UNIVERSITAT POLITÈCNICA DE VALÈNCIA

Escuela Técnica Superior de Ingeniería Industrial

Modelado unidimensional de un inyector de amoniaco para motores de encendido por compresión

Trabajo Fin de Grado

Grado en Ingeniería en Tecnologías Industriales

AUTOR/A: Plazas García, Laura

Tutor/a: Bracho León, Gabriela Cristina

CURSO ACADÉMICO: 2023/2024

Abstract

The increasing demand for sustainable energy solutions has directed research towards alternative fuels with lower environmental impact. This bachelor's degree Thesis focuses on the 1D modelling of an ammonia injector for a compression ignition engine, investigating its viability as a substitute for traditional diesel fuel. Ammonia presents a promising carbon-free alternative due to its zero carbon dioxide emissions during combustion. However, challenges such as its high ignition temperature and low flame speed necessitate detailed analysis and optimization.

This study employs the GT-Power software to implement a one-dimensional model of an ammonia injector, comparing its performance against a traditional diesel injector under various operating conditions. Key parameters such as operating pressure, temperature, and injection rate are analyzed to determine optimal conditions for ammonia combustion. The results indicate that while ammonia can potentially match the performance of diesel, specific modifications in the injection operation are essential to accommodate ammonia's unique properties. The findings contribute to the broader goal of achieving sustainable transportation solutions by providing insights into the practical application of ammonia in internal combustion engines.

Key words: 1D modelling, Ammonia injector, Internal combustion engine, Compression ignition engine, Combustion performance, Alternative fuels, GT-Power

Resumen

La creciente necesidad de soluciones energéticas sostenibles ha motivado la investigación de combustibles alternativos con menor impacto ambiental. Este trabajo Final de Grado (TFG) se centra en la modelización 1D de un inyector de amoníaco para un motor de encendido por compresión, investigando su viabilidad como sustituto del diésel tradicional. El amoníaco emerge como una opción libre de carbono muy prometedora, dado que su combustión no genera emisiones de dióxido de carbono. Sin embargo, desafíos como su alta temperatura de ignición y baja velocidad de llama requieren un análisis y una optimización detallados.

Este estudio utiliza el software GT-Power para desarrollar un modelo unidimensional de un inyector que opera con amoníaco, comparando su rendimiento con un inyector que utiliza diésel tradicional en diversas condiciones operativas. Se analizan parámetros clave como la presión de operación, la temperatura y el caudal másico para identificar las condiciones óptimas para la combustión del amoníaco. Los resultados sugieren que, aunque el amoníaco puede alcanzar un rendimiento similar al del diésel, es necesario ajustar las condiciones operativas para asegurar que el combustible permanezca en fase líquida. Los hallazgos contribuyen al objetivo más amplio de lograr soluciones de transporte sostenibles, proporcionando ideas sobre la aplicación práctica del amoníaco en motores de combustión interna.

Palabras clave: Modelización 1D, Inyector de amoníaco, Motor de combustión interna, Motor de encendido por compresión, Rendimiento de la combustión, Combustibles alternativos, GT-Power

Resum

La creixent demanda de solucions energètiques sostenibles ha dirigit la investigació cap a combustibles alternatius amb menor impacte ambiental. Aquest treball Final de Grau es centra en la modelització 1D d'un injector d'amoníac per a un motor d'encesa per compressió, investigