For this specific set of simulations, with both the discharging chamber temperature and the inlet total temperature set to 300 K, the best regression curve for the non-dimensional $L_{0.3}/D_{nozzle}$ is the following:

$$L_{0.3}/D_{nozzle} = 8.9096(NPR)^{0.4677} \quad (3.9)$$

3.5 Underexpanded jets in ICE conditions

After the definition of the correct numerical setup for under-expanded flows analyses and the subsequent validation, focus has been posed on the effect of the typical pressure and temperature conditions observed during ICE operation. The goal has been to determine whether unsteady phenomena could arise during the compression stroke, as well as to observe how significant is the impact of temperature on the fuel distribution along the jet.

3.5.1 Hysteresis phenomena

Underexpanded flows are known to show hysteresis phenomena influencing the gas-dynamic structure when the pressure ratio varies with time. To verify the presence of this kind of unsteady effect when injecting throughout the compression stroke, data regarding the ICE analyzed in [45] have been exploited as a reference, assessing and testing the NPR variation from the start of injection (SOI) to the end.

The engine in [45] is featured by an injector operating at 100 bar. It is also equipped with a turbocharger able to deliver up to 2.5 bar, and the compression ratio is 12.9. A rotational speed of 1700 RPM has been considered for the investigation, with the optimum SOI 80° before TDC; the injection spans for 50° CA. Trend of the in-cylinder static pressure during the compression stroke and the consequent variation of the NPR - both reported in Figure 3.14 - have been computed under the assumption of an isentropic transformation.

Unsteady simulations of the injection process have been performed starting from the solution characterized by a NPR equal to 16.3, which corresponds to the start of injection. For these simulations, a first-order implicit formulation has been adopted for the temporal discretization. Keeping the injection pressure constant, the discharging ambient pressure has been progressively increased following the profile in Figure 3.14(a). Consequently, the overall simulated process lasts 4.9 ms, and a timestep of 10^{-6} s has been adopted. 30 iterations per timestep have been set, ensuring at least a 4th orders drop for all residuals. The aim of this step has been the analysis of the differences between the steady and unsteady structure of the underexpanded jet under ICE conditions. Indeed, as reported in [98] [99] and [100], a hysteretic behaviour can be observed in the jet structure when NPR changes with time. The nature of this phenomenon has not been clarified, but it is known that it affects the underexpanded structure in two ways. Firstly, for a given NPR, position and diameter of the Mach disk can show a marked difference between the steady and the unsteady solution. Secondly, hysteresis determines a mismatch in the threshold NPR for which the regular reflection is replaced by the Mach reflection. This difference arises when comparing increasing and decreasing NPR histories.

Figure 3.15 shows the result of this analysis: no particular discrepancies have been

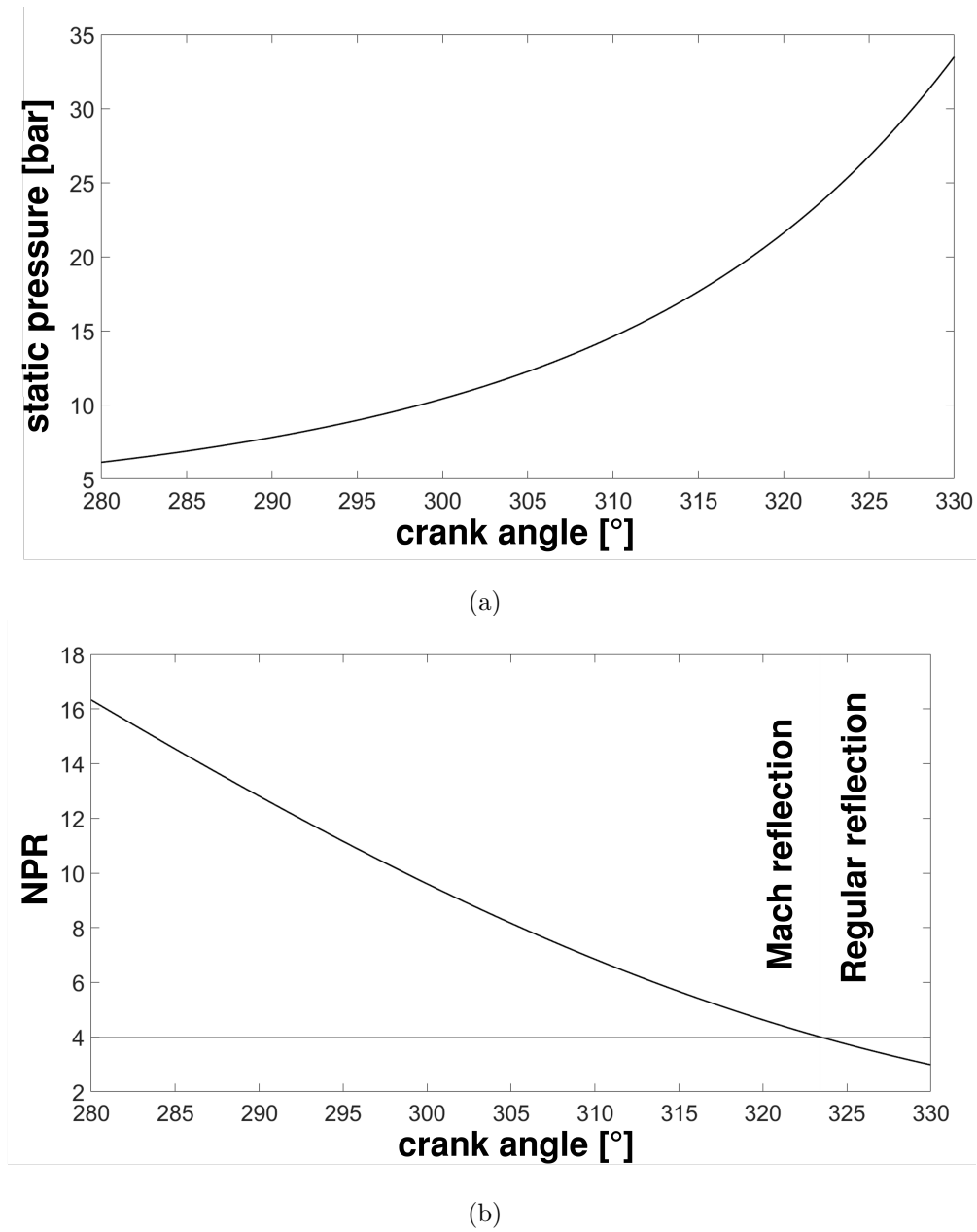


Figure 3.14: Evolution of (a) the static pressure during the compression stroke for the ICE reported in [45], and (b) the related NPR trend.

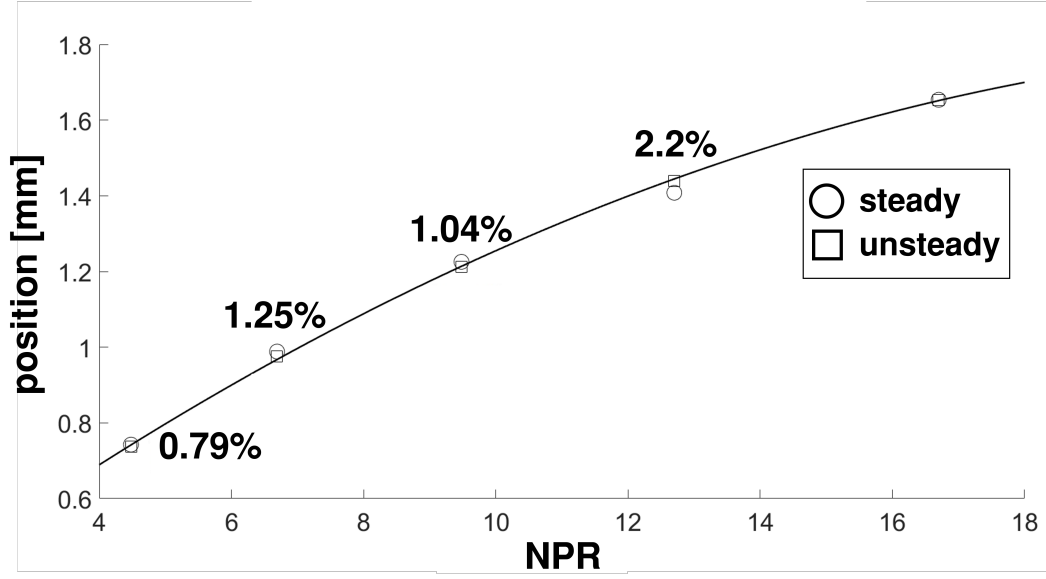


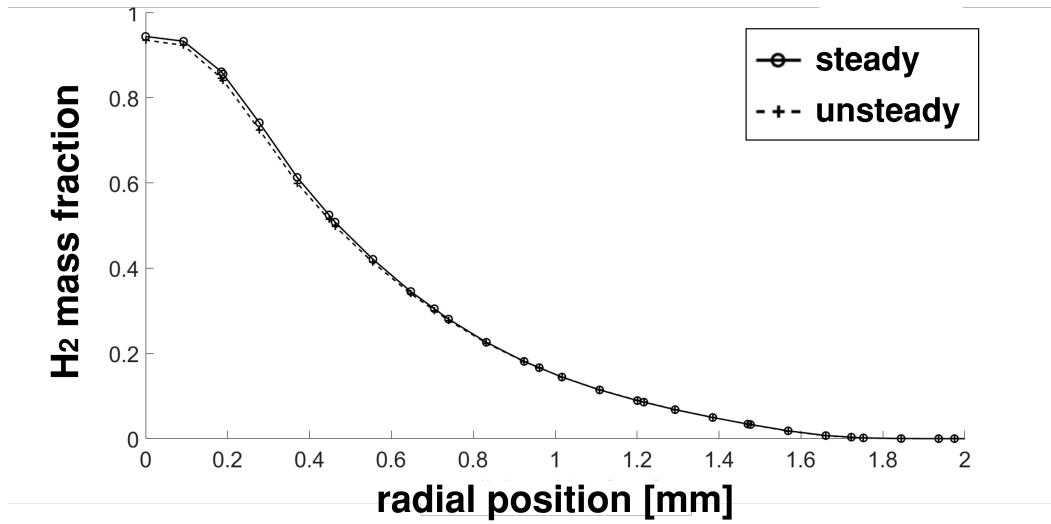
Figure 3.15: Comparison of the Mach disk position between steady and unsteady RANS simulations. For the characteristic variation rate of the NPR inside the ICE cylinder, no differences are observed regarding the Mach disk position.

found regarding the Mach disk position, since the maximum error is about 2%. In [100] higher differences, around 10%, are reported. This can be explained by considering that this kind of hysteresis depends on the NPR variation rate. The results shown by [100] refer to a dimensionless velocity $d(NPR)/dt' = 0.835$, being t' defined as:

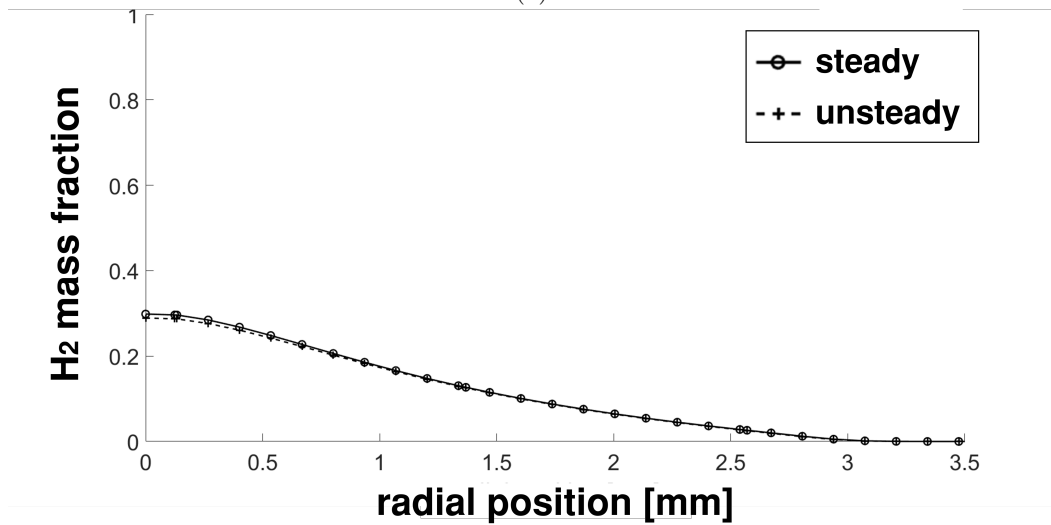
$$t' = \frac{ta_1}{\sqrt{k}d_{exit}} \quad (3.10)$$

The ICE injection process is characterized by a mean NPR variation rate of about 0.0015, hence almost 500 times slower. For this reason, the authors believe that no differences can be visible between steady and unsteady solutions at such a slow characteristic NPR rate.

Similarly, no differences are found when comparing the H_2 mass fraction distributions, either in the axial and radial direction. As an example, Figure 3.16 shows the radial distribution in the NPR 12.7 case at (a) 10 and (b) 20 mm from the nozzle exit plane. For all these reasons, it can be assumed that the H_2 jet evolution in ICE conditions can be captured by steady solutions and vice-versa, given the low dimensionless velocity of the injection process. Moreover, the validity of the correlations previously provided regarding the Mach disk features are still valid for ICE applications and the correlations can be confidently used in the mesh definition process. To complete the assessment of the hysteresis, an unsteady simulation has been carried out reversing the direction of travel in Figure 3.14(a). Indeed, another kind of hysteresis exists, due to which the threshold NPR of the regular to Mach reflection transition differs between in-



(a)



(b)

Figure 3.16: Comparison of the H₂ mass fraction radial distribution between steady and unsteady solution for NPR = 12.7: (a) at 10 mm and (b) at 20 mm from nozzle exit plane. As for the Mach disk position, because of the low NPR variation rate (defined in [?]), no remarkable differences are observed between the steady and unsteady solutions.

creasing and decreasing NPR histories [98] [99]. Although NPR does not increase during the ICE injection, it is interesting to analyze this aspect too. For the decreasing profile of Figure 3.14 (a), the transition takes place when the NPR is 4, while in the opposite direction it is visible for a NPR equal to 3.5. Therefore, the hysteresis associated to the increasing and decreasing NPR does not seem to be dependent on the NPR variation rate, in accordance with [98] and [99] where no effects of the variation rate have been reported.

3.5.2 Influence of the in-cylinder temperature

Inside an internal combustion engine, the injection takes place while the piston moves from the BDC to the TDC, causing not only a pressure rise but an increase of temperature as well. To assess this effect, RANS simulations have been performed by varying the discharging chamber temperature according to its evolution inside the combustion chamber. Numerically, this analysis has required the switch of the ambient vertical line (see Figure 3.3 (a)) from the wall condition to a velocity inlet condition. By doing so, it has been possible to impose different temperatures to the H₂ jet and the discharging chamber. Air velocity at the boundary has been set equal to 0.01 m/s in order to consider the discharging ambient almost steady. The temperature evolution during the compression stroke has been computed using the hypothesis of isentropic transformation:

$$T = T_{in} \left(\frac{p}{p_{in}} \right)^{\frac{k-1}{k}} \quad (3.11)$$

being T_{in} the temperature at the beginning of the compression stroke. Dealing with a turbocharged engine, T_{in} has been roughly considered equal to the exit temperature from the intercooler T_{ec} , assessed as follows:

$$T_{ec} = T_{amb} + \frac{T_{amb}}{\eta_c} \left[\left(\frac{p_c}{p_{amb}} \right)^{\frac{k-1}{k}} - 1 \right] - \Delta T \quad (3.12)$$

where η_c is the isentropic efficiency of the compressor (supposed equal to 0.86) and ΔT is the temperature drop imposed by the intercooler, supposed equal to 50 K. Figure 3.17 shows the temperature contour for the case with a NPR equal to 12.7 (1 ms after SOI). An ambient temperature equal to 491 K has been computed using the previous equations, while the H₂ temperature in the tank is still 300 K. In the expansion zone of the jet, just downstream of the nozzle exit section, a significant temperature drop can be observed, with a minimum of about 70 K before the Mach disk. Through this shock, the temperature rises up to 290 K. Surrounding the inner core, a layer where temperature is around 300 K can be observed, mainly made up of air cooled by the proximity to the H₂ jet.

Figure 3.18 shows the H₂ radial distributions at 3-15-30 mm from the nozzle exit

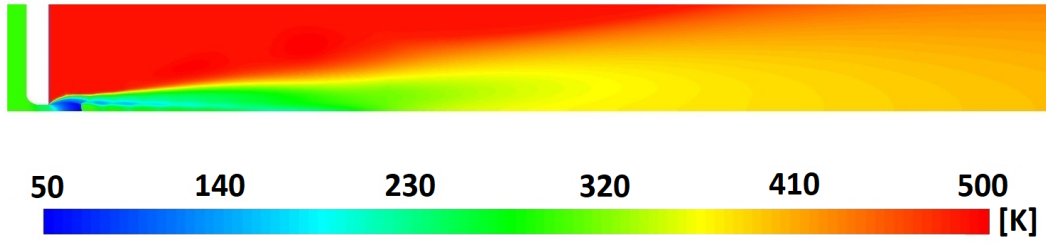


Figure 3.17: Contours of the static temperature, NPR 12.7. Air temperature in the ICE cylinder is fixed equal to 491 K.

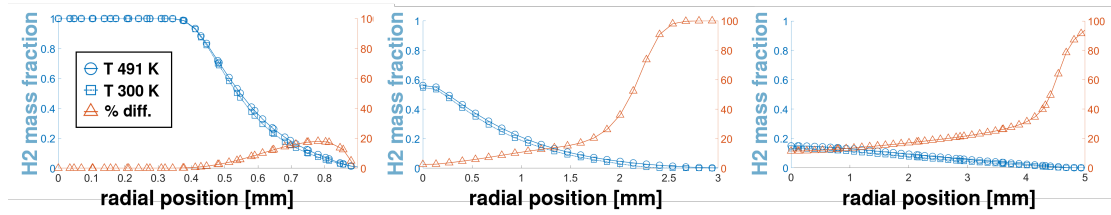


Figure 3.18: Impact of the different air temperature in the ICE cylinder (300 K vs 491 K): H_2 mass fraction value (light blue) and percentage difference (orange) in the radial direction at (a) 3 mm, (b) 15 mm and (c) 30 mm from the nozzle exit plane.

plane for the cases with the ambient temperature set at 300 K and 491 K. In all the plots the higher temperature determines an intensified diffusion of the H_2 , particularly far away from the nozzle exit plane, where jet momentum decreases and thermal diffusion becomes more relevant (Equation 3.4). At 3 mm from the exit, the maximum difference is about 20%, while at 15 and 30 mm both the percentage difference profiles show an almost linear increase of up to 30-40%, followed by a marked change of the slope at about 1.8 and 4.2 mm along the radial direction, respectively. At such radial positions, this trend is due to the H_2 diffusion towards zones where almost only air can be found in the 300 K case. Regarding the gas-dynamics structure, a perfect match in the Mach disk position can be observed between the two cases, further confirming that the position only depends on the NPR.

3.6 Conclusions

In this chapter, H_2 underexpanded jets have been examined by means of RANS and URANS simulations. Differing from the majority of the current literature, focus has been placed on the effect of ICE conditions on the jet structure and H_2 distribution. In particular:

- The correct numerical setup to get reliable results has been determined. The proposed mesh sensitivity analysis is a valuable tool to define the optimum cell

size, especially for ICE simulations reported in the next chapters.

- The correlations provided by the literature to assess the Mach disk features have been improved. Most of the authors propose constant values for C_H and C_D , while new correlations depending on NPR have been proposed. Therefore, the extension of the mesh refinement downstream of the nozzle can be defined more accurately.
- The axial position where the H_2 mass fraction drops to 30%, $L_{0.3}$, has been introduced as a parameter to determine the distance where the farfield zone begins. A deeper analysis of this parameter might be carried out in a future work, with the aim to develop a new notional nozzle approach for safety assessment.
- The dynamic behavior of the jet has been examined. Due to the NPR variation rate inside the combustion chamber, no hysteresis phenomena have been registered regarding both the Mach disk position and the H_2 distribution. Therefore, in ICE analyses, jet features at a specified crank angle (i.e., at a specified NPR) can be directly examined by means of a steady simulation, avoiding the analysis of the whole injection.
- The gas-dynamics features of the jet, such as the Mach disk height, are not dependent on the ambient temperature. Conversely, an enhanced H_2 diffusion is observed at higher temperatures, allegedly due to the Soret effect. The phenomenon is more evident far away from the nozzle exit, as the flow momentum diminishes.

Chapter 4

Influence of the cross section shape on under-expanded jets

Exploration of novel solutions for the direct injection of H_2 in internal combustion engines is a main topic for both academia and industry. In this context, injectors caps have received attention as a possible solution to quickly modify the exit section of the injector. For this reason, the physics of under-expanded jets discharged by non-circular sections is investigated, aiming at understanding the possibilities offered in ICE applications. Specifically, triangular and star sections have been compared against elliptical and rectangular ones. For the last two, the influence of the aspect ratio (AR) has been investigated as well. Studies regarding rectangular and elliptical sections are already present in the literature, but to the author's best knowledge some peculiarities that will be illustrated have not received enough attention.

Rajakuperan [101] numerically solved the under-expanded structure of elliptical jets, showing different shock patterns along the minor and major axis planes. A quicker growth of the boundary along the minor axis of the section was noted, ultimately leading downstream to the inversion of the axes (*axis switching* phenomenon). Menon and Skews [102] analyzed elliptical nozzles with aspect ratios (ARs) equal to 2 and 4 and pressure ratios from 4 to 6. They observed different dimensions of the Mach disk along the minor and major cross section axes, which confirmed the axis switching of the jet observed by Rajakuperan. The axis switching was generically attributed to the different curvature of the exit section in the minor and major axes. Menon and Skews [103] also observed that the barrel shock originates just after the nozzle exit section in the major axis plane, and later along the minor axis plane. Such trend was further intensified for the higher ARs. This behaviour was generically attributed to the variable curvature of the elliptical section, but a clear mechanism for the quicker onset of the barrel shock along the major axis plane was not provided. Chauhan and Aravindh [104] analyzed different elliptical jets with ARs of 2-4-6 and pressure ratios from 2 to 5, comparing results with a circular nozzle of the same area. They found superior levels of mixing for

all the tested NPRs. Interestingly, the influence of the AR on the mixing level seemed to be dependent on the under-expansion intensity. At the lower NPRs, jets released from section of ARs 4 and 6 featured a superior level of mixing, whereas a more intense mixing was promoted by the AR 2 nozzle at the higher NPRs. They attributed the higher mixing of the elliptical sections to the generation of eddies of different size (smaller in the major axis plane, greater in the minor) which enhance the different scales of the turbulent mixing. The same conclusions were drawn by Kumar [105] to explain the higher mixing provided by an AR 2 over-expanded elliptical jet issuing at Mach 2. As reported by the literature, rectangular jets provide an enhanced mixing as well, mainly due to the higher level of turbulence generated by the shape, as explained by [106]. [107] experimentally analyzed rectangular under-expanded jets for different ARs (2, 3, 4, 5, 62) and NPRs up to 500 using the Laser Induced Fluorescence (LIF) technique. Attention was paid to the transition from the regular to the Mach reflection of the incident shock waves. He noted that the Mach transition did not depend solely on NPR but an influence of the inlet total pressure was observed. No detailed description of the shock system was provided. Computational studies have been carried out by [108], who reported a quicker growth of the boundary along the minor axis of the exit section similarly to the elliptical cases, and the rounding of the corners due to the turbulent mixing. For square sections, a 45° rotation of the jet boundary was also noticed. [103] used the Laser Vapor Screen visualization technique to get "slices" of the flow field of underexpanded jets discharged by rectangular and square nozzles for pressure ratios of 4 and 6. To the authors' knowledge, he was the first to provide a detailed explanation of the near-field structure of such jets. Differently from circular nozzles, over-expanded conditions were recognized close to the corners of the outlet section, which caused the onset of four re-compression shock-waves but did not performed any consideration regarding the effects of the Mach disk features. Along the radial direction, saddle shape profiles in the velocity and mass distributions were also observed. To the authors' knowledge, these profiles have been mostly investigated in subsonic flows (see [109], [110]). [111] and [112] attributed the saddle-shaped profile to the development of 3D vortex rings shed from the nozzle lips, in synergy with the streamwise vorticity of the secondary flows developed inside the nozzle. The underexpanded flows in this chapter have been analyzed setting the NPR equal to 10, which corresponds to a highly underexpanded condition. Indeed, H₂ DI feed pressure is expected to increase in the near future. To such a purpose, 3D RANS simulations have been carried out, since the shock system development is mainly an inviscid phenomenon which does not require more advanced approaches (LES, DNS). Regarding the mixing analysis, although the LES simulations would provide closer results to the experiments (see [113]) than RANS, the latter are still reliable when one wants to perform analyses on a large number of cases.

4.0.1 Sections analyzed

In Figure 4.1, a sketch of the computational domain is shown. It is basically made up of three zones: a cylindrical body (green), with a sufficiently large diameter to minimize the total pressure losses, a convergent nozzle ending with a constant section duct, and a cylindrical discharging ambient with large dimensions to avoid confinement effects. Such a configuration creates a radial velocity field in the convergent section, which tends to zero in the constant section duct. Hence flow can be considered axial at the outlet section. For a generic cross section shape, $D_{nozzle,eq}$ has been defined as the diameter of the circular section with the same area.

Length of the discharging chamber has been set equal to $35D_{nozzle,eq}$. Position of the Mach disk is expected to be around $2D_{nozzle,eq}$ and length of the potential core about $26D_{nozzle,eq}$ (see [80]). Consequently, length of the discharging chamber has been deemed sufficient to solve the near-field zone of the jet. Diameter of the chamber has been set to $14D_{nozzle,eq}$, enough to avoid the interaction with the boundary condition along the lateral surface. The convergent nozzle has been preferred to convergent-divergent configurations in order to analyze flows at sonic condition (Mach equal to 1) in the exit section.

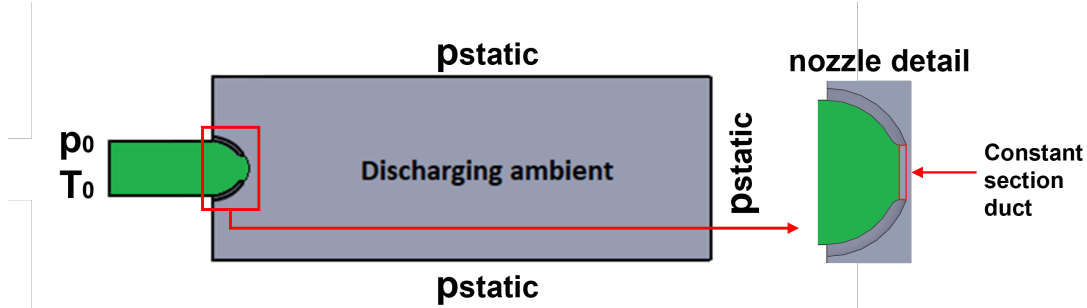


Figure 4.1: Section of the numerical domain used in this work with the boundary conditions applied to the domain boundaries. On the right, a detailed view of the nozzle exit.

The choice of the cross-section area is coherent with benchmark experiments on H_2 DI ICE. All the nozzles have the same outlet area of 1.67 mm^2 , which is the exit area of the circular injector equipping the H_2 optical engine tested at the Sandia National Laboratories [114].

Sketches of the sections are reported in Figure 4.2. For the rectangular and elliptical sections, aspect ratios (defined as the ratio between the major, A, to minor, B, sides for the rectangular section, and between the major to the minor axes for the elliptical one) equal to 1.5, 5.0 and 8.0 have been taken into account. The AR 8.0 has been selected on the basis of manufacturing considerations: for the chosen outlet area, an elliptical section featuring an even higher AR would result in an excessive curvature along the

minor axis plane. The minimum AR has been chosen to be close to one, while the AR 5 has been selected as a middle value between the maximum and minimum ARs. The triangular section is equilateral, while the star is composed of an inner central square sharing sides with four equilateral triangles. By examining this set of shapes, insights regarding the influence of constant curvature (circular section), continuously varying curvature (elliptical section), convex and concave angles (rectangular, triangular, and star section) can be obtained.

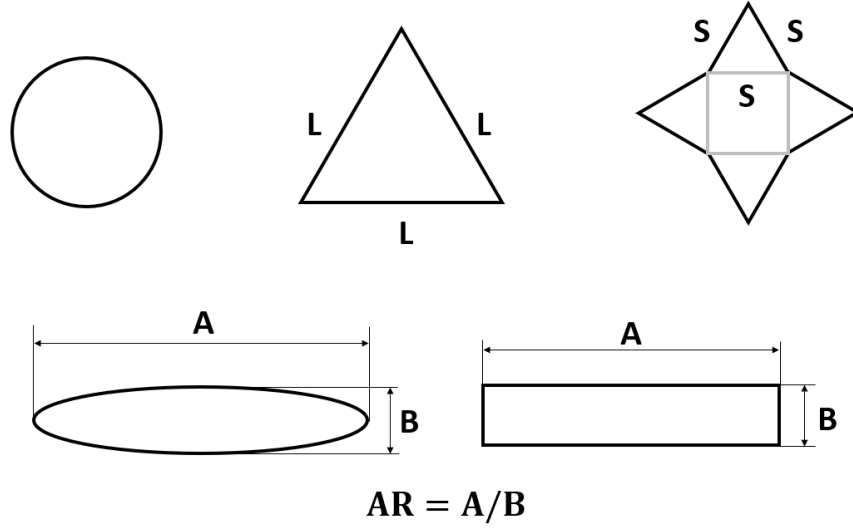


Figure 4.2: Sketch of the nozzle section shapes analyzed in this work. L, S, A, and B indicate the dimensions of the different cross sections. AR is the aspect ratio.

4.0.2 Numerical methods

In Figure 4.3, a cut plane of the mesh employed in this work is reported, along with an enlargement downstream of the nozzle exit section. Mesh is made up of tetrahedral elements, which is a useful feature at such stage of the study, in which no information about the orientation of the main eddies is available. Two levels of refinement can be observed in the enlargement. A mean cell size of $50 \mu\text{m}$ has been applied in the near-field zone of the jet, where intense gas-dynamic phenomena are expected to occur. Externally to the near-field zone, an average cell size of $100 \mu\text{m}$ has been deemed sufficient to effectively capture the mixing-layer of the jet, responsible for the diffusion of the H_2 into the ambient fluid (see [115] [42]).

The steady form of the conservation equations have been solved using the same numerical approach defined in the previous Chapter. As verified in the previous Chapter, the characteristic variation of the NPR during the injection in ICE applications is too small to produce hysteresis effects. Therefore, features of the shock system can be analyzed by means of a steady computation.

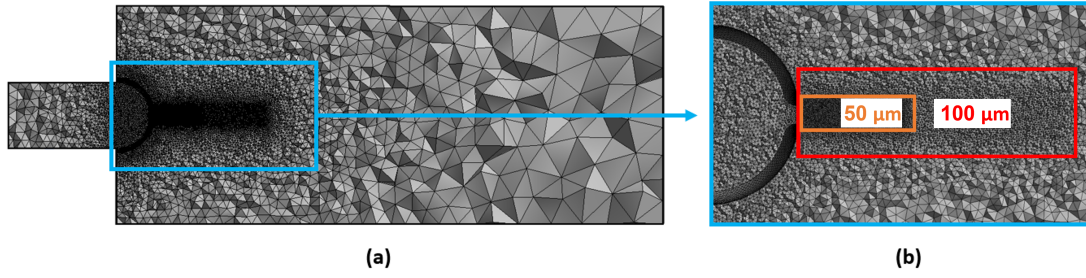


Figure 4.3: (a) Representation of the numerical grid on a section plane, (b) detail of the mesh refinement on two boxes downstream of the nozzle exit section.

Total conditions of 10 bar and 300 K have been imposed at the domain inlet. Both the right face and the lateral surfaces of the discharging cylinder have been treated as pressure outlet boundaries (see Figure 4.1), setting a static pressure equal to 1 bar. To reduce the computational time, water vapour in the air has not been taken into account, thus solving transport equations only for H_2 and O_2 . Significant variations of the temperature inside the jet are expected, leading to the adoption of the three parameters Sutherland law to model the local molecular viscosity. Spatial derivatives have been discretized by means of a second-order accurate upwind scheme.

Several studies are present in the literature to assess the most suitable RANS turbulence model for non-circular jets. According to [116], the Spalart-Allmaras model over-predicts the axial velocity decay rate and under-predicts the potential core length (i.e., the near-field zone where the gas-dynamic effects are predominant). The RNG $k-\varepsilon$ better captures the potential core length, but the axial decay rate is again over-predicted. The standard $k-\varepsilon$ computes an axial decay rate slightly slower than the RNG model, but under-predicts the potential core length. Tide ([117]) compared the Wilcox $k-\omega$ model against the SST $k-\omega$ using a jet at Mach number 0.9 as a benchmark. Both the models showed acceptable agreement with the experimental data, but the SST $k-\omega$ resulted to be less sensitive to the mesh density, which is a favourable characteristic to exploit when 3D simulations have to be carried out.

To define the most suitable turbulence model, and to test the validity of the setup previously described, a validation step has been deemed necessary. Two benchmarks have been carried out. In the first one, the experimental data provided by [118] have been exploited to assess the validity of the numerical results in terms of H_2 axial penetration. In this case, a rectangular nozzle (aspect ratio equal to 8) has been tested applying a NPR equal to 10.

In Figure 4.4, the reciprocal of the H_2 axial mass fraction has been plotted against the non-dimensional axial position (being r_{eq} the radius of the circular area with the same area). The $k-\varepsilon$, SST $k-\omega$ and RSM closures have been examined using the default configurations set by ANSYS Fluent[®]. As it can be observed, the SST $k-\omega$ provides the

closest outcomes to the experimental data, and consequently it has been chosen for the RANS closure.

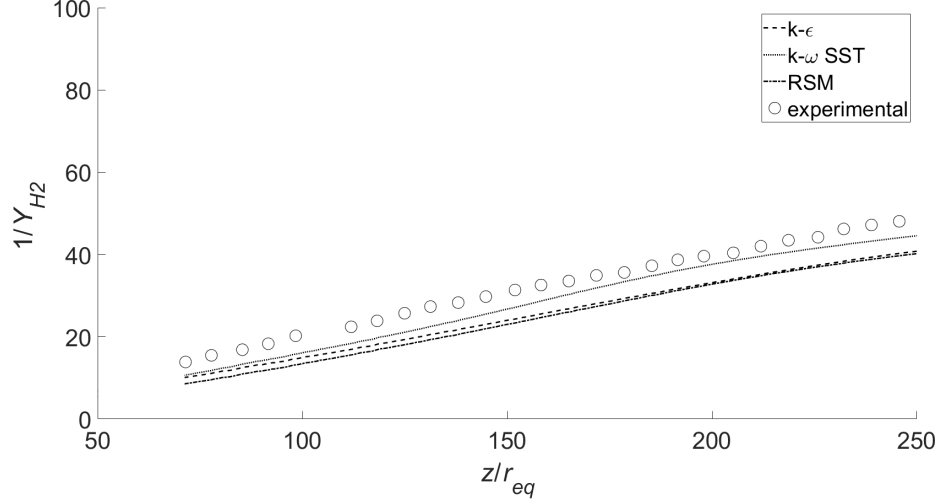


Figure 4.4: Comparison between the experimental [118] and numerical results of the reciprocal H_2 mass fraction (Y_{H_2}) along the axial direction (z) for an AR 8.0 rectangular jet, $NPR = 10$.

As a second step, the same validation based on the position of the Mach disk for a 1 mm circular nozzle under a NPR of 10 [93] has been carried out to test the overall validity of the numerical setup in the 3D domain. As already shown in the previous Chapter, the Mach disk is located at about 2 mm from the nozzle exit section (see Figure 3.4. The numerical position of the shock, reported in Table 4.1 for different refinement levels in the nearfield zone of the jet, is correctly captured by the simulations. A cell size of $50 \mu\text{m}$ has been considered a good compromise between the accuracy of the results and the required computational time.

Table 4.1: Mesh sensitivity analysis. Comparison of the Mach disk position for different grid refinements.

Near-field cell size [μm]	5	10	20	30	50	100
Disk position [mm]	2.02	2.00	1.99	1.96	1.95	1.89

4.1 Influence of the cross section shape

Triangular section

The equilateral triangular section has been selected to investigate the influence of acute angles on the shock-expansion system. In Figure 4.5, the longitudinal numerical Schlieren pictures are reported. Here, some major differences with respect to the classical circular nozzle are present. As it can be observed along the symmetry plane in Figure 4.5(a), the barrel shock forms almost immediately from the upper vertex, while the onset is delayed from the edge of the triangle.

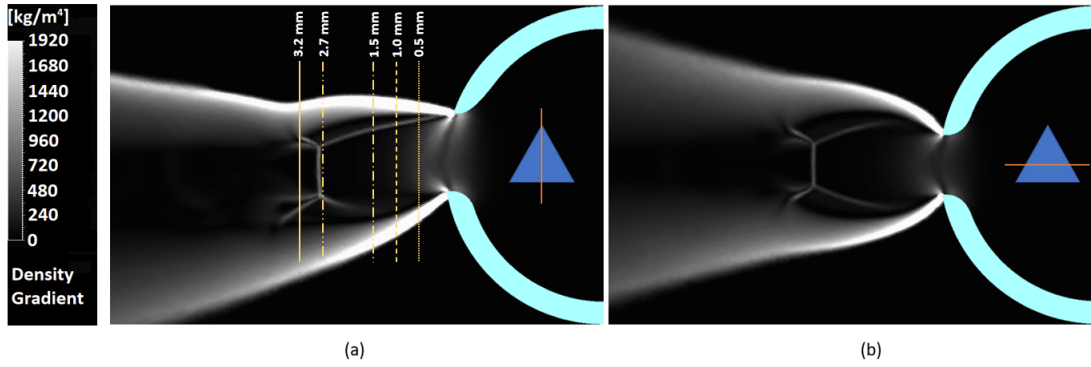


Figure 4.5: Longitudinal numerical Schlieren picture of the underexpanded jet from the triangular section: (a) in the symmetry plane and (b) in a plane parallel to the triangle base passing for the center of the triangle.

The reasons behind the shock formation are indeed quite different. At the vertex (convex zone), the interaction between the fans originating from two consecutive sides leads to a locally over-expanded flow: pressure drops below the ambient pressure, and consequently a shock wave quickly forms to re-compress the flow. The over-expanded condition is visible in Figure 4.6(a), reporting the static pressure contours at the exit section of the nozzle: while the static pressure is equal to 284000 Pa along the edges, a minimum of about 70000 Pa is reached at the corners, which is below the ambient pressure of 100000 Pa.

The re-compression shock wave is the barrel shock visible in Figure 4.5(a). At the basis, the classical formation of the barrel shock takes place. However, coalescence of the expansion waves is quicker for higher curvatures (i.e., for smaller radii of the osculating circles): in this case, the edge curvature equal to zero leads to a very delayed formation of the barrel shock. Such trend is visible in Figure 4.5(b), in which the shock-expansions system is symmetrical.

To clarify the structure of the shock system, the shock detection method proposed by Lovely and Haines (see [119]) has been exploited to produce Figure 4.6(b). Here, the three corner shocks are clearly visible. They result to point towards the axis, eventually reflecting and forming a Mach disk normal to the axis, followed by a reflected shock. In

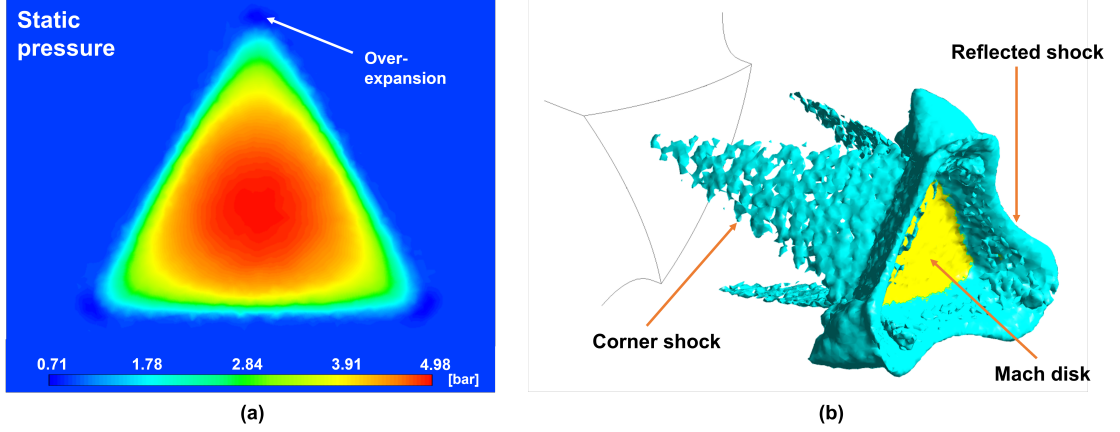


Figure 4.6: (a) Contours of the static pressure at the nominal exit section of the triangular nozzle and (b) 3D shock structure of the jet by means of shock detection proposed by Lovely and Haimes [119].

Figure 4.7, the numerical Schlieren pictures relative to five planes normal to the axis are shown to further draw insights of the shock system. At 0.5 mm from the nozzle exit, it can be observed that the over-expansion condition leads to the onset of the corner shock waves. Moving further downstream, the shock waves become wider (see Figure 4.7(b) and (c)) and eventually reflect (Figure 4.7(d)).

In this specific case, the reflection is irregular, hence a lateral Mach disk and the related reflected waves form. The incident shock system is then made up of the three corner shocks, their Mach disks and the lateral reflected waves. The incident shock system points towards the jet axis, causing the onset of a strong normal Mach disk. After this, the shear layer and the reflected shock propagate downstream (both shown in Figure 4.7(e)). Another distinctive feature observable in the Schlieren pictures is the growth of the jet boundary. The boundary expands faster from the center of the edges and slower from the vertices, resulting in a deformation which leads to a three-lobe jet. This behaviour is related to the higher level of the vorticity magnitude (i.e., the vorticity module) at the center of the edges.

In Figure 4.8(a), the vorticity magnitude distribution along the jet perimeter immediately downstream of the exit section is superimposed to the jet boundary of Figure 4.7(e). As it can be observed, the higher vorticity leads to a faster deformation of the boundary from the middle of the sides, ultimately generating the three-lobe shape observed at 3.2 mm from the exit section.

Thus, the high vorticity magnitude zones behave as *traction points* governing the deformation of the boundary. In Figure 4.8(b) the velocity magnitude is shown immediately downstream of the exit section. Higher velocities are found along the jet boundary, because the flow, ejected in the proximity of the wall, meets earlier the expansion fan with respect to the flow released from the inner of the section. As the velocity module

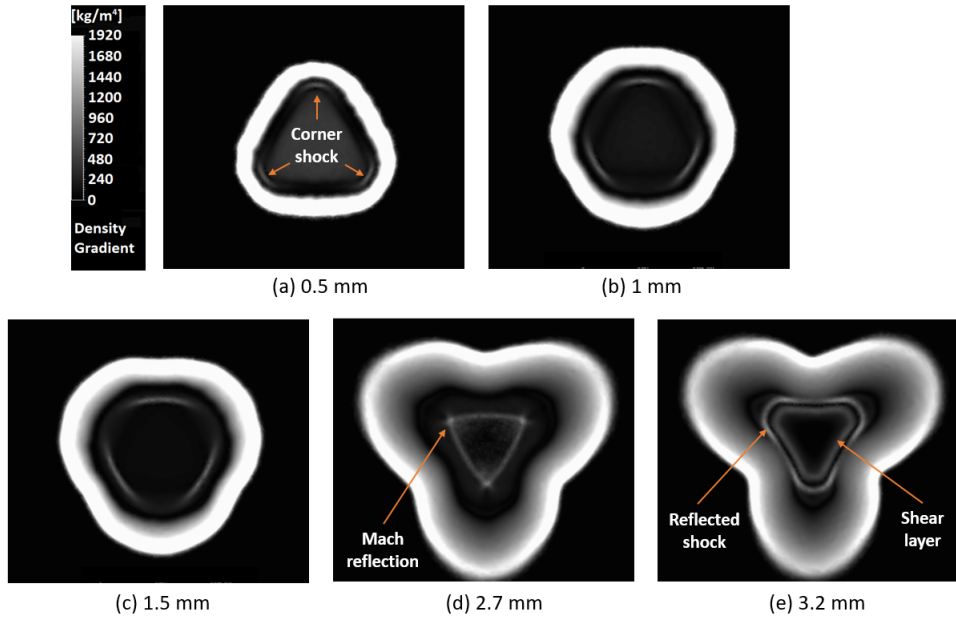


Figure 4.7: Normal numerical Schlieren pictures of the jet issuing from the triangular section on five different planes normal to the jet axis: (a) at 0.5 mm, (b) at 1.0 mm, (c) at 1.5 mm, (d) at 2.7 mm, and (e) at 3.2 mm from the exit section.

must be unique at the center of the shape, higher velocity gradients are expected where distance between the shape center and the triangle side is minimum (see Figure 4.8(b)). This can be considered the reason why a higher vorticity module has been observed in the middle of the side edges.

Star-shaped section

The triangular section has a convex shape. Consequently, it has been deemed interesting to analyze the jet structure developed by a nozzle section with convex and concave features: the star-shaped section. This shape has eight vertices: four equal to 60° and four equal to 210° , alternatively arranged. Figure 4.9(a) reports the numerical Schlieren along a plane passing through two opposite convex vertices. As already observed in the triangular nozzle, the onset of shock waves just downstream of the exit section is found. Conversely, in the plane passing through two opposite concave vertices, see Figure 4.9(b), the occurrence of the barrel shock is delayed.

As already discussed for the triangular section, the onset of the shock waves emanating from the convex vertices is due to the over-expanded condition occurring when the angle is acute, as shown in the pressure contours reported in Figure 4.10(a). In the same picture, it can be observed that concave vertices (obtuse angles) are not subject to the over-expanded condition, since the expansion fans do not cross in the proximity of concave vertices. The 3D shock-system is reported in Figure 4.10(b), where it can be observed that the re-compression corner shocks reflect along the axis forming a normal

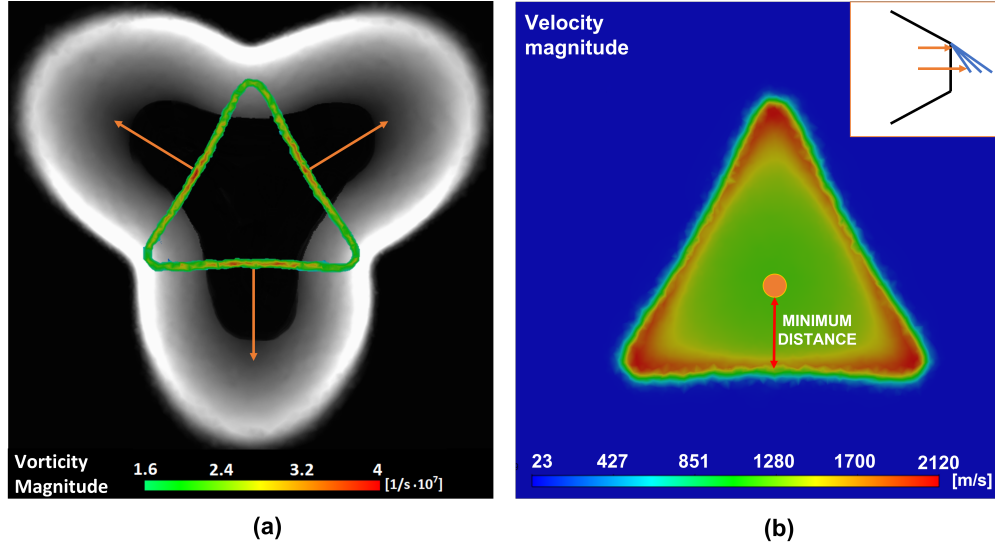


Figure 4.8: (a) Vorticity magnitude contours at the triangular nozzle exit section superimposed to the jet boundary developed further downstream. (b) Velocity magnitude immediately downstream of the exit section: higher velocity is observed along the perimeter due to the earlier expansion of the outer flow.

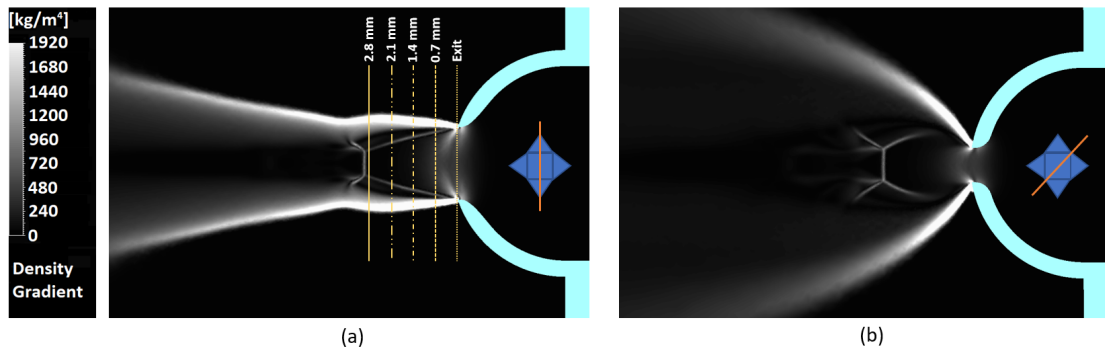


Figure 4.9: Longitudinal numerical Schlieren picture of the underexpanded jet from the star nozzle: (a) in a plane passing through the vertices of the triangles and (b) in a plane along the diagonal of the inner square.

Mach disk, followed by its reflected shock.

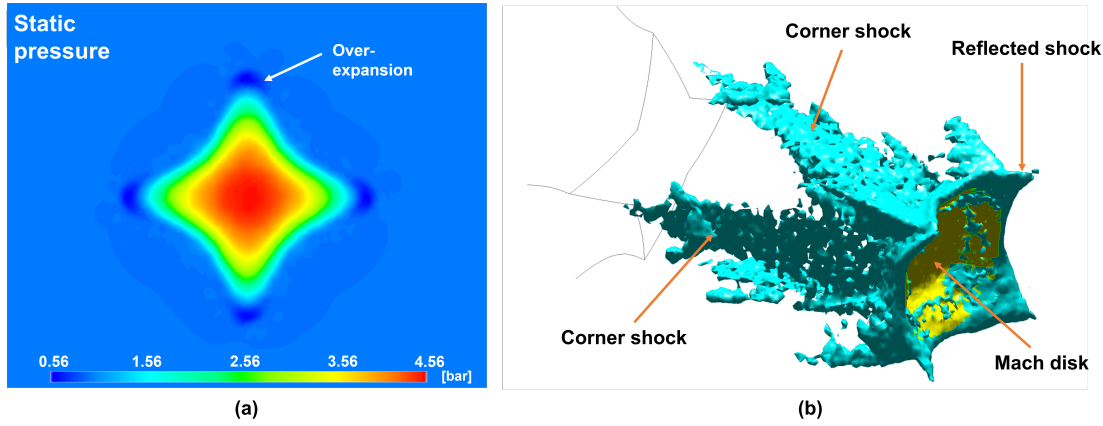


Figure 4.10: (a) Contours of static pressure at the exit section of the star shaped nozzle and (b) 3D visualization of the shock system developed by the star nozzle, reconstructed by means of the shock detection method proposed by [119].

Schlieren pictures normal to the jet axis are reported in Figure 4.11. At the exit section the jet holds the same shape of the nozzle. At 0.7 mm, the corner shock waves propagating from the convex vertices are visible. Further downstream, they expand (1.4 mm) and reflect each against the other in an irregular way (note, in the picture at 2.1 mm, the formation of the lateral Mach disks and reflected shocks). At 2.8 mm the Mach disk normal to the jet axis has already formed, and consequently the shear layer and the reflected shocks can be observed. Regarding the jet boundary, it can be noted that the growth is faster along the diagonals of the inner square with respect to the tip vertices of the triangles. This behaviour can be justified observing the vorticity contours immediately downstream of the nominal exit section (Figure 4.12): the higher values are found at the concave vertices, where the enhanced turbulent diffusion leads to a much quicker growth of the boundary along the diagonals of the square. Thus, as already discussed for the triangular case, zones characterized by a higher vorticity magnitude behave as *traction points*, quicker stretching the jet boundary towards the surrounding ambient. Such zones are once again the closest points to the shape center, confirming that greater vorticity levels are due to the higher velocity gradients.

Elliptical section

In Figure 4.13, the numerical Schlieren pictures are reported for a jet issuing from the AR 1.5 elliptical nozzle. It can be observed that the occurrence of the barrel shock is quicker along the major axis plane, whereas it has a lower intensity along the minor axis plane. This behaviour can be explained looking at Figure 4.14, which reports a sketch of the leading waves of the fans originating at the endpoints of the major and minor axes. Since the pressure $\bar{p}$ just after the expansion fans at the axis location must be unique,

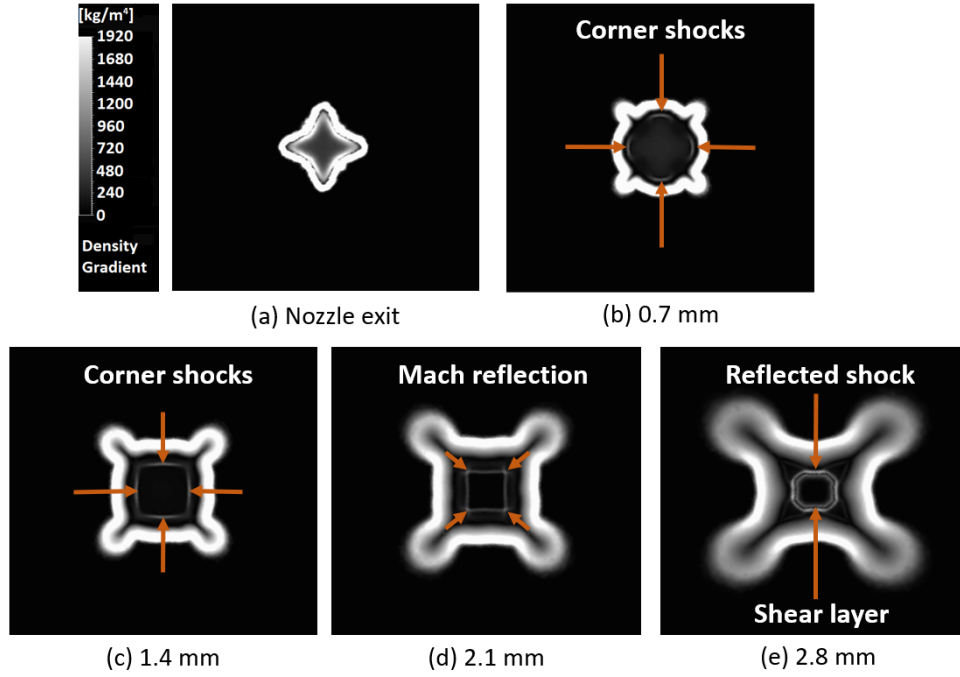


Figure 4.11: Normal numerical Schlieren pictures of the jet issuing from the star section on five different planes normal to the jet axis: (a) at the nozzle exit, and (b) at 0.7 mm, (c) at 1.4 mm, (d) at 2.1 mm, (e) at 2.8 mm from the exit section.

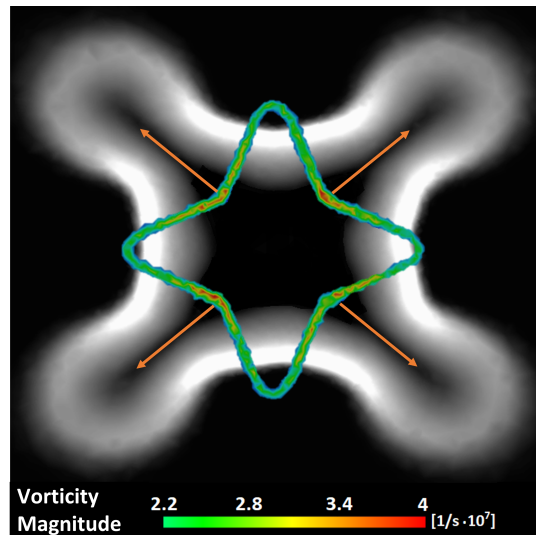


Figure 4.12: Vorticity magnitude contours at the star nozzle exit section superimposed to the jet boundary developed further downstream. Also in this case, the high vorticity zones behave as traction points, driving the deformation of the boundary.

inclination of the fan from the major axis must be lower (i.e., $\alpha < \theta$ in Figure 4.14). As a consequence, reflection of the expansion waves and coalescence of the compression ones is quicker along the major axis plane, resulting in an earlier formation of barrel shock. Hence, it can be concluded that the coalescence is faster for higher curvatures, and vice-versa.

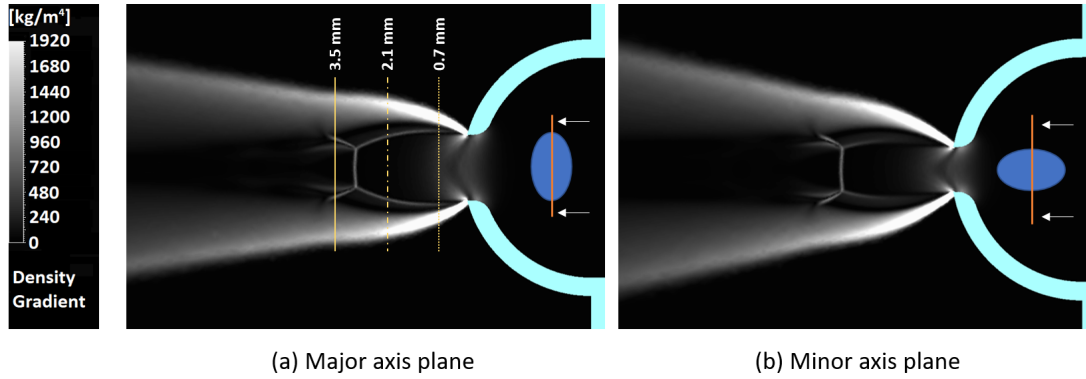


Figure 4.13: Longitudinal numerical Schlieren pictures of the jet issuing from the elliptical nozzle with $AR = 1.5$: (a) major axis plane and (b) minor axis plane.

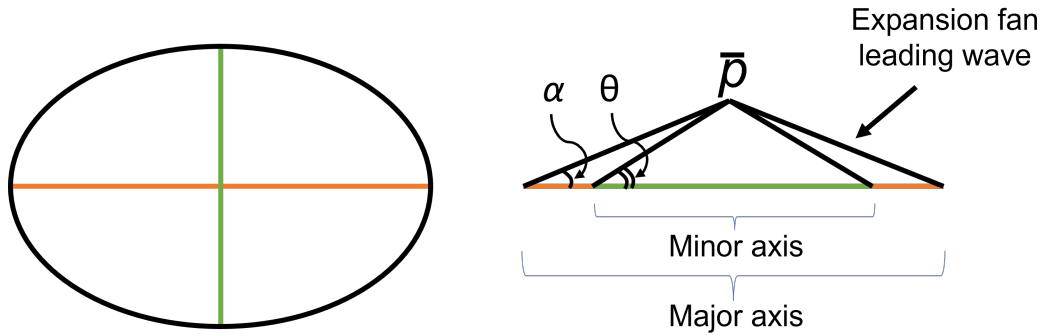


Figure 4.14: Sketch of the expansion fans leading waves emanating from the major and minor axes of the elliptical section. α and θ represent the wave inclination from the minor and major axes, whereas $\bar{p}$ stands for the pressure level at the axis just after the fans.

What has been described is confirmed by both the 3D shock system in Figure 4.15 and the normal Schlieren reported in Figure 4.16. At 0.7 mm from the nozzle exit, the incident barrel shock is only visible at the extremes of the major axis, whereas it begins to be observable along the minor axis at 2.1 mm from the exit section. At the imposed NPR of 10, the incident shock system reflects in an irregular way, forming a normal Mach disk followed by its shear layer and the reflected shock, both visible at 3.5 mm downstream of the exit section. In the sequence reported in Figure 4.16, the axis switching phenomenon can be observed: the boundary expands faster along the minor axis plane as an effect of the higher level of the vorticity magnitude (whose distribution

has not been reported for the sake of brevity).

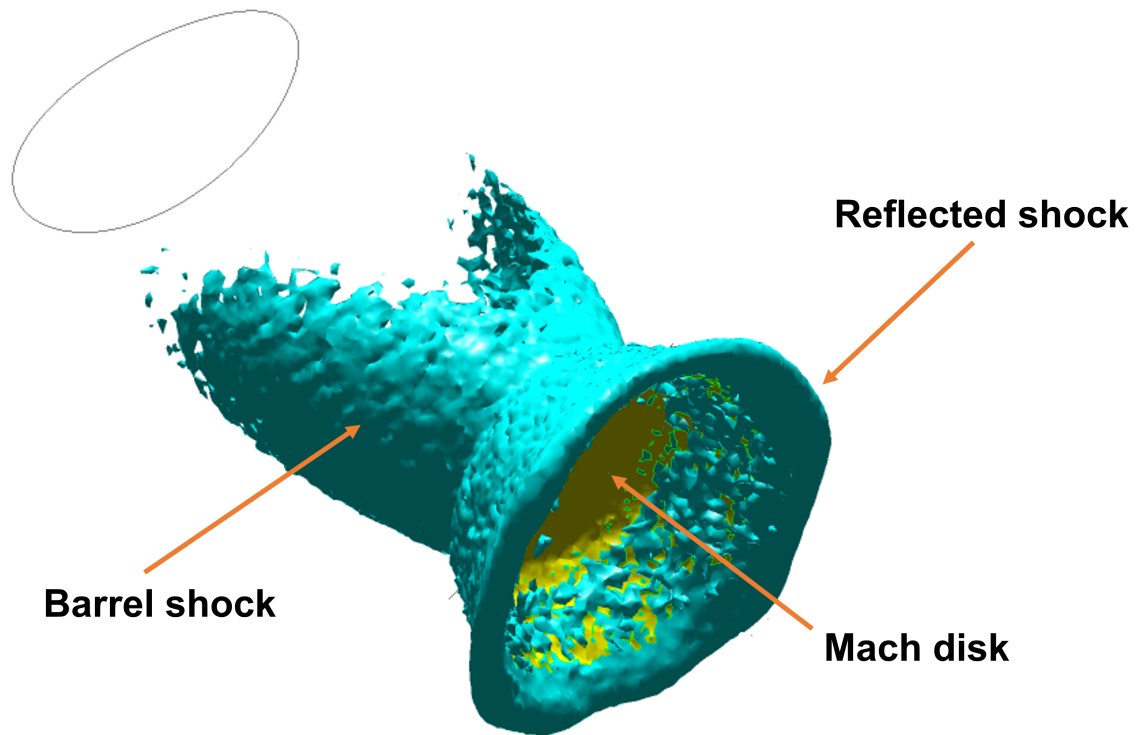


Figure 4.15: Shock system developed by the elliptical section, reconstructed by means of the shock detection method proposed by [119].

Rectangular section

The shock system developed by a rectangular nozzle of AR 1.5 is reported in the longitudinal planes in Figure 4.17. Also in this case, the barrel shock forms earlier along the major axis plane, resulting to be more intense here with respect to the minor axis plane. Differently from the elliptical case previously analyzed, such trend cannot be justified by different curvatures along the section perimeter. What has been observed can be explained by looking at Figure 4.18, which reports the static pressure contours at the nozzle exit section along with the 3D shock system, and Figure 4.19, which shows the normal Schlieren pictures. Similarly to the triangular and star-shaped sections, the coexistence of the expansion fans at the vertices of the exit section leads to an over-expanded condition.

As a consequence, four re-compression shock waves occur at the vertices, as visible in Figure 4.18(b) and Figure 4.19(a). At 2.1 mm from the exit section, the re-compression waves have met along the major axis plane, resulting in the barrel shock visible in Figure 4.17(a). Along the minor axis plane, the barrel shock is still not visible because the shock waves have not met yet. At 2.5 mm the reflection of the shock waves is irregular,

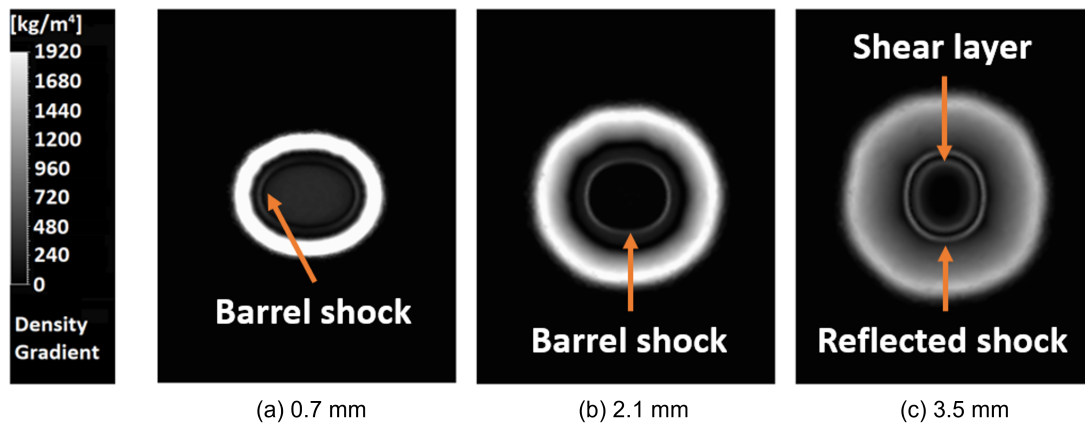


Figure 4.16: Normal numerical Schlieren pictures of the jet issuing from the elliptical nozzle with $AR = 1.5$, on three different planes normal to the jet axis: (a) at 0.7 mm, (b) at 2.1 mm, and (c) at 3.5 mm from the exit section.

leading to the formation of a lateral Mach disk and the related reflected waves. Similarly to the triangular and rectangular sections, the incident shock system is then made of the four corner shocks, the lateral Mach disk and the reflected shocks. The incident system points towards the axis and reflects forming a normal Mach disk, followed by the shear layer and the reflected shock, both visible at 3.0 mm from the exit section. The growth of the jet boundary results to be very slow at the corners and faster from the center of the sides. As in the previous cases, higher values of the vorticity magnitude have been observed in the center of the longer sides, which are once again the closest points to the section center (picture of the vorticity distribution has not been reported for the sake of brevity). Such high vorticity zones lead to a faster growth along the minor axis plane, resulting in the four-lobe boundary at 3.0 mm from the exit plane (Figure 4.19(d)).

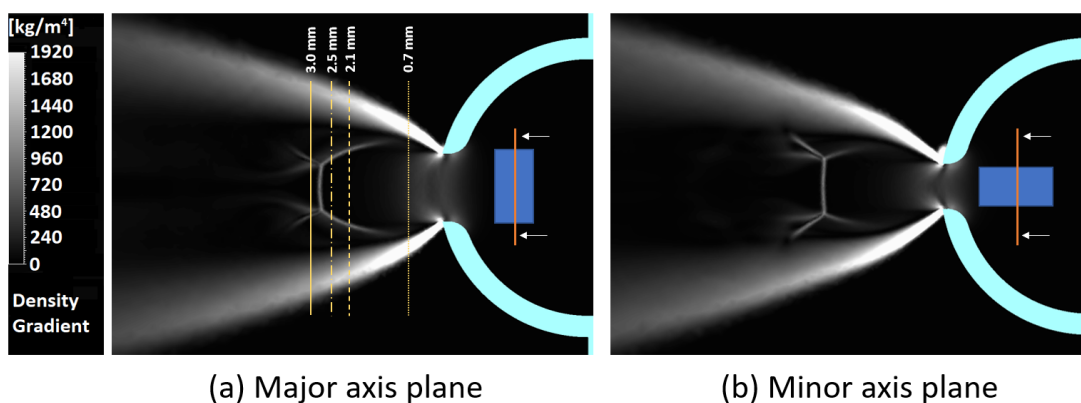


Figure 4.17: Longitudinal numerical Schlieren pictures of the jet issuing from the rectangular nozzle with $AR = 1.5$: (a) major axis plane and (b) minor axis plane.

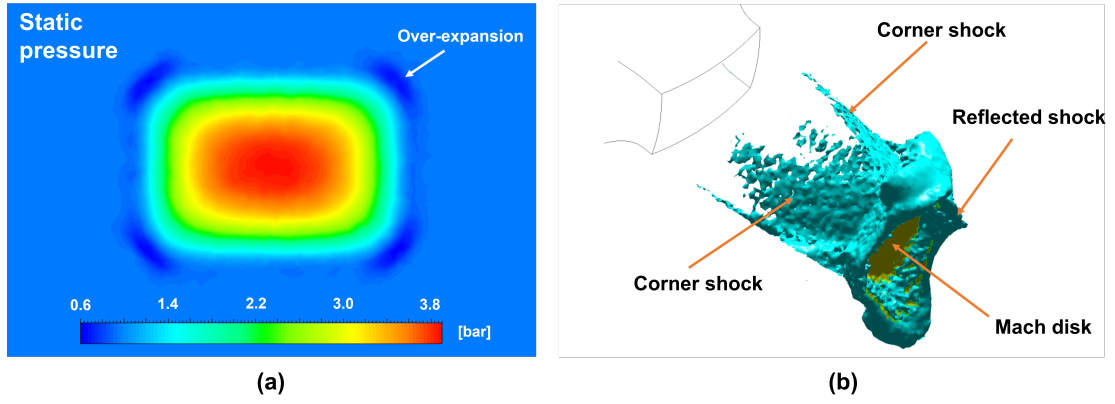


Figure 4.18: (a) Static pressure contours at the nominal exit section for the AR 1.5 rectangular nozzle and (b) visualization of the 3D shock system, reconstructed by means of the shock detection method proposed by [119].

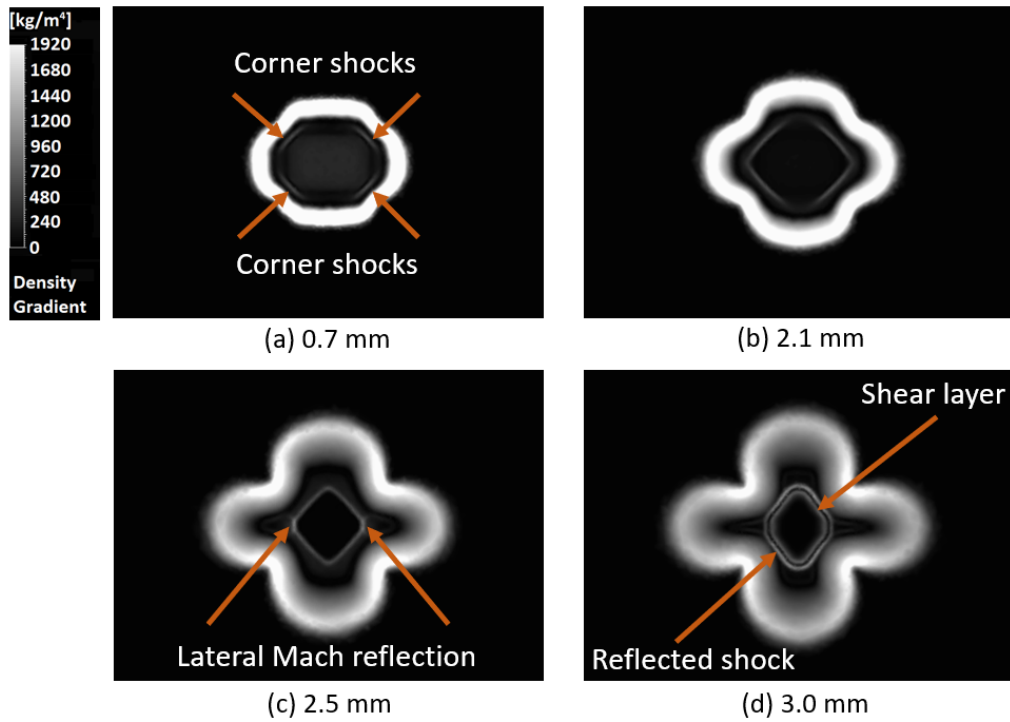


Figure 4.19: Normal numerical Schlieren pictures of the jet issuing from the rectangular nozzle with $AR = 1.5$ on four different planes normal to the jet axis: (a) at 0.7 mm, (b) at 2.1 mm, (c) at 2.5 mm, and (d) at 3.0 mm from the exit section.

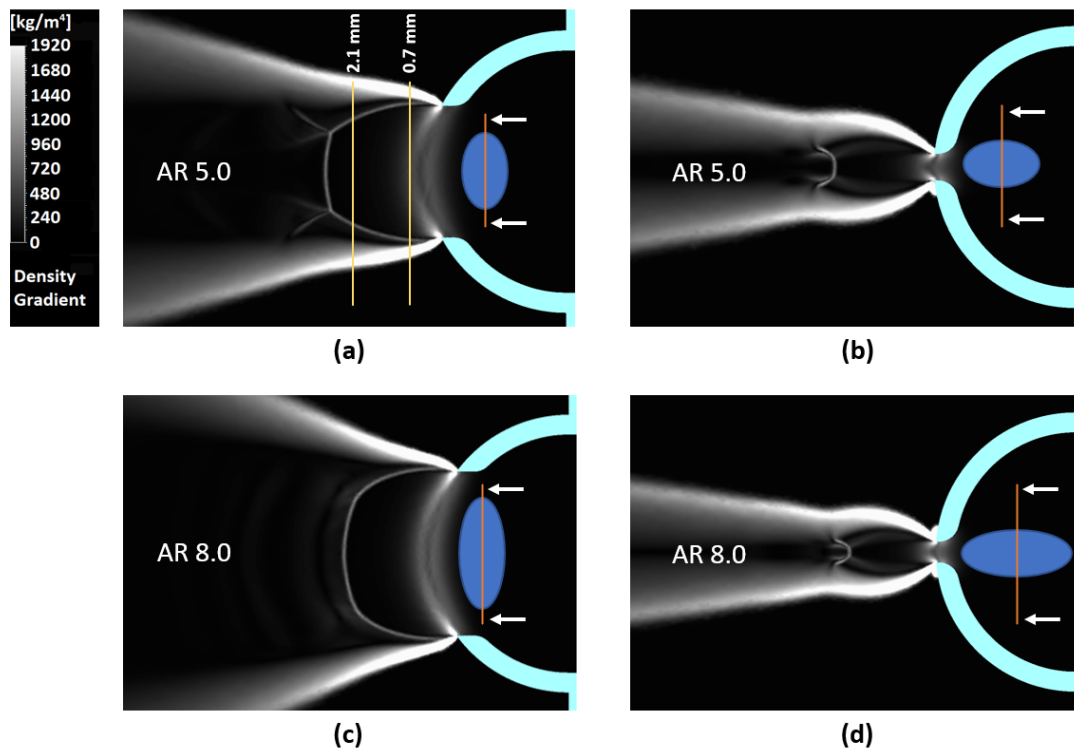


Figure 4.20: Longitudinal numerical Schlieren pictures for the elliptical nozzles: (a) AR 5.0 - major axis plane, (b) AR 5.0 - minor axis plane, (c) AR 8.0 - major axis plane, (d) AR 8.0 - minor axis plane.

4.1.1 Influence of the aspect ratio

The rectangular and elliptical sections previously described have been further analyzed. Holding the same total conditions and the same nozzle exit area, the AR has been varied to get insights of the influence on the structure and mixing characteristics of the jets. The results of the AR 1.5 cases have been compared to the outcomes relative to nozzles with ARs equal to 5.0 and 8.0. In Figure 4.20, the longitudinal Schlieren of the elliptical sections are reported. The first row refers to the AR 5.0 case, while the second one to the AR 8.0. In both the cases, the barrel shock along the minor axis plane is not well defined, looking like a band rather than a thin shock. This can be attributed to the progressively lower curvature of the section perimeter along the minor axis plane, as a result of which the weak compression waves are not able to coalesce. For both the sections, instead, the barrel shock along the major axis plane results to be well defined, forming just downstream of the exit section. While the normal Mach disk looks like a thin flat discontinuity for the elliptical section with an AR of 1.5, a rising curvature can be observed as the AR increases. The shear layer in the AR 5.0 case constitutes a convergent duct on the major axis plane (as already observed for the circular nozzle), whilst it looks straight along the minor. In the AR 8.0 case, the normal Mach disk and

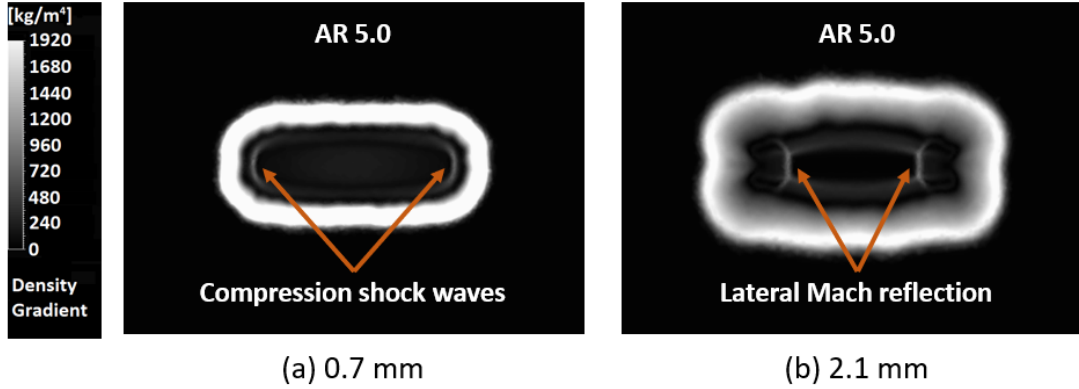


Figure 4.21: Normal numerical Schlieren pictures for the jet issuing from the elliptical nozzle with $AR = 5.0$ on two different planes normal to the jet axis: (a) at 0.7 mm and (b) at 2.1 mm from the nozzle exit section.

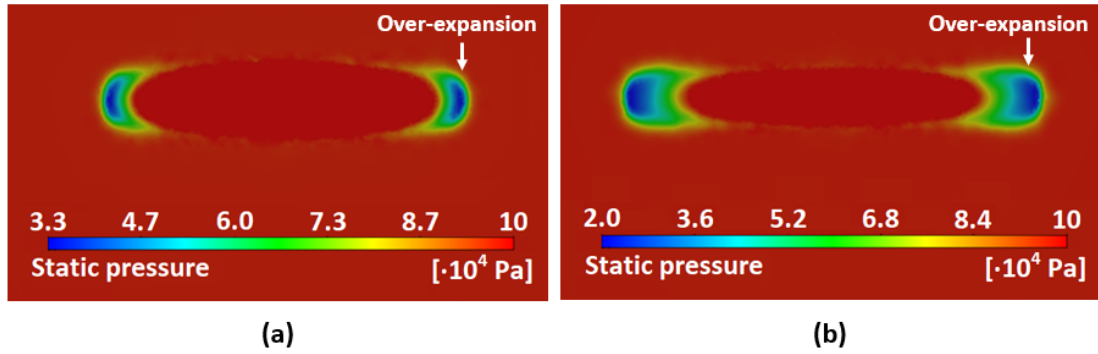


Figure 4.22: Static pressure contours at the nozzle exit section for (a) the AR 5.0 elliptical nozzle and (b) the AR 8.0 elliptical nozzle.

the barrel shocks form a single curve without any angular point along the major axis plane. Moreover, the subsequent shear layer does not look as a continuous surface, since it is not visible in the major axis plane. Hence, it can be imagined as formed by two surfaces which do not meet in the major axis plane. Looking at the normal Schlieren pictures reported in Figure 4.21, the onset of re-compression shock waves along the major axis can be appreciated, followed by a lateral Mach reflection as previously described for the rectangular sections. From the pictures of the static pressure contours reported in Figure 4.22, the origin of the shock waves can be attributed once again to an over-expanded condition, similarly to what already described for sections characterized by convex angles. For the AR 5.0 case, the minimum pressure is found along the major axis and is equal to 33000 Pa. For the AR of 8.0, drop is even greater, reaching a minimum of 20000 Pa. Hence, when increasing the ARs the high curvature profile at the extremes of the major axis acts like a convex angle, with an interaction between the fans that lowers the static pressure below the ambient pressure. Similarly to the elliptical cases, the AR has been found to deeply influence the flow field of the rectangular jets. The

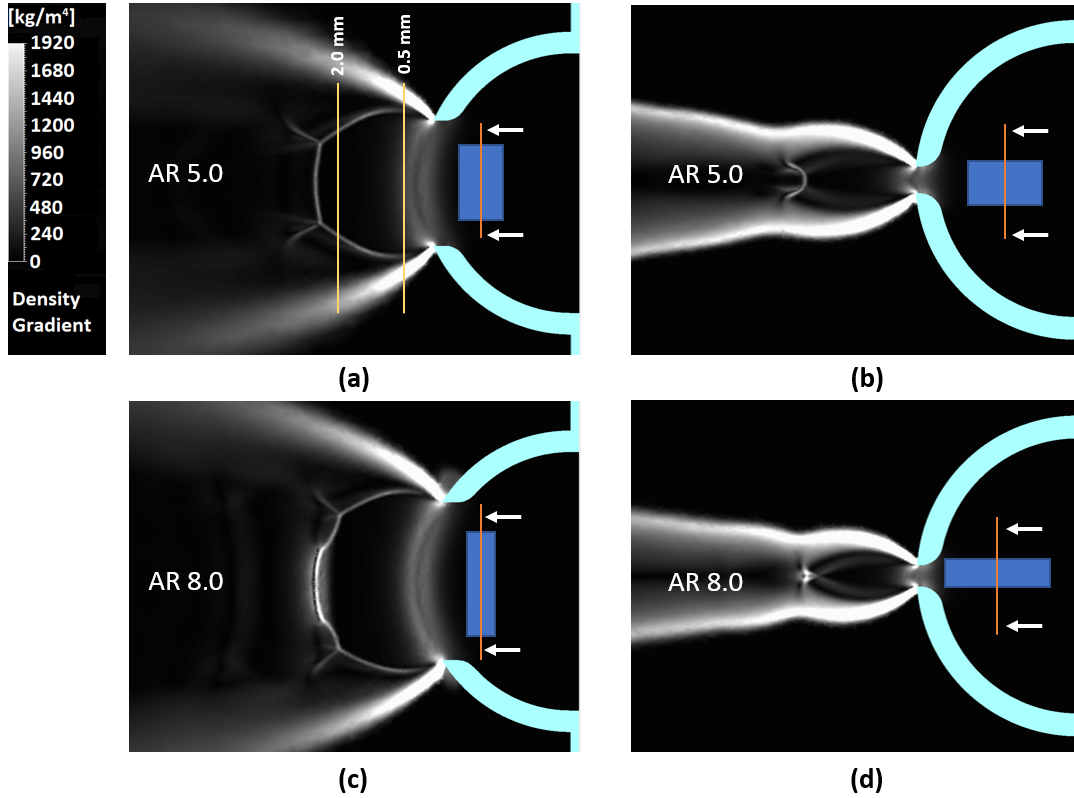


Figure 4.23: Longitudinal numerical Schlieren pictures for the rectangular nozzles: (a) AR 5.0 - major axis plane, (b) AR 5.0 - minor axis plane, (c) AR 8.0 - major axis plane, (d) AR 8.0 - minor axis plane.

longitudinal and normal Schlieren of the jets issuing from rectangular nozzles with AR equal to 5.0 and 8.0 are reported in Figure 4.23 and Figure 4.24, respectively. The genesis of the incident shock system is similar to AR 1.5 case, formerly described, with an over-expanded condition at the four corners of the exit section. For the AR 5.0 case, the minimum pressure is equal to 55000 Pa, dropping to 33000 Pa in the AR 8.0 case. Consequently, the barrel shock in the major axis plane forms as a consequence of the interaction of the re-compression corner shock waves, while the curvature equal to zero of the sides does not guarantee the coalescence of the weak compression waves in the minor axis plane. A slight curvature of the normal Mach disk is visible in the major plane in the AR 5.0 case. For the AR 8.0 case, the structure of the shock system in the same plane is quite different. As shown in Figure 4.23(c), the Mach disk is divided into three parts: a central outward curved disk and two lateral inward curved disks. Such condition might be dependent on the specific geometry employed in this work, and the authors are willing to deepen the causes in a future work.

In Figure 4.25 (a) and (b), the evolution of the Mach number along the axis is reported for the elliptical and rectangular cases, respectively. The circular case is shown for comparison too. For both the shapes, as the AR increases, the expansion process results

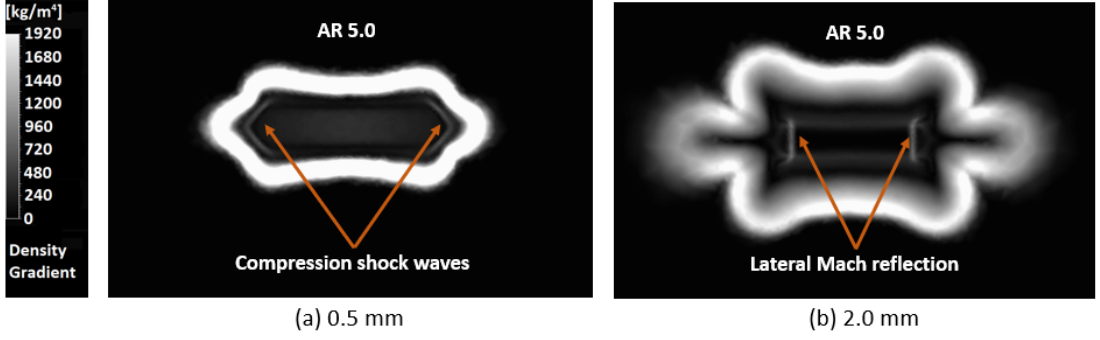


Figure 4.24: Normal numerical Schlieren pictures for the jet issuing from the rectangular nozzle with $AR = 5.0$ on two different planes normal to the jet axis: (a) at 0.5 mm and (b) at 2.0 mm from the nozzle exit section.

Table 4.2: Coefficients of the linear interpolation (and related coefficient of determination R^2) for the corrective factor: $C(AR) = m(AR) + q$.

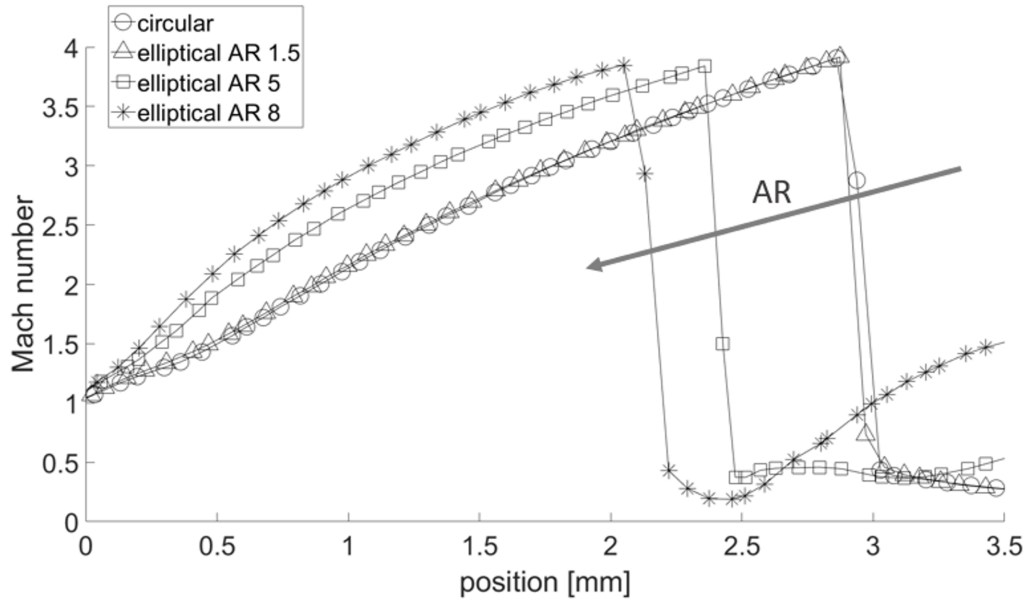
Section	NPR	m	q	R^2
Elliptical	10	-0.0389	1.0439	0.967
	15	-0.0402	1.0929	0.995
	20	-0.0355	1.0992	0.995
Rectangular	10	-0.0403	1.0003	0.987
	15	-0.0326	1.0132	0.989
	20	-0.0277	1.0168	0.991

to be faster and the position of the Mach disk progressively moves towards the nozzle exit section. Hence, the equation commonly reported in the literature to assess the position of the Mach disk [80] is here corrected as follows:

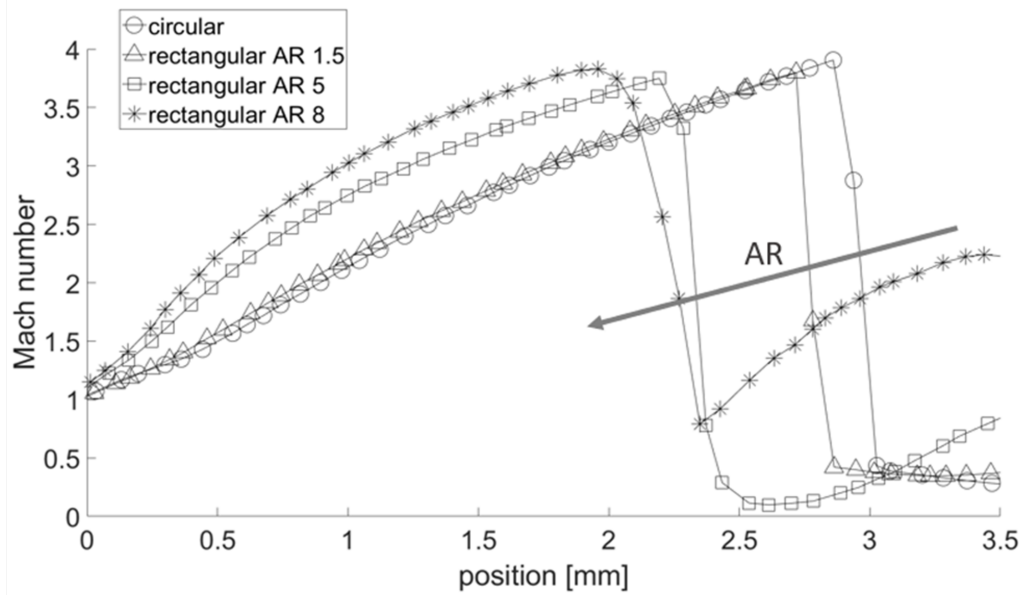
$$\frac{H_{disk}}{D_{nozzle,eq}} = C(AR)C_H\sqrt{NPR} \quad (4.1)$$

being $C(AR)$ a corrective coefficient depending on the AR. $C(AR)$ is reported in Figure 4.26 for three different NPR (10, 15, 20). Whatever the NPR, $C(AR)$ is well approximated by a linear regression, whose coefficients are reported in Tab. 4.2 along with the coefficient of determination R^2 .

An explanation for the drift of the Mach disk can be drawn looking at the shape of the static pressure iso-surfaces downstream the nozzle exit, which look like domes centered along the jet axis (Figure 4.27). The dome shape is the result of the different tilt of the expansion fans along the two axes, as previously shown in Figure 4.14. In the rectangular sections, for all the ARs considered, it has been observed that the fans originating from the major sides have the same inclination. Hence, as visible in Figure 4.28, when increasing the AR the distance between the major sides lowers, leading to a quicker pressure drop along the axis. As a result, the expansion fans from the minor



(a)



(b)

Figure 4.25: Mach number evolution along the jet axis for (a) the elliptical nozzles and (b) the rectangular, and its dependency on the AR.

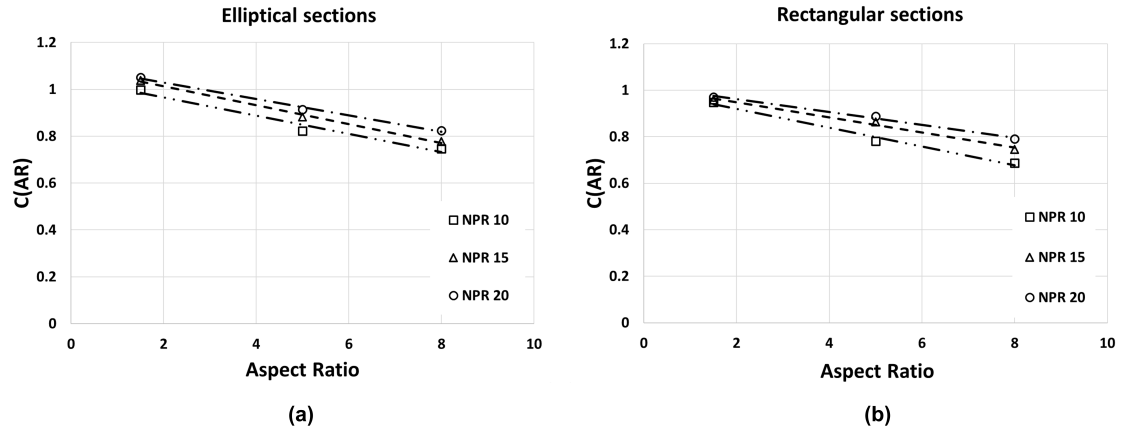


Figure 4.26: $C(AR)$ for (a) the elliptical sections and (b) rectangular sections at three different NPR (10, 15, 20).

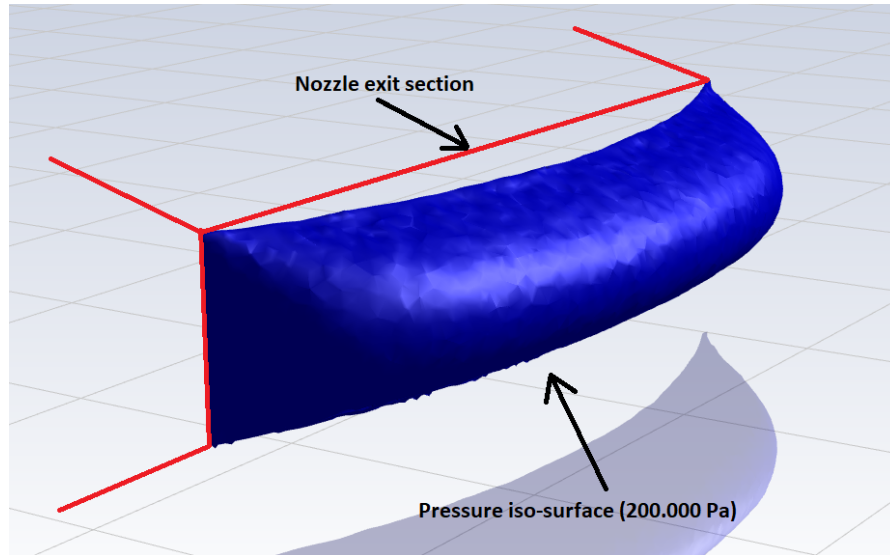


Figure 4.27: Example of an iso-surface pressure contour at the exit section of a rectangular nozzle (NPR = 10, AR = 5).

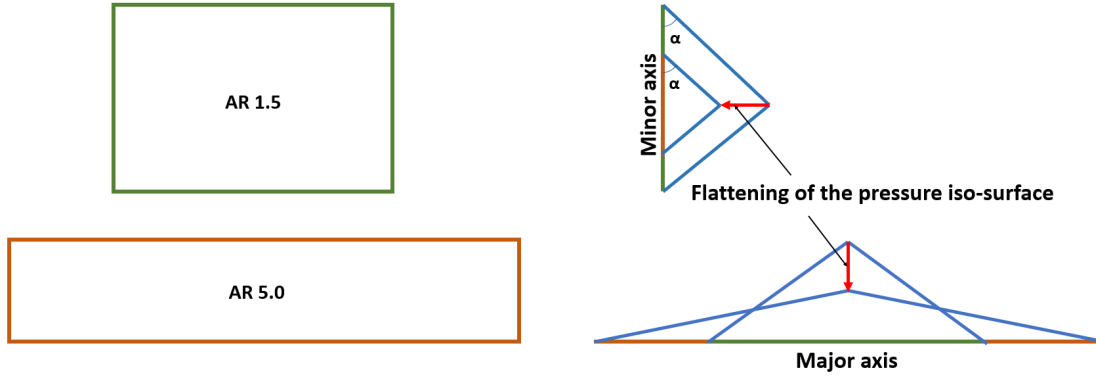


Figure 4.28: Sketch illustrating the influence of the area ratio over the expansion fans geometry.

sides must have a higher tilt angle (with respect to the streamwise direction), and the pressure iso-surfaces are progressively flattened towards the nozzle exit section. This can be considered the reason why a progressively higher pressure drop is found at the corners of the exit section. Because of this, the re-compression corner shocks must be more intense as the AR increases, therefore resulting to have a higher inclination with respect to the streamwise direction. The higher tilt of the re-compression corner shocks can be then considered the reason why the Mach disk moves towards the exit section. A similar mechanism takes place for the elliptical sections too. Fans from the minor axis are found to incrementally have a higher tilt as the AR increases, eventually reaching the same inclination found in the rectangular section when the AR is 8.0, because curvature tends to zero. Consequently, pressure iso-surfaces are flattened towards the exit section, leading to a higher level of over-expansion along the major axis. Also in this case, then, the re-compression shock waves must be more intense, resulting in a higher inclination and eventually shifting the Mach disk towards the nozzle exit section.

In Figure 4.29 and Figure 4.30, the H_2 axial mass fractions are reported. For both the shapes, the axial decay is similar to the circular section case when $AR = 1.5$. Conversely, as the AR increases, the axial decay results to be faster, suggesting a higher radial spread due to a quicker H_2 -air mixing in the external layer of the jet. The same trend is confirmed by the radial plots at ten equivalent diameters from the exit section, reported in Figure 4.31. In particular, a saddle-shaped profile is observed in the AR 8.0 rectangular nozzle, which is indicative of a split of the jet into two parts. The saddle-shaped profile has been analyzed by several authors in the literature, and it has been mostly ascribed to the vorticity developed by the rectangular section ([120], [121], [122]). At the same AR, the axial decay is faster for the rectangular section than the elliptical. The triangular and star-shaped sections show an axial decay similar to the AR 1.5 rectangular case and to the AR 5.0 elliptical case, respectively (see Figure 4.29 and Figure 4.30). The faster mixing and the axial decay rate can be linked to lower hydraulic diameter,

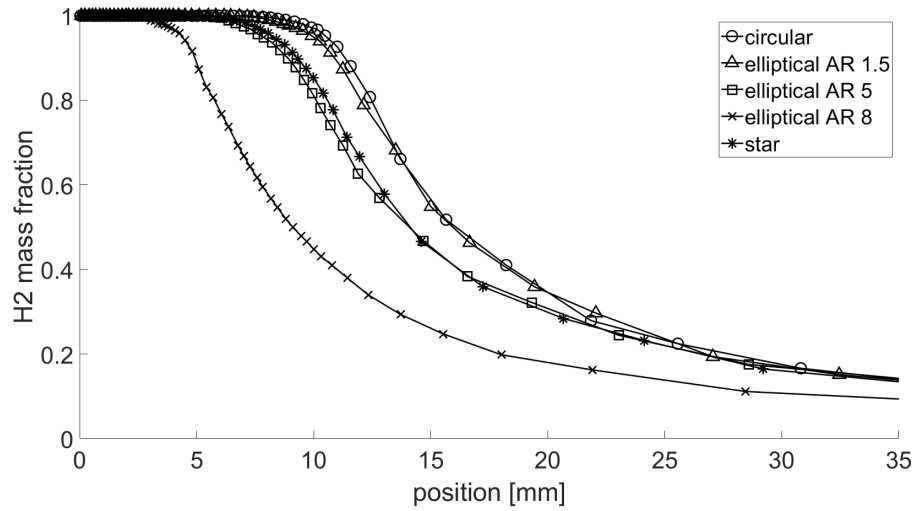


Figure 4.29: H₂ axial distribution for the circular, elliptical and star nozzles.

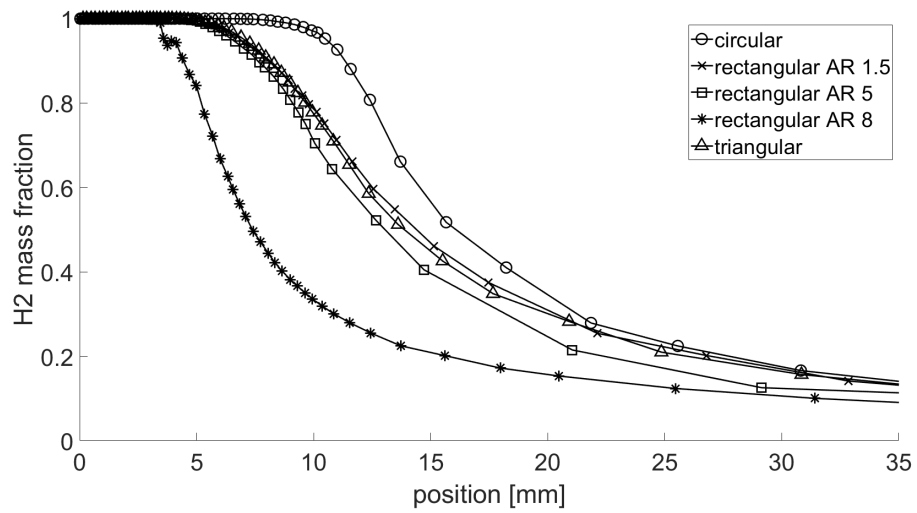


Figure 4.30: H₂ axial distribution for the circular, rectangular and triangular nozzles.

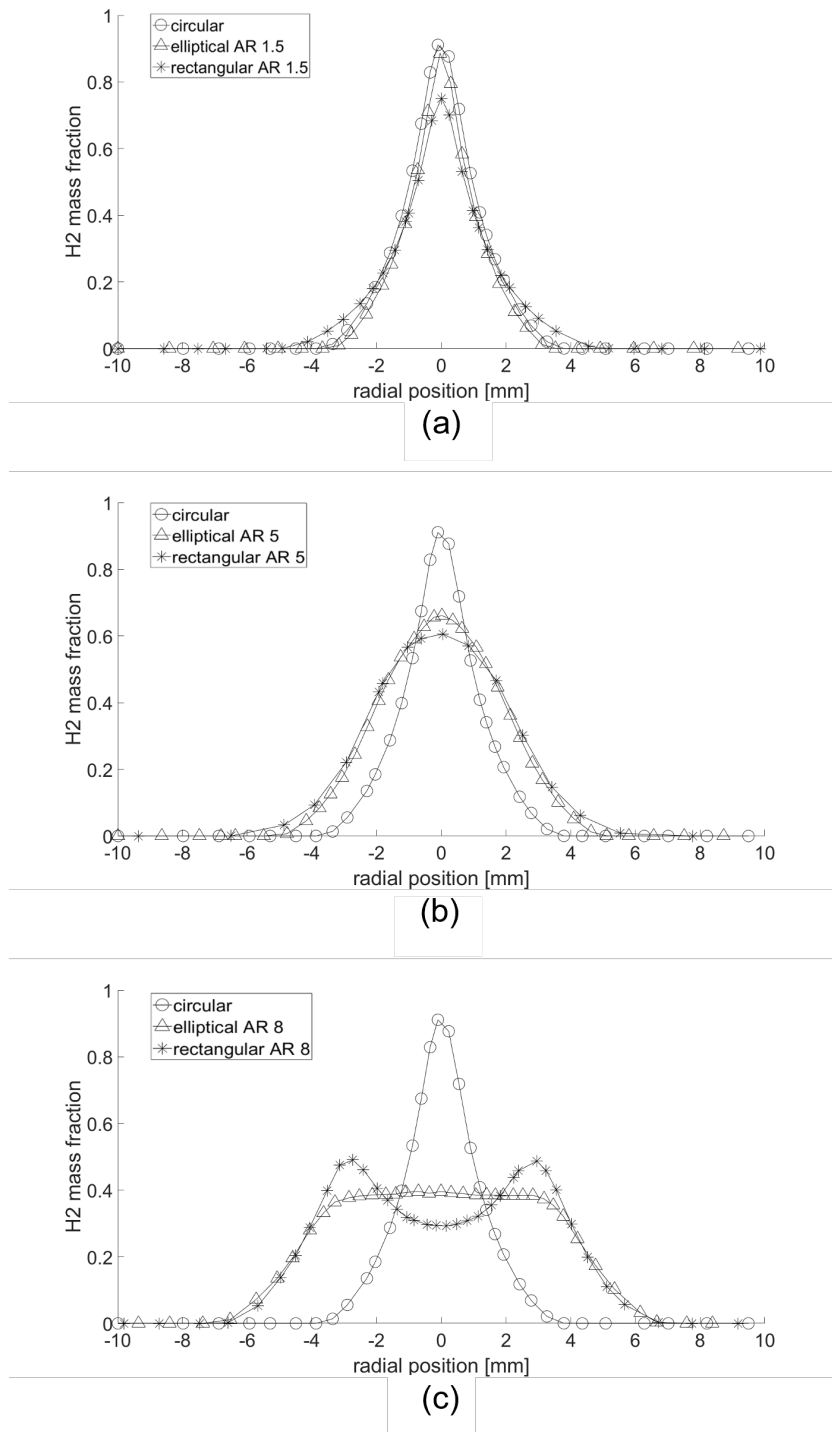


Figure 4.31: H₂ radial distributions at 10 equivalent diameters from the exit section for the circular, elliptical and rectangular sections: (a) AR 1.5 cases (b) AR 5.0 cases and (c) AR 8.0 cases.

Table 4.3: Mean vorticity (1/s) computed on the iso-surface characterized by a mass fraction of hydrogen equal to 0.1.

AR	circular	triangular	star	elliptical	rectangular
-	219460	238374	252046	-	-
1.5	-	-	-	219731	238118
5.0	-	-	-	244528	264188
8.0	-	-	-	266531	286428

i.e, to the larger perimeter of the section. At the same time, they can be associated to the level of the vorticity magnitude generated in the mixing layer. In Tab. 4.3, the mean levels of vorticity magnitude, computed on the iso-surface characterized by a H_2 mass fraction of 0.1, are reported. For the elliptical and rectangular sections, it can be seen that the vorticity increases with the AR, suggesting a more intense mass exchange promoted by the turbulent eddies. Moreover, at a fixed AR, vorticity is higher for the rectangular section with respect to the elliptical one, reflecting the faster axial decay of the rectangular sections. The triangular section has a level of vorticity close to AR 1.5 rectangular one, and the star to the AR 5.0 elliptical section. Hence, the authors believe vorticity can be the basic parameter to explain the different levels of mixing shown in Figure from 4.29 to 4.31.

4.2 Conclusions

In this Chapter, the influence of the nozzle cross section shape on under-expanded jets has been investigated by means of RANS approach. The aim has been to discover whether some of the solutions tested could be relevant for the direct injection, for instance allowing for a faster mixing. The conventional circular exit section has been compared to triangular, star, elliptical, and rectangular shapes. Significant differences have been observed in terms of the shock structure. Overexpansion conditions have been found at the convex corners of the sections, leading to the onset of re-compression shock waves. For the elliptical section, a faster formation of the barrel shock has been noticed along the major axis plane, due to the higher curvature of the perimeter. Increasing the aspect ratio of the elliptical and rectangular cases leads to a progressive shift of the Mach disk towards the nozzle exit section, phenomenon stemming from the stronger and stronger interaction of the expansion fans developed along the section perimeter. The elliptical and rectangular sections also enhance the radial mixing as the aspect ratio increases, due to the higher vorticity generated along the jet boundary. This opens to the possibility to exploit the intensified mixing to create different levels of the charge stratification. This opportunity will be verified in the next Chapter, which addresses the variable of the design space influencing the mixture formation process.

Chapter 5

Direct Injection strategies for hydrogen ICEs

The previous analyses have focused on the understanding of the phenomena featuring the under-expanded flows. This kind of jets are observed in direct injection engines due to the high pressure required to deliver the fuel in a short time frame. The preliminary investigation on such flows has been deemed of paramount importance for the subsequent analysis focusing on the mixing process, the topic of this Chapter. Herein, numerical simulations have been run to delve into the influence of the start of injection and injection pressure on the mixture formation, focusing on charge distribution and motion. Moreover, different ways to stratify the charge have been tested, because of the ultra-lean conditions adopted in this study (equivalence ratio of 0.25). Elliptical and rectangular nozzle sections have been tested to verify whether the increased radial mixing discussed in the previous Chapter could be helpful for the fuel stratification. The second approach relies on multi-injection strategies to locally create a richer composition around the spark, increasing the turbulent kinetic level as well. For specific combinations of the mixture deemed interesting, the combustion phase has been investigated too. Burning the most homogeneous ultra-lean mixture is a slow process whereas the combustion of the less uniform charge allows to significantly increase the peak pressure, but NO_x emissions are not negligible. The multi-injection approach shows the potential to be an optimal solution under ultra-lean conditions.

5.1 Introduction

As already stated in Chapter 2, the DI technology allows to overcome some of the H_2 detrimental features, such as the low volumetric efficiency of the PFI architecture, as well as high chance of backfiring events. The DI approach introduces the start of the injection (SOI) as a new degree of freedom. Intuitively, an early injection is expected to yield an almost homogeneous mixture, whereas a delayed injection can be a way to

stratify the fuel. The early injection strategy is expected to be beneficial when dealing with lean and extremely lean mixtures, in order to avoid volumes where the equivalence ratio is below the flammability limit [67]. Conversely, a stratified mixture could represent a favourable solution for higher loads, to create a richer and easily ignitable mixture around the spark while ensuring a leaner composition close to the walls to reduce heat losses [39] [123]. Retarding the injection leads also to a beneficial reduction of the compression work, further increasing the engine efficiency [124] [125] [126].

Due to the short time available to inject the fuel, DI injectors able to operate with tens to hundreds bar are currently under-development [42] [92] [127]. The higher the injection pressure, the shorter is the injection duration. Thus, in the DI approach the injection strategy has a profound impact on the equivalence distribution, which in turns influences the engine performance and emissions.

Several numerical and experimental studies have examined the mixture formation process. In [128], the velocity field and the H_2 distribution in a single-cylinder engine have been analyzed for pre-IVC and post-IVC injections using a 6-hole nozzle. Early injection produced a nearly uniform mixture, while intermediate and late injections showed leaner and richer regions due to fuel jet interaction with walls. The influence of the SOI has been also investigated in [129], demonstrating that an optimized SOI can increase the efficiency while reducing the emissions. Moreover, both in [129] and in [45] it has been observed that the jet-jet interaction, which can arise using multi-hole injectors, has a strong influence on the mixing process.

In this Chapter, the Sandia Optically Hydrogen (SOpHy) engine has been used as a reference geometry due to the availability of experimental results regarding the fuel distribution and the charge motion. Both numerical and experimental works have delved into the mixing process inside the SOpHy cylinder for different SOI timings and nozzle configurations (geometry, position, and number of holes) [130] [131] [132].

All of these publications have highlighted how the fuel distribution at spark timing is deeply affected by several design variables. Therefore, accurate numerical simulations are a valuable tool to assess the mixing process for different operating points allowing to optimize the combustion chamber geometry and the injection strategy. However, the complex flow field inside the combustion chamber makes challenging to get the correct prediction of the H_2 distribution throughout the compression stroke.

For instance, in [46] and [47], a good agreement with the PLIF results of the SOpHy engine has been observed for the H_2 jet shape and penetration using ANSYS Fluent, but the fuel distribution resulted under-predicted towards the end of the compression stroke. To improve the results, different turbulence models have been tested ($k-\varepsilon$ standard, RNG, realizable) in [47], while [133] the effect of the turbulent Schmidt number has been analyzed.

More recently, the same kind of validation has been carried out using the commercial code Converge CFD, as for instance in [134] and [135]. Here, attention has been paid

to the mesh strategy and turbulence modeling. The main suggestions are to adopt second-order discretization methods for the momentum equation, to set the turbulent Schmidt number equal to 0.5 and to align the mesh according to the H_2 jet direction to solve the shocks system. Several studies about the influence of mixing process over the engine performance, based on Converge numerical simulations, are available in the literature. In [136], a comparison between PFI modality and DI for several injection timings has been performed. DI has proven to provide both higher indicated thermal efficiency (ITE) and higher power output. In [137], several nozzle positions and jet orientations have been numerically tested, and remarkable differences in terms of power output and brake thermal efficiency (BTE) emerged.

In this Chapter, the challenging goal to define a suitable numerical setup has been addressed using ANSYS Fluent. The SOpHy low tumble configuration has been selected to this aim. Once defined the best practice to get reliable simulations, the effect of the injection timing and injection pressure has been assessed. The mixture formation has been analyzed for several injection strategies in terms of uniformity index (UI), fuel distribution, and charge motion. As the current research is addressed towards ultra-lean operation (i.e., equivalence ratio between 0.25 - 0.4), the need to properly stratify the fuel arises, in order to ensure a fast combustion under any condition. For this reason, two ways have been studied to differentiate the fuel concentration inside the combustion chamber, trying to create a richer mixture close to the spark. The first approach has been based on the adoption of non-circular nozzle exit sections, while the second is based on multi-injection strategies. Experimentally, this solution has been tested in [52] revealing the potential to reduce NO_x emissions while increasing the BTE for an equivalence ratio around 0.45. Here, multi-injection has been tested under leaner condition, being the mixture equivalence ratio 0.25.

5.2 SOpHy Engine and injection strategies

SOpHy is an optical pent-roof engine featured by fused-silica walls. The main geometrical features are reported in Table 5.1 while the related CAD is shown in Figure 5.1(a).

Table 5.1: SOpHy engine features

Displacement volume [cm^3]	590
Compression ratio	10.9
Bore [mm]	92
Stroke [mm]	85
Number of injector holes	1
Injector exit section diameter [mm]	1.42
Piston surface	flat

The displaced volume, spanned by a flat piston, is equal to 590 cm^3 and the compression ratio is 10.9. The intake manifolds have been designed to realize a low-tumble motion, which can be increased by means of adjustable tumble-plates. In this context, the low-tumble configuration has been taken into account. In such a way, all the differences regarding the charge distribution can be directly attributed to the tested injection strategies. The single-hole injector is placed in the symmetry plane of the cylinder, tilted by 50° with respect to the cylinder axis to direct the H_2 plume towards the intake valves as reported in the engine section reported in Figure 5.1(b).

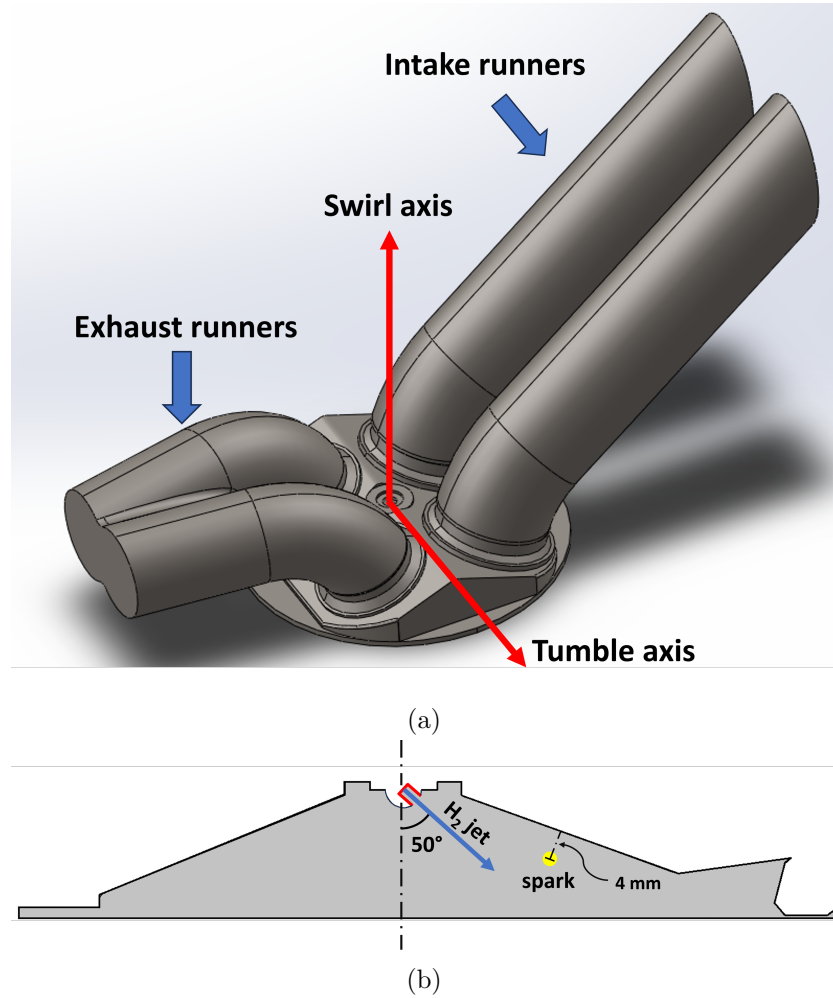


Figure 5.1: (a) CAD of the SOpHy engine and (b) section highlighting the direction and the H_2 and the spark position.

Experimental data - averaged over motored 200 cycles - are freely available [138]. Measurements for the low-tumble configuration are relative to an injection starting at 137°CA bTDC and lasting for 17.5°CA . The injection profile is trapezoidal, including opening and closing ramps both lasting for 1°CA , as reported in Figure 5.2. This early injection strategy will be named as "reference injection" hereafter.

Several other injection timings have been studied. Depending on the SOI, all the strategies can be clustered into three groups: early (SOI = 137 °CA bTDC), intermediate (SOI = 90 °CA bTDC), and late injections (SOI = 50 °CA bTDC). In addition, for each group different pressure levels have been compared. Whatever the pressure, the H_2 flow is choked during the injection. Consequently, for a constant amount of H_2 to be injected, increasing the pressure determines a lower duration of the process and viceversa. Therefore, the three pressure levels chosen - 12, 23 and 70 bar - lead to overall durations of the injections (DOI) of 35 °CA, 17.5 °CA and 6 °CA, respectively. A sketch of the injection strategies is reported in Figure 5.2. The combination SOI 50 °CA - DOI 35 °CA has not been considered because the in-cylinder pressure would rise over the 12 bar of the injection pressure towards the TDC. A ninth injection strategy, the dotted profile in Figure 5.2, has been studied too. It is characterized by a DOI of 6 °CA and a SOI set at 125.5 °CA bTDC, to obtain the same end of injection (EOI) of the reference case. In this way, it will be possible to determine whether the differences in mixing between the SOI 137 °CA - DOI 6 °CA case and the reference case are primarily due to the variation in mixing time (i.e., the different EOI) or the difference in the injection pressure.

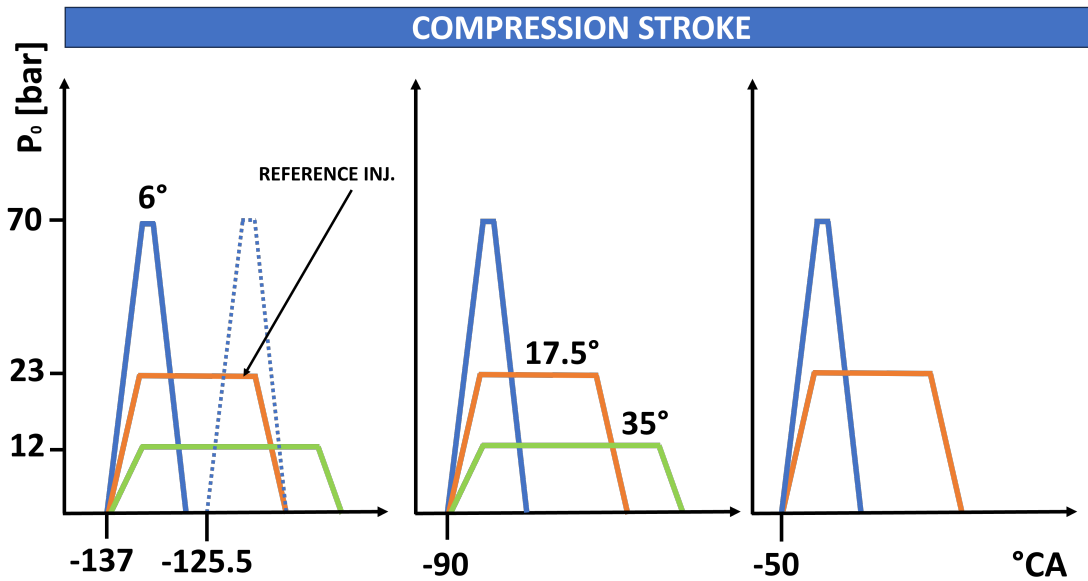


Figure 5.2: Sketch of the injection strategies (note: not in scale).

Beyond timing and pressure, the work has been also dedicated to the nozzle section shape, which could be changed by means of injector caps [139]. As already discussed, nozzle cross section shapes other than the circular one can have an effect on the jet spreading [140] [118] [111] [104]. Rectangular and elliptical sections have been tested setting the aspect ratio equal to 5. Lower values are not expected to produce significant differences when compared to the circular case while higher aspect ratios could not be taken into account due to geometrical and manufacturing constraints. Additionally,

the multi-injection approach has been examined to speed up the combustion while still burning the ultra-lean mixture feature by the equivalence ratio of 0.25.

Since the SOpHy engine has been exploited to run mixing analyses only, the freely available CAD does not include a spark. Therefore, for the combustion analysis later discussed, spark has been modeled by a simple spherical energy source, placed in the symmetry plane close to the intake ducts due to the wider available room in the cylinder head, as indicated by the yellow dot in Figure 5.1(b).

5.3 Numerical methodology and validation

Unsteady RANS simulations have been carried out by means of the CFD code ANSYS Fluent. Mesh has been realized accordingly to the workflow established by the ANSYS Internal Combustion Engine module, which applies a hybrid approach to discretize the domain.

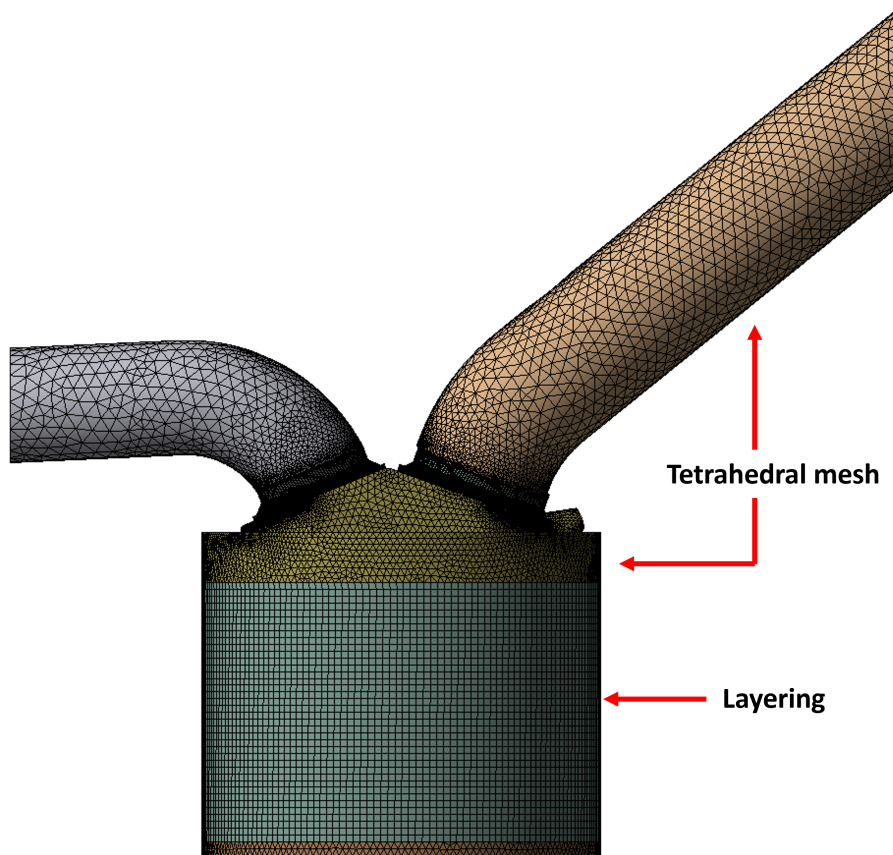


Figure 5.3: Typical mesh for ICE simulations in ANSYS Fluent: the cylinder head and intake and exhaust ducts are discretized by means of tetrahedral elements, whereas a layering approach is used for the volume spanned by the piston.

Figure 5.3 shows the typical mesh for ICEs simulations in ANSYS Fluent. The intake

and exhaust ducts are discretized by means tetrahedral elements, as well as the upper volume of the cylinder. A layering approach is instead provided to solve the flow inside the remaining of the cylinder and through the gap between valves and their seats. Following the mesh sensitivity analysis provided for the SOpHy engine in [133], the cylinder has been discretized with cells of 1.6 mm. Attention has been paid to the refinement near the injector where a grid size of 80 μm has been applied to solve the under-expanded H_2 flow. To account for the high pressure injection phenomena, mixture has been modeled as a real gas according to the Redlich-Kwong equation of state.

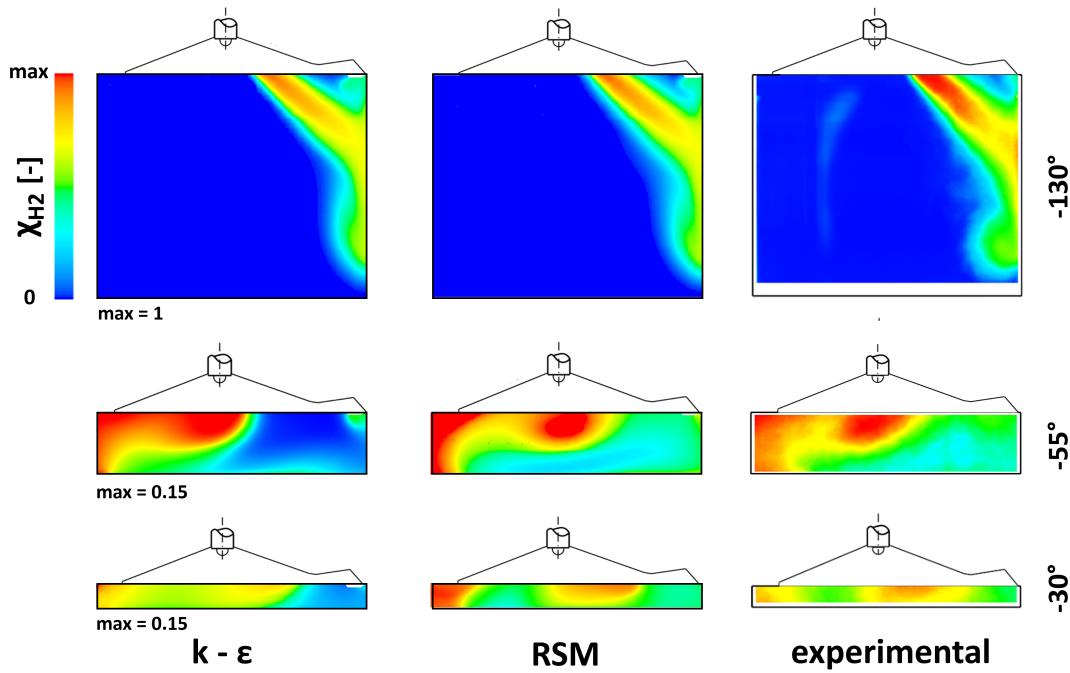


Figure 5.4: Numerical validation of the mixing process in the SOpHy engine by means of the H_2 mole fraction distribution. Left column: injection and mixing using the $k-\epsilon$ turbulence model; central column: RSM model; right column: experimental contours of the H_2 mole fraction distribution.

For the turbulence closure, the standard $k-\epsilon$ model has been compared against the Reynolds Stress Model (RSM). Figure 5.4 shows the distributions computed using the two turbulence models against the experimental results at different crank angles during the compression stroke. Whatever the model, the jet penetration and its morphology (130 °CA bTDC) are well captured by both the models. Differences arise later throughout the mixing process. At 55 °CA bTDC, the tumble motion of the H_2 fuel is properly captured by the RSM, whereas in the $k-\epsilon$ contour the reader can observe a lack of H_2 on the right side of the combustion chamber with respect to the experimental data. The same issue is found also at 30 °CA bTDC, where the experimental distribution

is properly reproduced by the RSM. The better performance of the RSM can be attributed to the capability to take into account the anisotropy of the flow-field, which in the end can be beneficial for the solution of highly strained flows such as the air inside the cylinder [141], subject to tumble and swirl motion at the same time. To solve the governing equations, the PISO pressure-velocity coupling algorithm has been selected, with first-order accurate discretization schemes for both spatial and time derivatives.

Table 5.2: Boundary and initial conditions

Boundary Conditions	
Intake manifolds inlet	Pressure: experimental traces [138] Temperature: 309 K
Exhaust manifolds outlet	Pressure: experimental traces [138]
H ₂ injector inlet	Mass flow profile Temperature: 300 K
Initial Conditions	
Cylinder	Pressure: 1.005 bar Temperature: 353 K
Intake manifolds	Pressure: 1.005 bar Temperature: 309 K
Exhaust manifolds	Pressure: 0.944 bar Temperature: 353 K

Table 5.2 reports the boundary and initial conditions imposed. Pressure and temperature at the intake manifolds inlet, as well as the exhaust manifold exit pressure, have been applied according to the experimental data provided by [138]. At the inlet of the injector, specific mass flow profiles have been applied for each of the cases, designed in such a way that the choked mass-flow rate corresponds to the desired pressure level (12, 23 or 70 bar). As an initialization strategy, a first whole cycle - without fuel injection - has been run starting from the exhaust valve opening (EVO) to reach a realistic turbulence level. Therefore, all the analyses refer to the second cycle.

5.3.1 Combustion model

The combustion phase has been computed according to the Partially-Premixed Model available in ANSYS Fluent, which allows to solve premixed flames in non-homogeneous mixtures. Chemistry tabulation has been preferred to a detailed chemistry approach, due to the lower computational time required. In the Partially-Premixed Model, the combustion is implemented by two additional transport equations, one for the mixture fraction Z and one for progress variable c . In ANSYS Fluent, Z is defined after Bilger [141], and results to be numerically equal to the fuel mass fraction when dealing with premixed systems. Under the assumption of an infinitely thin flame front, the progress variable c defines the separation surface between burnt and unburnt gases. The progress

variable c is defined as follows:

$$c = \frac{\sum_{Products} Y_i}{\sum_{Products} Y_i^{eq}} \quad (5.1)$$

where Y_i represents the actual mass fractions of the species in the burnt gases, while Y_i^{eq} is the species mass fraction at chemical equilibrium. Following this definition, c spans between 0 (unburnt gases) and 1 (burnt gases). The evolution of the flame front is tracked by the following transport equation for c :

$$\frac{\partial \rho c}{\partial t} + \nabla \cdot (\rho \vec{v} c) = -\nabla \cdot \left(\left(\frac{k}{c_p} + \frac{\mu_t}{Sc_t} \right) \nabla c \right) + \rho S_c \quad (5.2)$$

being ρ the density of the fluid, $\vec{v}$ the velocity vector, k the thermal conductivity, c_p the specific heat at constant pressure, μ_t the turbulent viscosity, Sc_t the turbulent Schmidt number, and S_c the reaction progress source term. The mean reaction rate ρS_c in Equation 5.2 is modeled in the following way:

$$\rho S_c = \rho_u U_t |\nabla c| \quad (5.3)$$

where U_t is the turbulent flame speed, evaluated in this study according to the Zimont model [141]. In the flamelet approach, the turbulent flame is considered as an ensemble of flamelets [142], whose properties are pre-computed and stored in tables as a function of the mixture fraction Z and the scalar dissipation χ , which accounts for the strain of the flamelets.

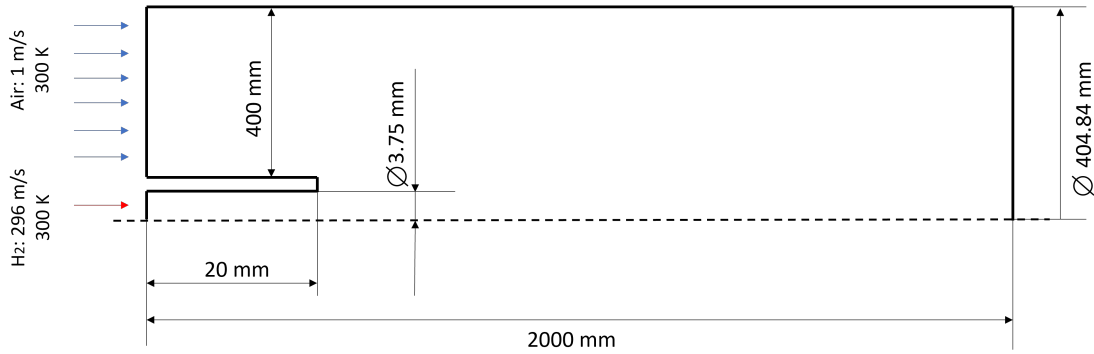


Figure 5.5: Sketch of the SANDIA burner [143] used to validate the Partially-Premixed combustion model in ANSYS Fluent (note: sketch not in scale).

Due to the lack of experimental results regarding fired-operation in the SOpHy engine, the numerical approach for the combustion process has been validated against the open experimental data of a non-premixed hydrogen - air burner reported in [143], whose sketch is provided in Figure 5.5. The burner is a 2000 mm long tube with pure H₂ en-

tering along the axis at 296 m/s with a total temperature of 300 K, while the 300 K air co-flow enters through the annular outer section of the device at 1 m/s. The resulting turbulent diffusive flame has been solved in ANSYS Fluent in a 2D axisymmetric configuration testing the Partially-Premixed Model. Two different chemical kinetic schemes have been compared, namely the San Diego (69 species) and the GRI-Mech v3.0 (53 species), both including their own nitrogen chemistry.

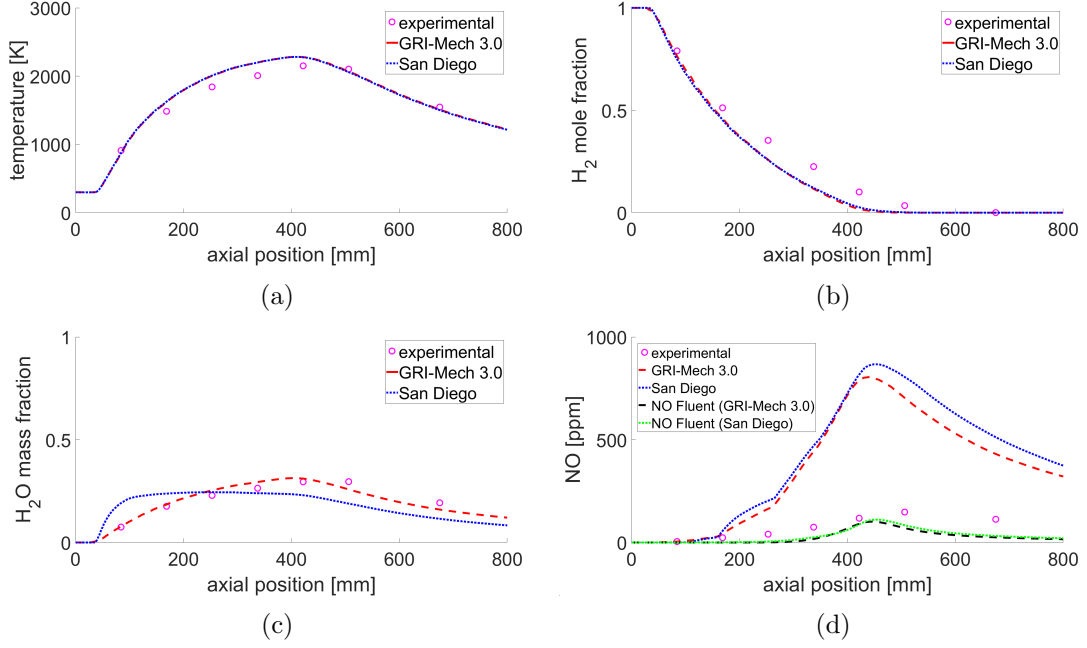


Figure 5.6: Comparison between the numerical and experimental results of the SANDIA burner used to validate the combustion setup: (a) temperature trend along the burner axis (b) H₂ trend along the burner axis (c) H₂O trend along the burner axis and (d) NO trend along the burner axis.

Trends of the temperature, H₂ consumption, H₂O production, and NO emissions along the axis of the flame are provided in Figure 5.6. As it can be observed, the temperature trend is properly captured by both the schemes, and the numerical curves result overlapped. Slightly higher temperatures are reported in the numerical results, which might be due to an under-prediction of the heat losses. Curves are also overlapped for the H₂ consumption along the axis of the flame, whereas the GRI-Mech 3.0 provides a closer agreements with the experimental data in terms of H₂O production. The prediction of the NO emissions is more challenging. As reported in [144] [145] [146], the flamelet approach, based on the assumption of fast chemistry, results deficient in predicting the NO formation, which is a process featured by large timescales. This can be clearly observed in the results provided in Figure 5.6(d), in which NO concentrations using the flamelet approach are about one order-magnitude higher than the experimental outcome whatever the kinetic scheme (both implementing their own nitrogen chemistry). To over-

come this issue, ANSYS Fluent provides a NO model based on the following Zeldovich mechanism:



The model relies on the assumption of a quasi-steady state for the N radical in the first reaction of the Zeldovich mechanism, which is a reasonable hypothesis for lean mixtures. Under such an assumption, the NO formation rate is described by:

$$\frac{d[NO]}{dt} = 2k_{f,1}[O][N_2] \frac{1 - \frac{k_{r,1}k_{r,2}[NO]^2}{k_{f,1}[N_2]k_{f,2}[O_2]}}{1 + \frac{k_{r,1}[NO]}{k_{f,2}[O_2]k_{f,3}[OH]}} \quad (5.7)$$

where $k_{f,i}$ and $k_{r,i}$ are the forward and reverse constant rates of the i -th reaction in the Zeldovich mechanism. According to Equation 5.7, the O and OH radicals have a strong influence on the NO formation. To compute their concentration, ANSYS Fluent provides several options. For the O radical concentration, the equilibrium model has been adopted, which relies on the hypothesis that the slow forming NO species can be assessed after the combustion has reached the equilibrium. Conversely, the OH radical has been neglected in the computation, under the assumption that:

$$k_2[O_2]_{eq} \gg k_3[OH]_{eq} \quad (5.8)$$

which is reasonable for a lean combustion. The outcomes of the Fluent NO model, shown in Figure 5.6(d), are much closer to the experimental measurements. Consequently, the approach has been deemed satisfactory for the following engine simulations.

5.4 Results

In the following, the effects of the injection timing, pressure, and nozzle geometry are addressed, highlighting the differences in terms of uniformity index (UI), equivalence ratio distribution, and charge motion. Additionally, for specific injection strategies which have led to marked differences of the fuel distribution, the combustion process has been analyzed to draw information about the velocity of the process and the emissions produced.

5.4.1 Uniformity index and equivalence ratio distribution

As a first analysis, the homogeneity of the mixtures has been characterized by evaluating the UI, which is a parameter defined as follows [147] [148] [149]:

$$UI = 1 - \frac{1}{2} \frac{\sum_{i=1}^N |\phi_i - \phi_{mean}| V_i}{\phi_{mean} V} \quad (5.9)$$

being ϕ_i the local equivalence ratio in the i_{th} cell featured by the volume V_i , and V the volume of the chamber at the crank angle in which the UI is assessed. The volume weighted equivalence ratio ϕ_{mean} is computed as follows:

$$\phi_{mean} = \frac{1}{V} \sum_{i=1}^N \phi_i V_i \quad (5.10)$$

According to this definition, the maximum UI value is 1 for a perfectly homogeneous mixture. The UI of the different injection strategies has been calculated at 10 °CA bTDC, which has been considered a plausible ignition angle. Values are reported in Table 5.3.

Table 5.3: Uniformity Index (UI) of the different injection strategies analyzed, at 10 °CA bTDC.

SOI [°CA bTDC]	DOI [°CA]	EOI [°CA bTDC]	UI
137	6	131	0.99
137	17.5	119.5	0.90
137	35	102.5	0.90
90	6	84	0.97
90	17.5	72.5	0.86
90	35	55	0.80
50	6	33	0.77
50	17.5	32.5	0.44
125.5	6	119.5	0.97

As shown in Table 5.3, early injections (SOI = 137 °CA bTDC) generally yield a nearly uniform charge, while slightly lower values of the UI are found for the medium SOI of 90 °CA bTDC. The influence of the injection pressure (which leads to the different DOIs) is remarkable, too. The higher the pressure, the higher the UI, due to a greater momentum of the jet which allows H₂ to spread through the combustion chamber more easily. The effect seems to be less relevant in the early injections cases, because the UI is the same for the DOI 17.5 °CA and DOI 35 °CA case. Differently, for the same DOIs and the SOI fixed at 90 °CA bTDC, the UI reduces from 0.80 to 0.77 when pressure lowers from 23 to 12 bar. The UI of the SOI 90 °CA - DOI 6 °CA is slightly lower than the SOI 137 °CA - DOI 6 °CA strategy, suggesting a strong influence of the injection pressure over the timing.

To confirm this observation, the SOI 125.5 °CA - DOI 6 °CA has been simulated, in such a way that the EOI is the same of the SOI 137 °CA - DOI 17.5 °CA case. Once again, the higher pressure leads to a UI very close to 1, confirming the strong influence of the injection pressure and jet momentum. The UI of SOI 50 °CA cases drops significantly, either due to the short time available to develop the mixture and due to the interaction of the jet with the walls of the cylinder and the piston, as shown for example in Figure 5.7 for the SOI 50 °CA - DOI 17.5 °CA at 40 °CA bTDC.

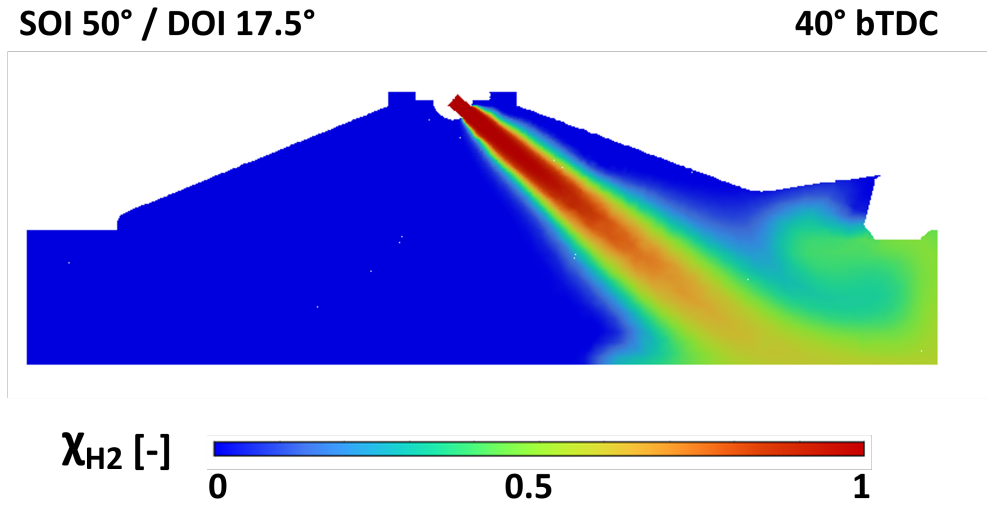


Figure 5.7: H₂ mole fraction contours for the SOI 50 °CA - DOI 17.5 °CA at 40 °CA bTDC. The jet-piston interaction is evident, leading to the drop of the UI observed in the late injection strategies.

Further insights can be drawn by looking at Figure 5.8, reporting the distributions of the equivalence ratio. The SOI 137 °CA bTDC - DOI 6 °CA yields a uniform mixture, whose equivalence ratio is 0.25 all-over the cylinder volume. The reduction of the injection pressure (DOI 17.5 °CA - DOI 35 °CA) produces scattered distributions, both centered on the global equivalence ratio of 0.25. Interestingly, the extension of the distribution is almost the same, which confirms the UI equal to 0.90 for both the strategies. Therefore, the injection pressure might have a less significant role for early injections, probably due to the similar density of the bulk gas.

When retarding the SOI to 90 °CA bTDC, the influence of the injection pressure becomes more relevant. For the pressure of 70 bar, a narrow distribution centered on the equivalence ratio of 0.25 is obtained again, but the mixture is not perfectly homogeneous, as in the SOI 137 °CA case, because of the shorter time for the mixing. A progressively widening of the distributions can be observed reducing the injection pressure to 23 and 12 bar. It is also worth noting that a significant fraction of the volume is featured by an equivalence ratio lower than 0.25 for both the injection strategies. This can lead to an excessively slow combustion, affecting the efficiency of thermodynamic cycle. Moreover,

for the longest DOI, richer zones characterized by an equivalence ratio between 0.25 and 0.5 can be observed. Nonetheless, also for this strategy NO_x should not be expected to be significant, as the threshold value over which emissions quickly increase is exactly 0.5.

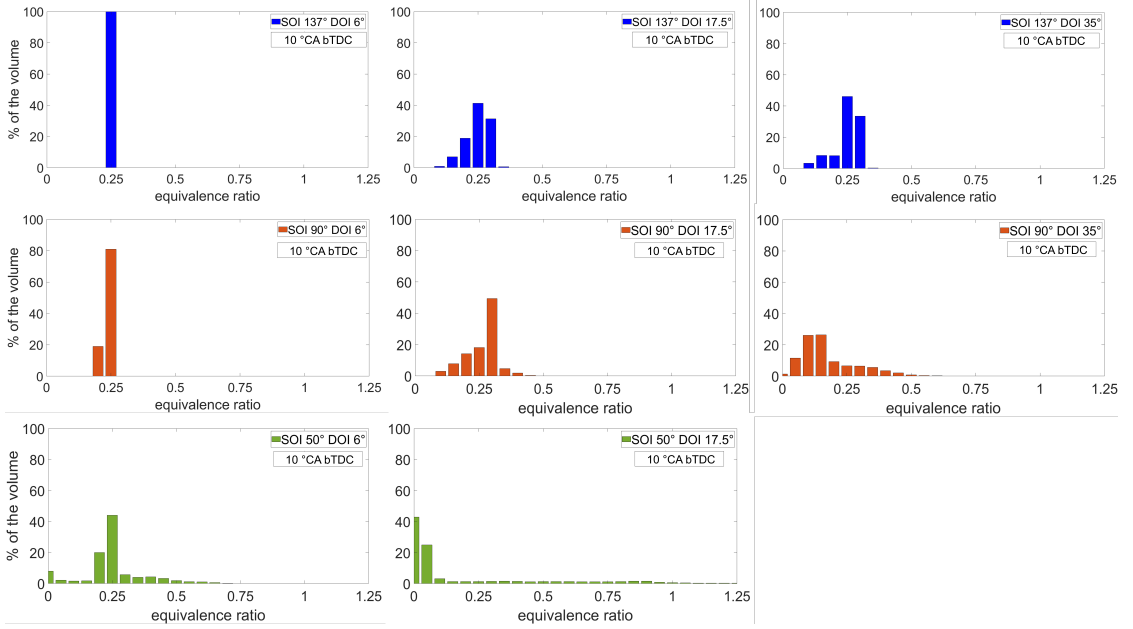


Figure 5.8: Equivalence ratio distributions at 10 °CA bTDC (spark timing). Upper row: early injections (SOI 137 °CA); central row: intermediate injections (SOI 90 °CA); lower row: late injections (SOI 50 °CA). Left column: high injection pressure (DOI 6 °CA); central column: mid-pressure injection (DOI 17.5 °CA); right column: low pressure injection (DOI 35 °CA).

For the SOI 50 °CA bTDC, mixtures are far from being uniform. In the DOI 6 °CA case, the distribution resembles a gaussian shape centered on the mean equivalence ratio. Nonetheless, a fraction of the cylinder has not been reached by the fuel, as well as small volumes present equivalences ratio beyond the 0.5 threshold. This trend is intensified for the longer DOI case, in which around the 40% of the volume has not been reached by fuel, and, particularly, significant fractions exceeds the threshold of 0.5.

5.4.2 Charge motion

In Figure 5.9, the effect of the injection on the charge motion and its relative evolution is presented in terms of swirl ratio (SR) and tumble ratio (TR), defined as follows:

$$SR = \frac{L_s/I_s}{2\pi N/60} \quad (5.11)$$

$$TR = \frac{L_T/I_T}{2\pi N/60} \quad (5.12)$$

being L and I the angular momentum (positive if it is clockwise, negative otherwise) and the inertia of the bulk gas with respect to the swirl and tumble axes. As a general confirmation, the geometry of the engine - and particularly the intake manifolds, do not produce a strong swirl motion. Indeed, before the injection the SR is almost zero in all the cases. A slight increase takes place after the injection, and it is more intense as the injection pressure increases. Conversely, tumble is clearly the main pattern of the charge motion, as observable by the TR which is generally one-order of magnitude higher than the SR.

For the early and middle SOI, a rapid increase of the tumble takes place as the injection starts. For a fixed SOI, the effect is clearly more pronounced as the injection pressure increases because of the higher momentum of the fuel jet. In particular, in the SOI 137 °CA and SOI 90 °CA bTDC, an increase of the TR can be noticed also after the EOI due to the onset of a main vortex in the symmetry plane of the chamber. As the piston moves towards the TDC, the TR increases to preserve the angular momentum of the vortex, until it gets destroyed by the distortion imposed close to the TDC. The same trend is identifiable - in a less marked way - also in the other SOI 137° CA cases, whereas for the SOI 90 °CA - DOI 17.5 °CA / 35 °CA strategies the intensity of the tumble decreases as the injection is over. This might be attributed to the progressively increase of the viscosity of the bulk gas with temperature, strengthening the friction losses that damp the intensity of the tumble vortex.

As it results from the plots, the SOI 50 °CA cases show an opposite trend of the TR, which indicates a different development of the charge motion. Indeed, due to the proximity of the piston to the cylinder head, the fuel jet quickly hits the walls (Figure 5.7) without triggering the tumble motion observed in the former cases. For instance, in Figure 5.10 two different velocity fields are compared along the injection plane. Figure 5.10(a) is a snapshot of the velocity distribution of the SOI 137.5 °CA - DOI 6 °CA case at 85 °CA bTDC, which is the angle of the maximum TR observed for this injection strategy (as shown in Figure 5.9). As it can be noticed, the flow field is mainly characterized by a central single tumble vortex entirely spreading along the plane. In Figure 5.10(b) the SOI 50 °CA - DOI 6 °CA case at 30 °CA bTDC is taken into account as representative of the late injections. In this case, the velocity field is mainly characterized by the entrainment of the air triggered by the hydrogen jet, explaining the opposite tumble sign observed in Figure 5.9) in the late injection strategies.

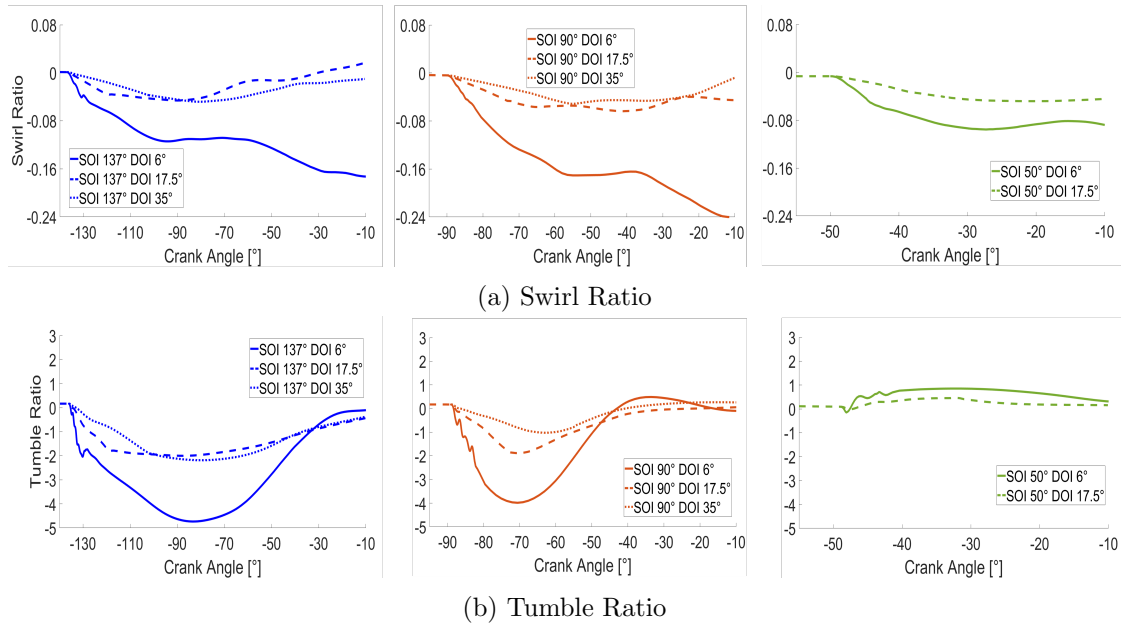


Figure 5.9: Comparison of the evolution of (a) the swirl ratio and (b) the tumble ratio throughout the injection phase for the tested strategies.

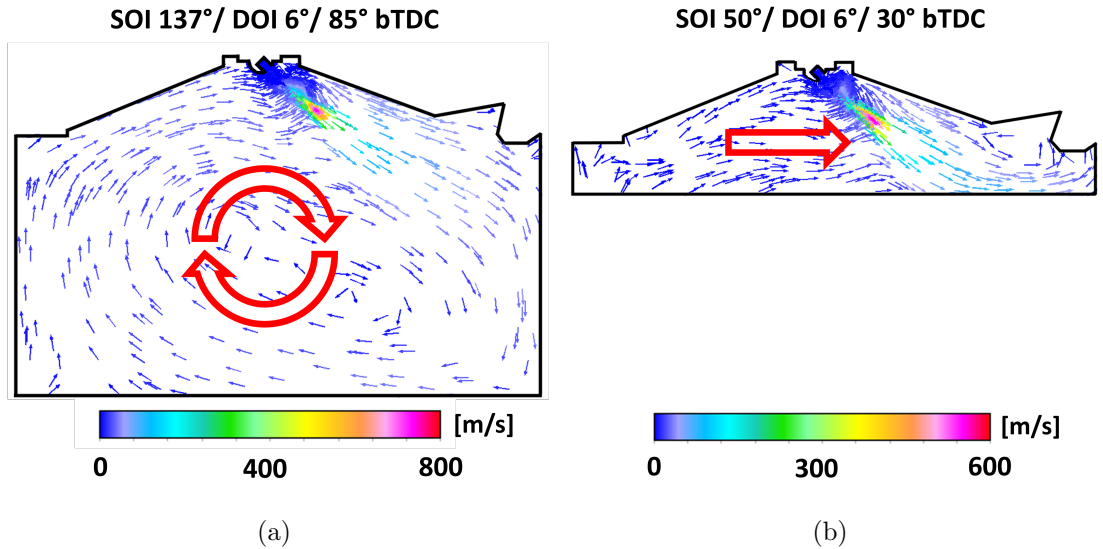


Figure 5.10: (a) Velocity field of the SOI 137 °CA / DOI 6 °CA at 85 °CA bTDC, featuring a clear tumble pattern. (b) Velocity field of the SOI 50 °CA / DOI 6 °CA at 35 °CA bTDC, mainly characterized by the entrainment triggered by the injection.

5.4.3 Towards the charge stratification: influence of the nozzle shape

The ongoing development of the injector caps, which allow to easily and quickly change the geometry of the nozzle [139] [150] [151], has pushed to analyze the influence of the injector exit section on the mixing process. As observed in the previous Chapter, the jet penetration reduces when switching from a circular to an elliptical section holding the same exit area. The lower jet penetration is related to a strengthened radial mixing, and the effect is more and more evident as the aspect ratio of the section (i.e., major to minor axis ratio) increases. The same results have been drawn for rectangular sections too, observing an even stronger radial mixing when compared to elliptical sections featuring the same aspect ratio.

Under this framework, the circular nozzle has been compared against either an elliptical or a rectangular one, both characterized by an aspect ratio equal to 5. Referring to the previously mentioned literature, lower values of the aspect ratio have been discarded because they are not expected to produce a significant difference in terms of jet behavior. Higher values have not been taken into account as well, because they could potentially lead to manufacturing issues. The goal has been to verify whether such nozzle configurations could produce a significant stratification of the charge thanks to the lower fuel penetration and stronger radial mixing.

The comparison has been run for both the SOI of 137 °CA bTDC and 90 °CA bTDC. In all of the cases, the DOI has been fixed at 17.5 °CA. The UIs are reported in Table 5.4 and the related equivalence ratio distributions are reported in Figure 5.11, which can be compared with the circular section distributions reported in Figure 5.8 for the same SOI and DOI.

Table 5.4: Uniformity Index (UI) at 10 °CA bTDC (spark timing) for the circular, elliptical, and rectangular sections.

SOI [°CA bTDC]	DOI [°CA]	section shape	UI
137	17.5	circular	0.90
137	17.5	elliptical	0.93
137	17.5	rectangular	0.88
90	17.5	circular	0.86
90	17.5	elliptical	0.85
90	17.5	rectangular	0.83

When considering the SOI 137 °CA cases, contrary to expectations, the elliptical injector results in a slightly higher UI with respect to the circular section (0.93 vs 0.90), whereas the rectangular provides a slightly lower level of homogenization (UI 0.90 vs UI 0.88). As a confirmation, more than 40% of the combustion chamber presents an equivalence ratio equal to 0.25 (the global value) in the elliptical case. When employing the rectangular section, this value is slightly lower than 40%. Whatever the case, the distributions are narrow around 0.25, and no volumes are characterized by an equivalence

ratio higher than 0.5.

These observation are confirmed by looking at Figure 5.12, where the contours of the equivalence ratio are displayed along the injection plane and its normal plane through the axis of the cylinder. Here, the distribution of the elliptical section is slightly more homogeneous when compared to the circular nozzle, particularly along the injection plane. On the same plane, the mixture is richer for the rectangular injector, with a smaller area on the right where the equivalence ratio is lower 0.2.

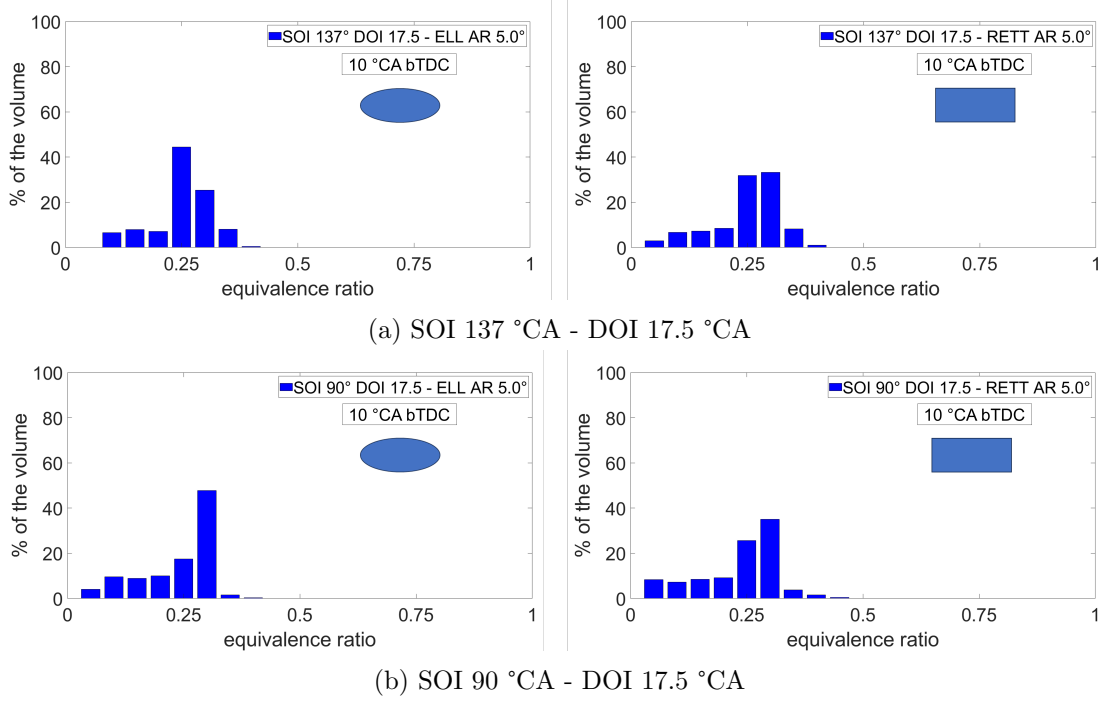


Figure 5.11: Equivalence ratio distributions at 10 °CA bTDC (spark timing) for (a) the early injections (SOI 137 °CA) and (b) intermediate injections (SOI 90 °CA). Left column: elliptical section; right column: rectangular section.

Anyway, it is possible to say that the shape of the injector section at early injection (SOI 137 °CA) plays a minor role, whereas injection timing has again a major role in driving the mixing, resulting in high UIs and narrow fuel distributions. Therefore, the same investigation has been run with the SOI delayed to 90 °CA bTDC to reduce the available mixing time.

Now, the UI of the circular injector is the highest, followed by the elliptical and the rectangular nozzles. Nonetheless, the difference is again not markedly high. In the elliptical case, around half of the volume is characterized by an equivalence ratio of 0.26 (versus the global of 0.25), which is mainly shown along the injection plane (Figure 5.12). The rectangular distribution features more volumes characterized by an equivalence ratio between 0.25 and 0.5, mainly concentrated along the cylinder axis (Figure 5.12). Summing up, non circular sections have an influence on the mixture formation, but the

UIs are close to the circular nozzle UIs, and on the top of that a clear pattern of the fuel distribution cannot be found. Hence, other solutions must be explored to properly stratify the charge.

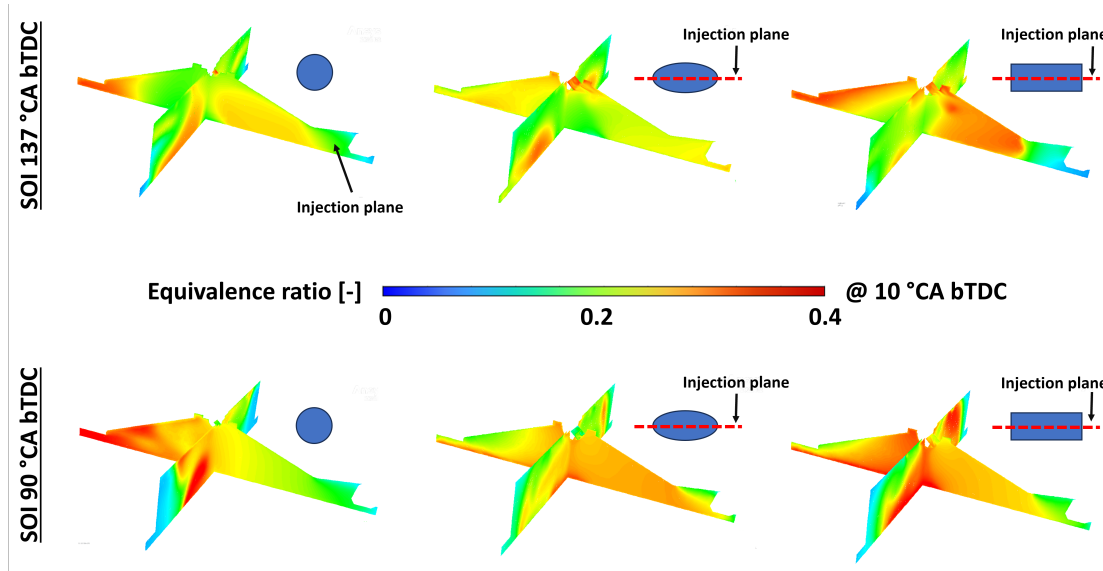


Figure 5.12: Contours of the equivalence ratio distributions at spark timing (10 °CA bTDC). Upper row: SOI 137 °CA bTDC; lower row: SOI 90 °CA bTDC.

5.4.4 Towards the charge stratification: the multi-injection approach

Non-circular injection sections have proven to influence the spreading of the hydrogen jet, and consequently the final distribution of the charge at spark timing, but only marginally. Therefore, other strategies need to be considered; hence, an approach based on splitting the injection into two steps during the compression stroke has been tested, aiming at achieving a more evident stratification of the charge. Indeed, a richer mixture close to the spark can be beneficial to start and stabilize the combustion of ultra-lean mixture which, in turn, are useful to reduce thermal losses [11] [152]. As previously stated, the spark plug location has been selected close to the intake ducts. This configuration results beneficial, because the fuel jet orientation enables the possibility to locally increase the equivalence ratio and the turbulent kinetic energy in the spark region.

The high pressure injector (70 bar) has been taken into account to allow extremely late injections. It has been hypothesized to split the SOI 137.5 °CA - DOI 6 °CA strategy into an early trapezoidal injection lasting 4 °CA and a late trapezoidal injection spanning for 3 °CA. For the second injection, two different SOI have been tested, 25 °CA and 15 °CA bTDC, as reported in Figure 5.13.

In such a way, the overall amount of H_2 injected is the same of the single injection cases. Regarding the dynamic behavior of the injector, both opening and closing ramps have been kept equal to 1 °CA, assuming that the same 70 bar injector employed for

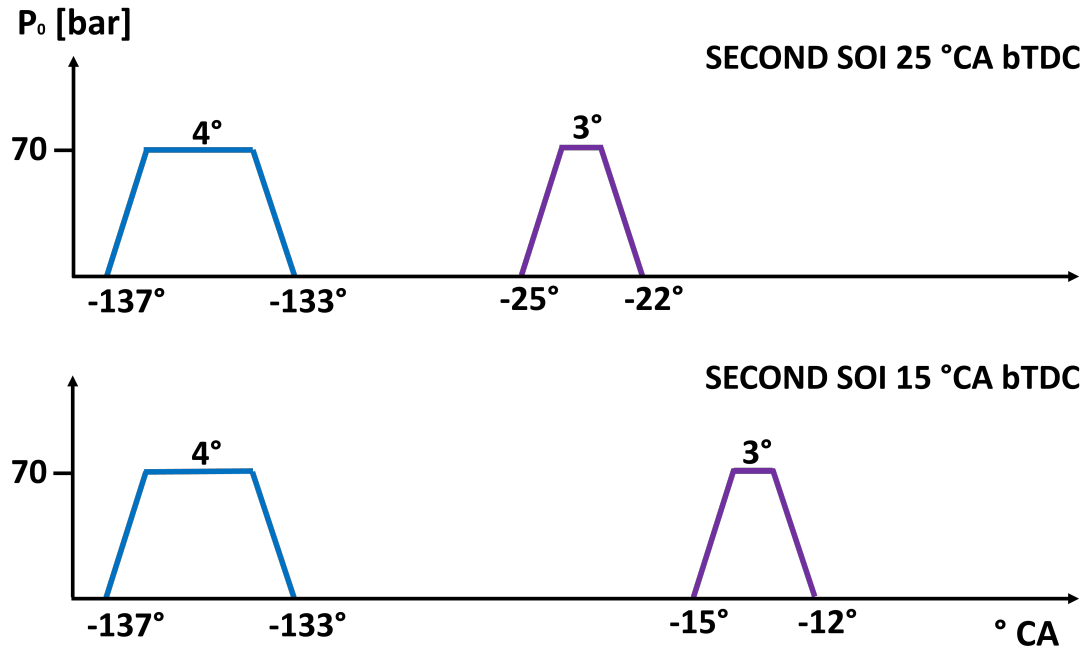


Figure 5.13: Sketch of the two multi-injection strategies tested in this work (note: not in scale).

the single injection cases could be used for multi-injections without any change in its dynamics. With respect to the SOI 137.5 °CA - DOI 6 °CA single injection, the UI lowers from 0.99 to 0.86 for the strategy featured by the second injection starting at 25 °CA bTDC. The UI further reduces to 0.82 when the second injection is delayed to 15 °CA bTDC. Indeed, when looking at the distributions of the equivalence ratio reported in Figure 5.14, the reader can observe a lean mixture for the first multi-injection strategy, along with smaller volumes of the cylinder featuring nearly stoichiometric and even rich mixture, that are expected to improve the speed of the combustion.

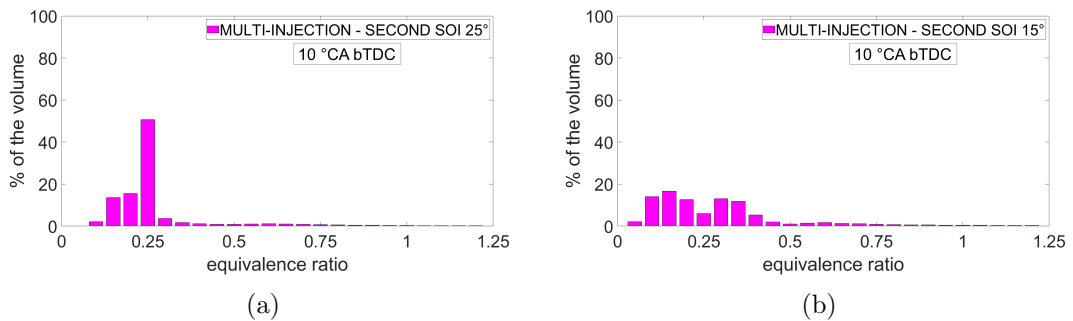


Figure 5.14: Equivalence ratio distributions, at 10 °CA bTDC (spark timing), for the multi-injection strategies, both featured by a first injection at 137 °CA bTDC. In (a) the second injection starts at 25 °CA bTDC, whereas in (b) at 15 °CA bTDC.

For the second strategy, the distribution results even less homogeneous, due to the lower time to spread the fuel before the spark timing. Also the interaction of the jet with the walls, and particularly the piston, is more pronounced, as visible in Figure 5.15, which reports the contours of the equivalence ratio, for both the multi-injection strategies, along the injection plane and its normal plane through the spark.

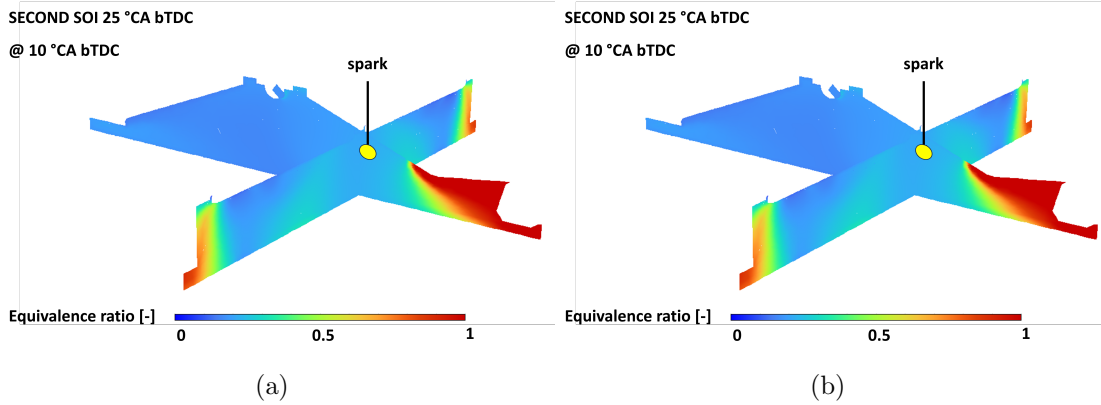


Figure 5.15: Equivalence ratio contours, at 10° CA bTDC, for the multi-injection strategies, both featured by a first injection at -137 °CA. In (a) the second injection starts at -25 °CA, whereas in (b) at -15 °CA. The yellow dot indicates the spark position.

In the first case, H_2 is confined in the pocket on the right of the chamber, whereas in the second case fuel has also been confined by the piston, resulting in a more extended fuel cloud close to the spark location. Lastly, in both of the cases the second injection is also beneficial in enlivening the turbulent kinetic energy level in the spark region, as visible from the contours reported in Figure 5.16. The effectiveness of the multi-injection strategies will be highlighted in the next paragraph.

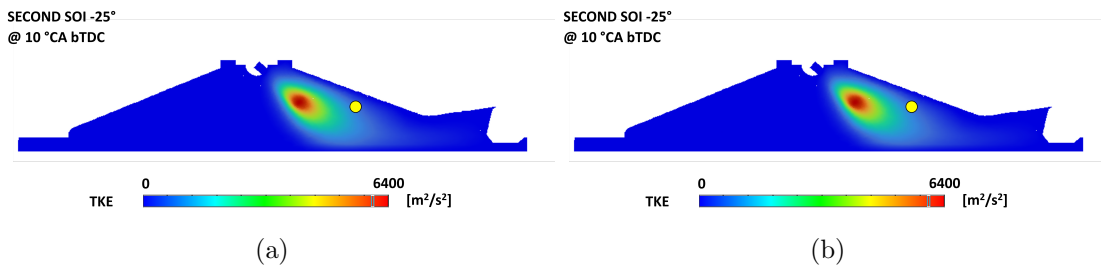


Figure 5.16: Turbulent kinetic energy contours, at 10° CA bTDC (spark timing), on the injection plane for the multi-injection strategies: (a) with the second SOI at 25 °CA bTDC and (b) with the second SOI at 15 °CA bTDC. The yellow dot indicates the spark position.

5.4.5 Combustion

In this section, some of the previous cases have been selected to run a comparison regarding the combustion process. Only circular injection sections are considered. Keeping in mind that in all the reactive cases the global equivalence ratio does not change, as well as the position and timing of the spark, all the differences observed can be directly attributed to the differences in the charge distribution.

The first selected case is the SOI 137 °CA - DOI 6 °CA, which is representative for the combustion of a perfectly homogenized mixture ($UI = 0.99$). The SOI 90 °CA - DOI 17 °CA has been deemed representative of an intermediate level of charge stratification, whereas the SOI 50 °CA - DOI 17 °CA injection has been taken into account for a strongly non-homogenous mixture. The SOI 50 °CA - DOI 35 °CA would result in a even lower UI, but the mixture resulted to have a too evident separation between air and pure H_2 to be significant from an engineering point of view. The effectiveness of the multi-injection strategies has been analyzed as well, testing the combustion for both of the cases previously discussed.

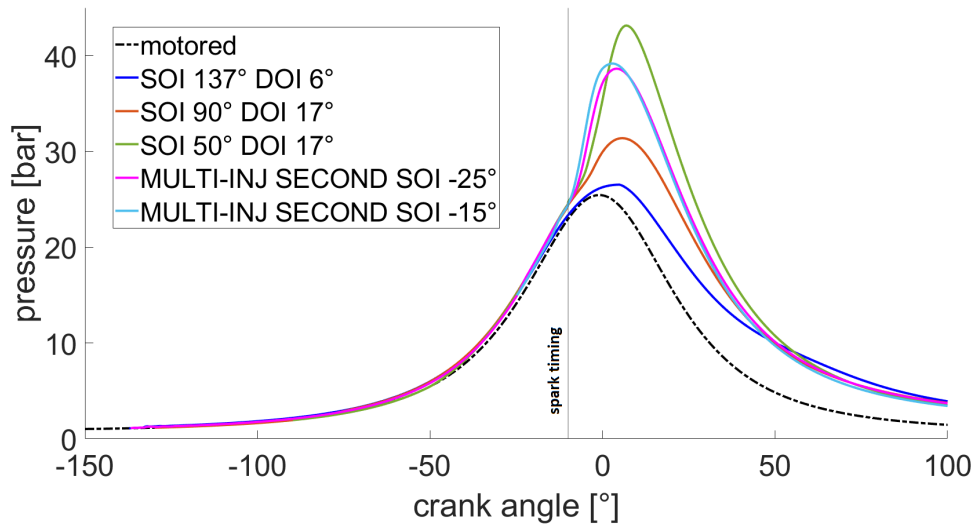


Figure 5.17: Pressure traces for the different injection strategies taken into account for the combustion. Spark timing is fixed at 10 °CA bTDC; the motored cycle is reported for comparison.

In Figure 5.17 the pressure traces inside the combustion chamber are shown. In all the cases, spark timing has been set at 10 °CA bTDC, and the motored cycle has been reported as a reference. As a first interesting observation, the reader can note the small difference in the peak pressure between the motored cycle and the SOI 137 °CA - DOI 6 °CA case. This can be attributed to the uniform mixture featuring an equivalence ratio as low as 0.25. Thus, combustion results to be significantly slow, and a tuning of the spark timing would be probably required to obtain a more effective expansion stroke. Anyway,

this result highlights the remarkable problem to reach an efficient thermodynamic cycle when burning a uniform mixture at a such low equivalence ratio.

Retarding the injection to 90 °CA bTDC leads to a more stratified charge (UI 0.86). This improves the combustion speed and results in a higher pressure peak (31 bar) at 6 °CA aTDC. Retarding the SOI to 90 °CA bTDC reduces the compression work during the angular span from 137.5 °CA to 90 °CA bTDC, but approaching the TDC the SOI 90 °CA - DOI 17.5 °CA results in a slightly higher pressure with respect to the SOI 137 °CA - DOI 6 °CA. This can be attributed to the charge distribution as well. The significant homogenization of the SOI 137.5 °CA - DOI 6 °CA case increases the specific heat of the mixture leading to a slower increase of the temperature as the piston approaches the TDC. Conversely, the increase of the specific heat is lower in the more stratified cases, resulting in the higher pressure approaching the TDC. The highest pressure peak is reached by the SOI 50 °CA - DOI 17.5 °CA due to a strongly stratified mixture, featuring a peak pressure of 43 bar at 8 °CA aTDC. In this case, the faster combustion can be attributed to the fractions of the volume characterized by a rich mixture. Differently from the previous cases, as reported in the distribution in Figure 5.8, non negligible fractions of the chamber feature an equivalence ratio greater than 0.5, promoting a markedly faster combustion.

Taking the emissions into account, the picture changes dramatically, as reported in Table 5.5. Both the SOI 137 °CA - DOI 6 °CA and SOI 90 °CA - DOI 17.5 °CA cases can be considered zero-emission cycles, due to the H₂ distributions never exceeding the equivalence ratio threshold of 0.5 and consequently the lower temperatures. Conversely, a NO_x concentration of around 270 ppm has been observed at the EVO in the SOI 50 °CA - DOI 17.5 °CA case, which can be directly attributed to the richer zones with equivalence ratios spanning from 0.5 up to 1.25. The low performance of the early and intermediate injections, along with the high emissions of the late injection, push towards the research of a balanced solution. Under this framework, the combustion of the two multi-injection cases has been analyzed too. As it can be observed from Figure 5.17, both of the cases provide similar results in terms of pressure traces, resulting in a higher pressure peak with respect to the early and intermediate injection cases, and slightly lower (11%) when compared with the late injection strategy.

SOI [°CA bTDC]	DOI [°CA]	NO _x [ppm]
137	6	0
90	17.5	0
50	17.5	278
137-25	4-3	95
137-15	4-3	183

Table 5.5: NO_x emissions in the combustion cases analyzed. The last two rows refer to the multi-injection strategies.

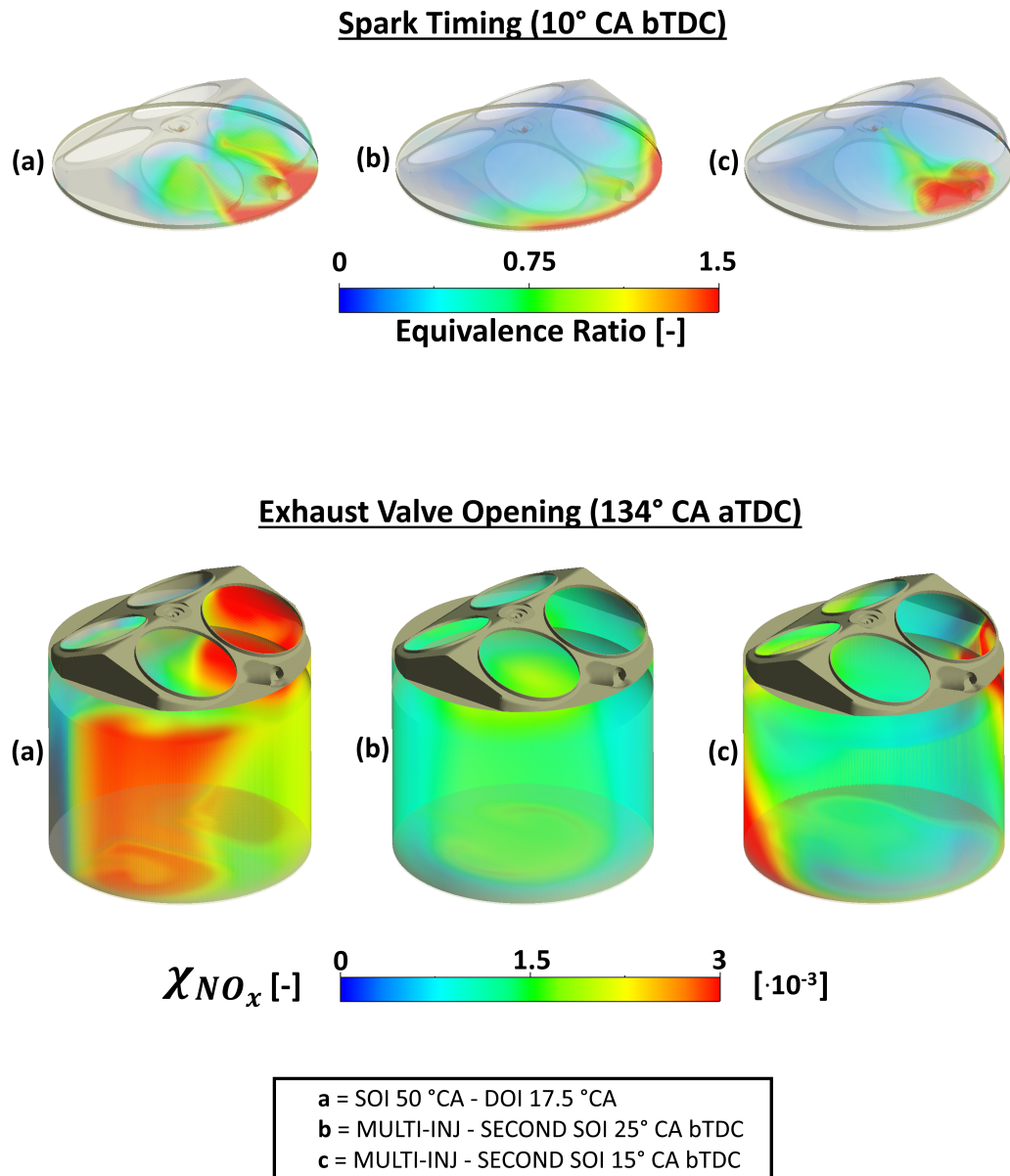


Figure 5.18: Upper: equivalence ratio distributions at 10 °CA bTDC (spark timing) for the three cases in which NO_x emissions are not negligible. Lower: NO_x distributions at the exhaust valve opening in the same cases.

Looking at the emission reported in Table 5.5, the multi-injection approach comes as a balanced solution too. The strategy with the second SOI at 15 °CA bTDC reduces the NO_x emissions from 270 to around 180 ppm. The case with the second SOI at 25 °CA provides the best solution, reducing the NO_x emission by the 60%, up to less than 100 ppm, thanks to the smaller fraction of almost-stoichiometric mixture. Therefore, the multi-injection approach can be deemed a promising solution for balancing performance and emission of the engine, providing room for a further optimization thanks to the wider design space. Insights of the emissions production can be drawn by looking at Figure 5.18, which reports the equivalence ratio distributions at spark timing (10 °CA bTDC) and NO_x distributions at the EVO for the three cases in which emissions are not negligible. The SOI 50 °CA - DOI 17.5 °CA case (on the left) clearly shows the highest NO_x content, with two symmetrical volumes featured by a considerable NO_x concentration, which can be related to the symmetrical equivalence ratio distribution at spark timing. For the multi-injection cases, when the second SOI is fixed at 25° CA bTDC (central pictures), a rich mixture forms at the wall, but volumes with an equivalence ratio around 0.8 - which leads to the peak of NO_x production - are more internal. Thus, the NO_x distribution becomes more concentrated moving from the walls to the cylinder axis. For the last case, with the second SOI at 15 °CA bTDC (right pictures), mixture did not have enough time to distribute along the liner. Volumes featured by an equivalence ratio around 0.8 are again more internal, and consequently most of the NO_x is similar to the previous case. Nonetheless, two high NO_x regions can be observed in the upper right and lower left of the figure, which justify the higher average NO_x concentration of this case with respect to the former.

5.5 Conclusions

In this Chapter, the effect of the injection strategy in a H_2 fueled ICE has been addressed. For a fixed ultra-lean equivalence ratio of 0.25, several combinations of the injection pressure and injection duration have been tested to delve the mixing between fuel and air and the influence on the combustion. The main findings are the following:

- numerically, two-equation turbulence models are able to capture the jet penetration and morphology acceptably. Conversely, capturing the mixing process after the injection is more challenging. The RSM model has been proven to provide better results, presumably due the anisotropic flow-field in the combustion chamber.
- either advancing the SOI or increasing the injection pressure increases the UI of the mixture. For early injections, the influence of the pressure is less relevant, due to the large amount of time to mix fuel and oxidizer. For instance, setting the EOI at 119.5 °CA bTDC and reducing the injection pressure from 70 to 23 bar, the UI decreases by only 7%.

- for early injections, mixing is driven by a strong tumble motion triggered by H_2 jet. Delaying the SOI, the TR decreases. For late injections, the fuel flow impinges both the liner and piston, without the possibility to create an evident tumble pattern.
- for early injections, rectangular and elliptical nozzle sections have a negligible influence on the charge homogeneity. Retarding the SOI, a slight decrease of the UI is observed with respect to the circular section for the same SOI and DOI. Nonetheless, it is not possible to recognize a specific pattern in the fuel distribution.
- multi-injections provide a way to control charge stratification. Moreover, this approach is useful to revamp the TKE level just before the ignition event.
- under ultra-lean conditions, the homogeneous mixture resulting from the early SOI and high pressure injection leads to a slow combustion. Retarding the SOI leads to faster combustion because of the progressively stratification of the charge, but NO_x emissions increase as well. Multi-injections are a balanced solution, providing a richer mixture close to the spark while substantially reducing emissions.

Chapter 6

Hydrogen thermodiffusive effects in the G-equation model

In this Chapter, a procedure to include the H_2 thermodiffusive (TD) instabilities in the context of the G-equation combustion model is discussed. The methodology has been applied to the simulations of a single cylinder H_2 research engine of the *Clean Mobility & Thermofluids* Institute of the Polytechnic University of Valencia. The focus of this Chapter is the validation of a methodology, based on the comparison of the numerical against experimental pressure traces for three operating points tested at the engine bench.

6.1 Phenomenology of H_2 flame instabilities

Laminar flames can be subject to two different kinds of instabilities. Darreius [153] and Landau [154] independently found that the flame sheet could be subject to an unconditionally instability caused by the gas expansion, σ , defined as the ratio of the unburnt to burnt gas densities.

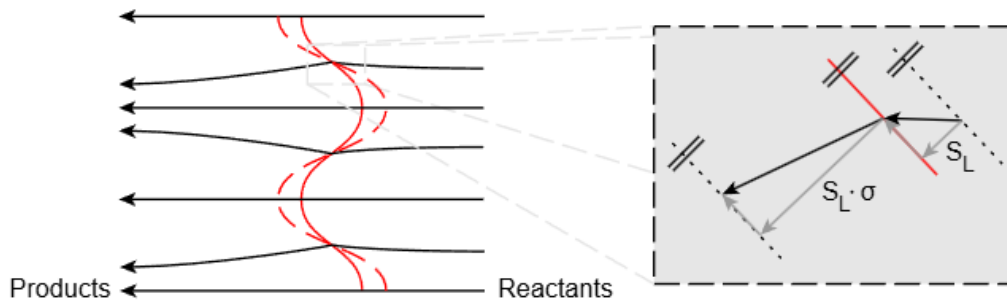


Figure 6.1: Sketch of the Darreius-Landau instability mechanism [155].

The fundamental mechanism of the Darreius-Landau instability is shown in Figure

6.1. Flow accelerates while passing through the flame as a consequence of the density drop. As visible on the right of the Figure, the velocity component normal to the flame increases while the tangential is unaffected. As a consequence, convex regions of the flame, being the center of curvature in the product region, produce a convergence of the streamlines, and vice-versa. The convergence increases the flame speed propagation, whereas concave regions experience a reduction of the flame speed. Ultimately, this mechanism will lead to an increase of the flame stretch. Darreius-Landau instability solely depends on the thermal expansion, resulting independent of the kind of fuel. The growth rate ω_{DL} of the Darreius-Landau perturbation is expressed as follows:

$$\omega_{DL} = \frac{1}{\sigma + 1} (\sqrt{\sigma^3 + \sigma^2} - \sigma - \sigma) \quad (6.1)$$

H₂ flames are also affected by the thermodiffusive instability, arising from the high molecular diffusivity of the fuel (Figure 6.2).

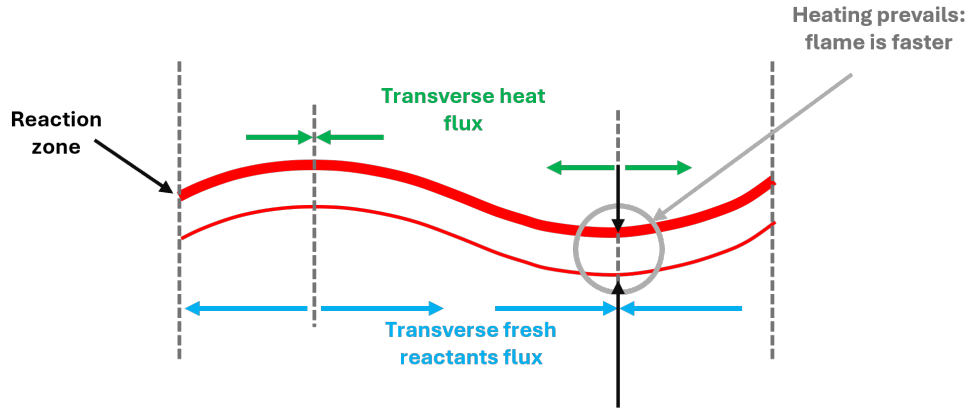


Figure 6.2: Sketch of the thermodiffusive instability mechanism [12].

TD instabilities arise when mixture is characterized by a molecular diffusivity higher than the thermal diffusivity, i.e., when the effective Lewis number (Le_{eff}) is lower than a critical threshold (Le_{cr}). Under this condition, if a perturbation is applied to the planar flame sheet, concave sections of the reaction sheet (being the center of curvature in the unburnt region) will experience an increased flux of fresh gases along with a lower dissipation of the generated heat, both resulting in a localized increase of the flame speed. In turns, the perturbation will step up according to the TD growth rate ω_2 defined as:

$$\omega_2 = -[B_1 + \beta(Le_{eff} - 1)B_2 + PrB_3] \quad (6.2)$$

being Bi parameters depending on the thermal expansion σ , the Prandtl number of the mixture, Pr , and the effective Lewis number, Le_{eff} , defined as:

$$Le_{eff} = \begin{cases} \frac{Le_o + ALe_f}{1+A}, A = 1 + \beta(\phi^{-1} - 1), \phi < 1 \\ \frac{ALE_o + Le_f}{1+A}, A = 1 + \beta(\phi - 1), \phi > 1 \end{cases} \quad (6.3)$$

where ϕ is the equivalence ratio of the mixture and β the Zeldovich number. Figure 6.3 shows an example of the ω_2 distribution as function of the mixture properties, being the unburnt temperature equal to 650 K. Reader can observe that for a fixed equivalence ratio, ω_2 increases with pressure up to a maximum. Beyond the maximum, ω_2 decreases as pressure increases. The initial growth of ω_2 is related to higher values of the Zeldovich number. This, in turns, is caused by the increased role of the termolecular reaction $H + O_2 + M \rightleftharpoons HO_2 + M$ which removes the H radical from the flame pool producing the relatively inactive HO_2 . Further increasing the pressure, reactions producing H and OH radicals starting from HO_2 and H_2O_2 become predominant, reducing the Zeldovich number and ω_2 as a consequence [156].

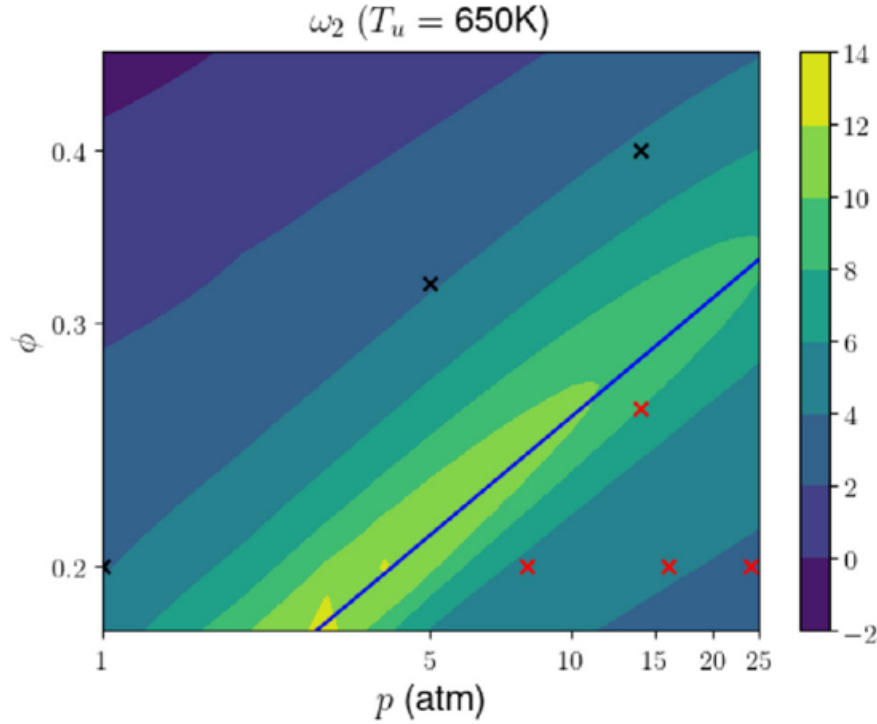


Figure 6.3: Distribution of the TD growth rate ω_2 as a function of the mixture properties [156].

Markers in Figure 6.3 indicate a subset of pressure/temperature/equivalence ratio conditions for which DNS simulations have been carried out to compute the laminar flame speed under the effect of several levels of the TD instabilities (i.e, for several values of ω_2). In such a way, Howarth [156] has been able to provide correlations for the ratio between the perturbed flame velocity s_F and s_L as a function of ω_2 , as reported in Figure 6.4. For a specific ω_2 , two ratios can be distinguished. One is relative to the low

pressure region, where the previously discussed termolecular reaction is preponderant, while the second is relative to the high pressure region where ω_2 decreases as pressure increases.

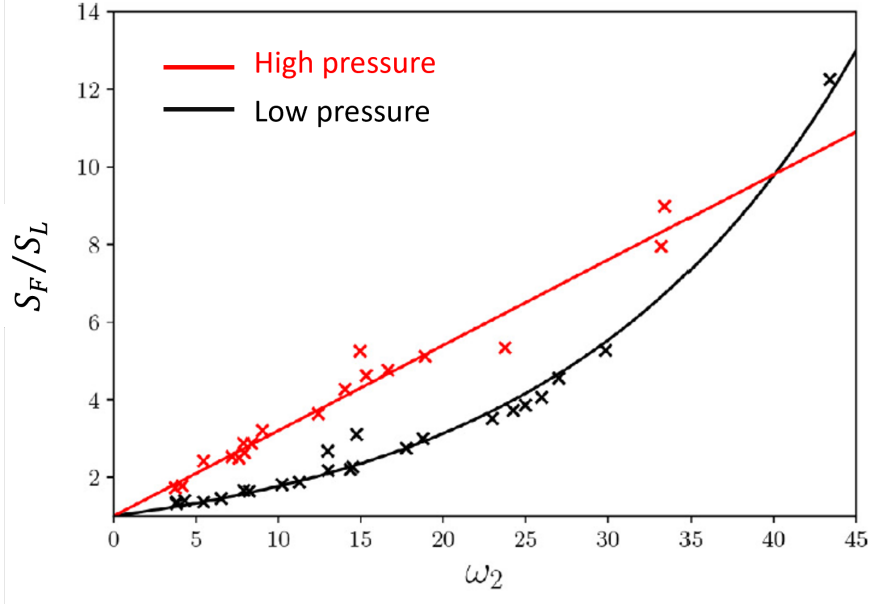


Figure 6.4: Correlations for the ratio between the perturbed flame velocity s_F and s_L as a function of ω_2 [156].

The interpolations of the two curves are the following:

$$\frac{s_F}{s_L} = \begin{cases} e^{0.057\omega_2}, & \text{low pressure region} \\ 1 + 0.22\omega_2, & \text{high pressure region} \end{cases} \quad (6.4)$$

The availability of such relations opens to the possibility of including the TD instability effects into the simulations of ICEs, as discussed in the next paragraph.

6.2 Methodology, case study, and preliminary results

Converge CFD is a widespread commercial CFD code, suitable for ICEs simulations. The G-equation is one the combustion models available in the code, and is based on a level-set approach. G is a scalar field, identifying regions of unburnt gases ($G < 0$), burnt ($G > 0$), and the flame front ($G = 0$). Converge CFD solves the following transport equation to track the evolution of the flame front:

$$\frac{\partial G}{\partial t} + \mathbf{u} \cdot \nabla G = -\rho D_t k |\nabla G| + \rho s_T |\nabla G| \quad (6.5)$$

being ρ the gas density, u the velocity field, k the local curvature of the flame, and s_T the turbulent flame speed. In the following, s_T has been computed according to the

Peter's correlation [157]:

$$s_T = s_L + u' \left(-\frac{a_4 b_3^2}{2b_1} Da + \left(\left(\frac{a_4 b_3^2}{2b_1} Da \right)^2 + a_4 b_3^2 Da \right)^{\frac{1}{2}} \right) \quad (6.6)$$

where u' is the turbulent intensity, Da the Damköhler number, and a_4 , b_1 , b_3 calibration constants. In the CFD code Converge, s_L can be computed by means of the chemical solver and stored in a table. This allows to modify the tabulated laminar flame speed according to the correlations 6.4, once coded a script to compute ω_2 for each combination of the equivalence ratio/pressure/temperature stored in the table, according to the scheme reported in Figure 6.5.

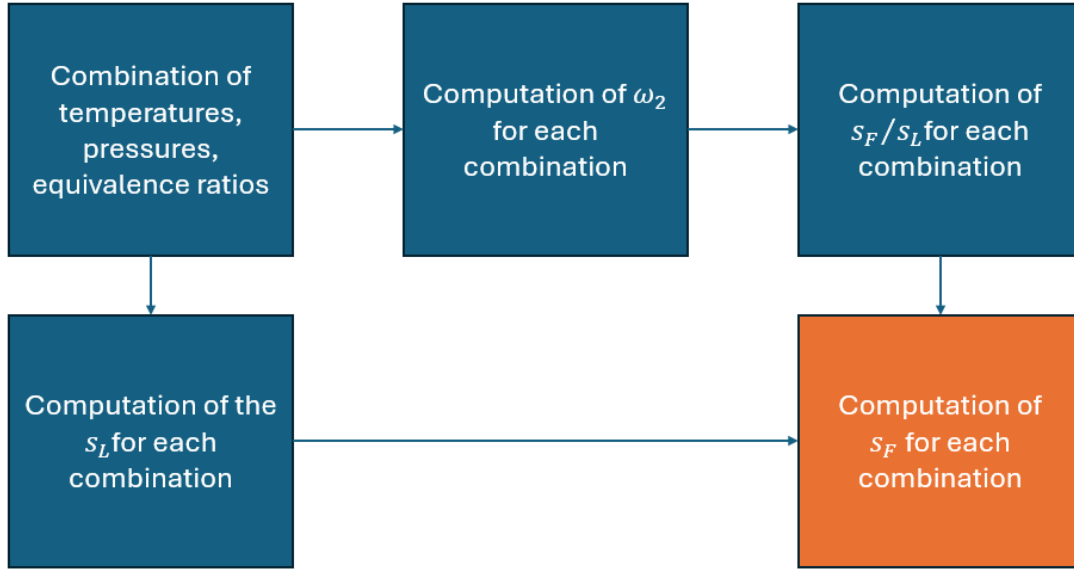


Figure 6.5: Scheme of the procedure to add the TD flame speed s_F in ICEs simulations.

The script to update the flame speed table has been written in Python and is based on the Cantera library. For each combination of pressure, temperature, and equivalence ratio of the original table, a 1D-flame premixed is solved. This allows to compute the density ratio σ needed to evaluate the grow rate of the Darreius-Landau instability ω_{DL} . Subsequently, the coefficients B_i of the thermo-diffusive grow-rate are assessed according to the following equations [156]:

$$B_1 = \frac{\sigma}{2(\sigma + (\sigma + 1)\omega_{DL})} \left(\frac{\sigma(2\omega_{DL} + \sigma + 1)}{\sigma - 1} \int_1^\sigma \frac{\tilde{\lambda}(x)}{x} dx + \int_1^\sigma \tilde{\lambda}(x) dx \right) \quad (6.7)$$

$$B_2 = \frac{\sigma(1 + \omega_{DL})(\sigma + \omega_{DL})}{2(\sigma - 1)(\sigma + (\sigma + 1)\omega_{DL})} \int_1^\sigma \log \left(\frac{\sigma - 1}{x - 1} \right) \frac{\tilde{\lambda}(x)}{x} dx \quad (6.8)$$

$$B_3 = \frac{\sigma}{\sigma + (\sigma + 1)\omega_{DL}} \left((\sigma - 1)\tilde{\lambda}(\sigma) - \int_1^\sigma \tilde{\lambda}(x) dx \right) \quad (6.9)$$

being $\tilde{\lambda} = \lambda(T)/\lambda_{unburnt}$ the non-dimensional Prandtl number and $x = T/T_{unburnt}$ the non-dimensional temperature of the mixture. Both the ratios are evaluated in Cantera considering a homogeneous mixture. As a last step, the Zel'dovich number β is computed. For a single-reaction scheme, the Zel'dovich number is defined as:

$$\beta = \frac{E_a(T_{burnt} - T_{unburnt})}{RT_{burnt}^2} \quad (6.10)$$

while for multi-reaction schemes, a generalized activation energy has been computed following an approach proposed by Law & Sung [158]:

$$E_a = -2R \frac{d(\log(f_0))}{d(1/T_{burnt})} \quad (6.11)$$

being $f_0 = \rho_{unburnt}s_L$ the laminar burning flux. Varying the adiabatic flame temperature T_{burnt} to compute the derivative without altering the fundamental conditions (equivalence ratio, unburnt temperature, pressure) is not straightforward. Reference [158] suggests that, when studying fuel-air flames, small amounts of nitrogen can be replaced with an equally inert gas, such as argon, to assess the changes in burning flux and adiabatic temperature. Once computed the Zel'dovich number, finally the laminar flame speed can be updated and used for the CFD simulations.

Table 6.1: H₂ single cylinder engine of the Polytechnic University of Valencia.

UPV H2 single cylinder engine	
Displacement volume	454 cm ³
Compression ratio	10.9
Stroke	86 mm
Connection rod length	144 mm
Bore	82 mm
Injection system	PFI/DI
Ignition mode	spark

The methodology has been tested exploiting the experimental results of a single cylinder H₂ engine of the Polytechnic University of Valencia, which can be operated either in PFI or DI mode. The main engine properties are reported in Table 6.1. As a preliminary assessment, the PFI mode has been taken into account to eliminate the numerical uncertainty regarding the mixing process of the DI cases.

An operating point featured by a mean effective pressure of 7 bar, 1500 RPM, and λ equal to 3.4 has been considered. The numerical results reported in Figure 6.6 refer to simulations carried out using the new flame speed tabulation which takes into account the TD instabilities effect. The dotted line refers to the pressure trace without any

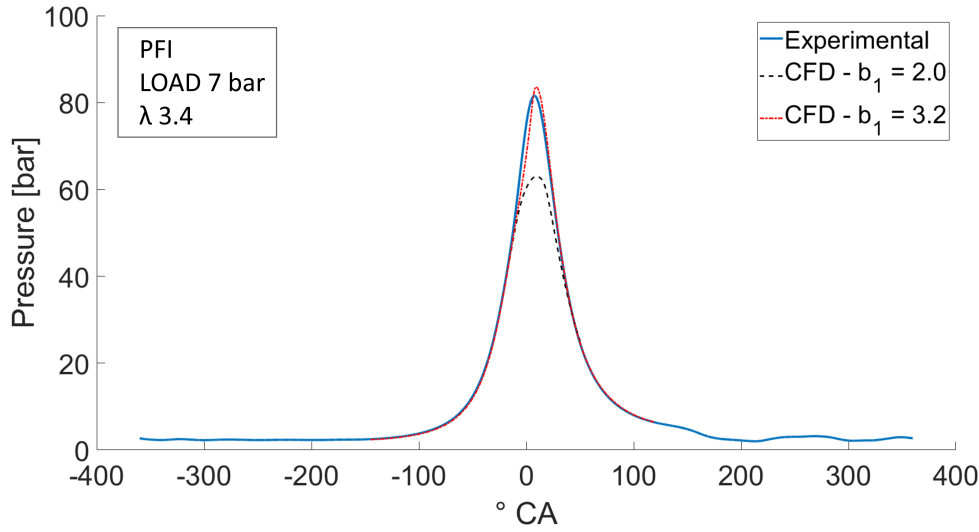


Figure 6.6: Test of the methodology on a PFI operating point. 1500 RPM, λ 3.4.

calibration of the Peter's correlation for the turbulent flame speed. Even including the TD effects, the peak pressure results significantly underestimated (20% lower than the experimental), though the phasing is acceptable.

Therefore, a calibration has been carried out for the b_1 parameter of the Peter's correlation, which determines the intensity of the flame stretch applied by the turbulent intensity. Setting $b_1 = 3$ results in a fairly better agreement with the experimental data. After this step, three operating points of the DI mode have been considered. The first one, considered as a base case, is featured by a mean effective pressure of 4 bar, SOI fixed at 130 °CA bTDC, 1500 RPM, and λ equal to 2.6. The second case only differs for the SOI set at 70 °CA bTDC. The last one shares the same data of the first case, but the mean effective pressure is equal to 7 bar.

For the first case, a quick calibration of b_1 has been run starting from the PFI experience, which resulted in a perfect match of the pressure curves setting b_1 equal to 3 as reader can observe in Figure 6.7. Without running any further calibration, the same setup has been used to test the second and third operating points. As reader can notice, the outcomes are acceptable for both the cases characterized by the delayed SOI (Figure 6.8) and the case featured by a higher load condition (Figure 6.9).

The difference in terms of peak pressure is 2.8% in the second case and 3.8% for the third. For both the cases, phasing of the peak pressure is tightly close to the experimental. Therefore, it seems that the combination of TD effects included in the simulations, along with a calibration of the combustion on a single case, can establish a reliable framework for DI H₂ ICEs analysis. Nonetheless, these cases share the same λ . Further tests should be carried out at leaner and richer conditions.

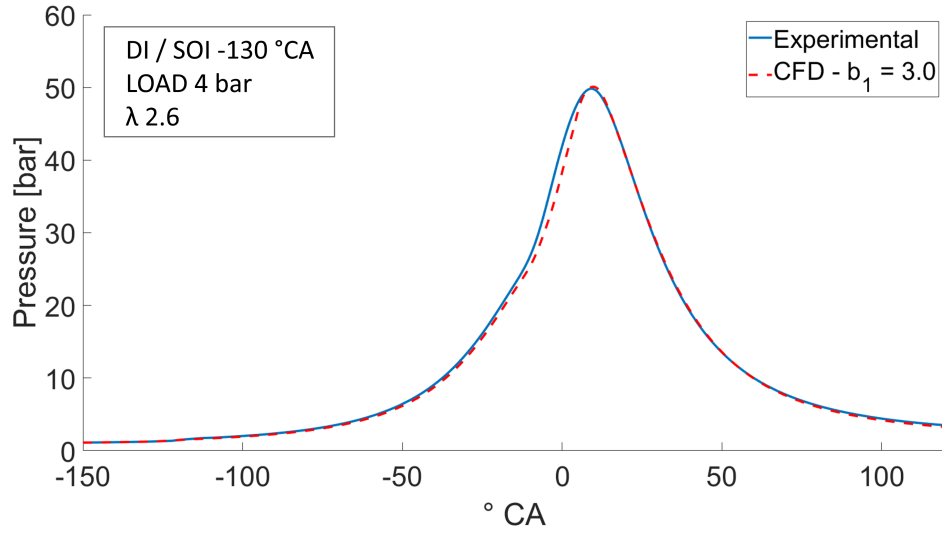


Figure 6.7: Pressure traces of the DI case featured by a $\text{SOI} = -130^\circ\text{CA}$, $\lambda = 2.6$, and load equal to 4 bar. This case has been used to calibrate the DI configuration. A good match is achieved setting b_1 equal to 3.

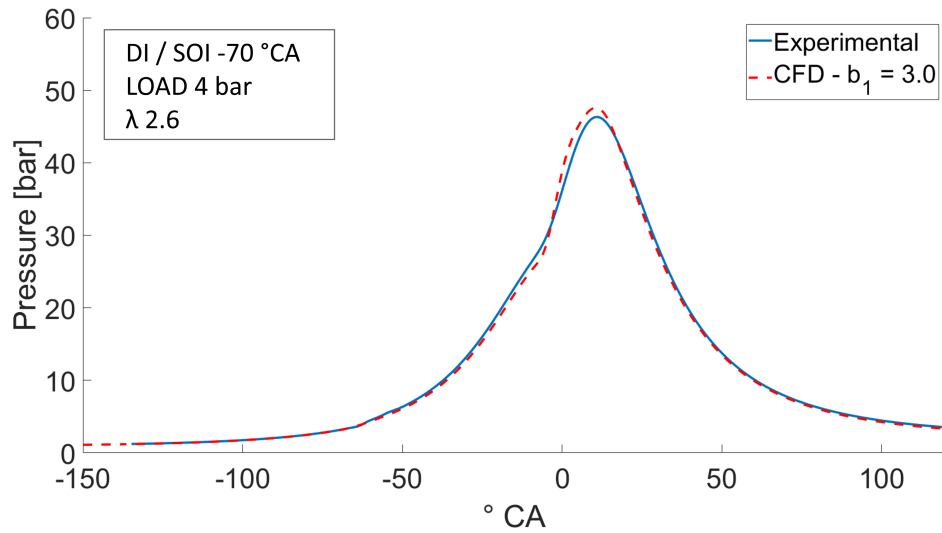


Figure 6.8: Pressure traces of the DI case featured by a $\text{SOI} = -70^\circ\text{CA}$, $\lambda = 2.6$, and load equal to 4 bar. For this case, no further calibration has been carried out.

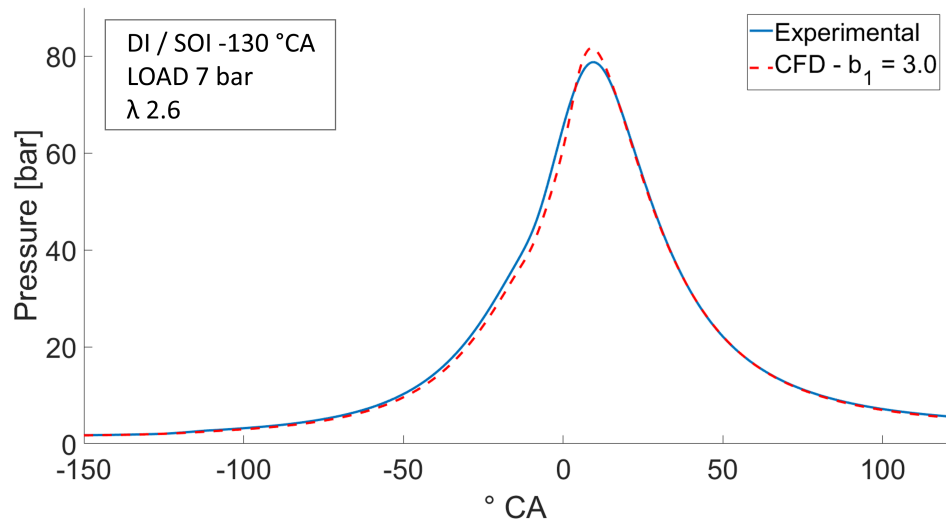


Figure 6.9: Pressure traces of the DI case featured by a SOI = -130 °CA, $\lambda = 2.6$, and load equal to 7 bar. For this case, no further calibration has been carried out.

Conclusions

Hydrogen for internal combustion engines is a promise which needs further intense investigation to extract all its potential. The main conclusions drawn by this thesis work are the following:

- the nature of the injected H_2 flow is complex, due to the mutual interaction of shocks and expansion fans. To correctly simulate the process, both the numerical setup and mesh must be carefully determined. Correlations have been provided in this work to describe the most relevant features of the high pressure H_2 jets. Such correlations can be useful to decide where the mesh refinement should be applied.
- In engine operation, the characteristic time of the process is too slow to trigger hysteresis phenomena. Therefore, a specific configuration of the jet structure can be analyzed by means of a steady simulation applying the correct NPR.
- Non-circular sections develop a markedly different gas-dynamic of the flow. For geometries featured by sharp corners, over-expanded conditions have been observed in a globally under-expanded flow. A shift of the Mach disk has been also observed and explained in terms of the intensity of the over-expansion. Corrective factors have been also determined to establish the position of the Mach disk for elliptical and rectangular nozzles a-priori.
- Mixing between jet and the surrounding ambient can be enhanced by using elliptical and rectangular nozzles, especially for high aspect ratios. This trend has been explained in terms of vorticity generated at the jet boundary. Also, the deformation of the jet boundary is driven by the vorticity distribution along the exit section perimeter.
- Mixing inside the combustion chamber is mainly driven by the SOI and injection pressure. For a fixed position of the injector, switching from the classical circular shape to elliptical or rectangular has a marginal influence on the final distribution of the fuel.
- Under ultra-lean conditions, retarding the SOI is useful to create a stratification of the charge thanks to the interaction between the fuel jet and piston. This results is

a much faster combustion, but the localized richer mixture leads to non-negligible NO_x emissions. The multi-injection approach is the way to optimize performance and emissions.

- A significant effort is still required to model H_2 ICEs. In this work, a preliminary analysis regarding the inclusion of the TD instabilities in the G-equation combustion model has been tested. Even with the new tabulated flame speed, a calibration of the turbulence-flame interaction is required. Fortunately, it seems that the calibration can be run just on a single engine point, and used successfully under other engine conditions. In any case, this highlights the need for novel numerical and experimental studies to shed light on flame-turbulence interaction under ICEs conditions.

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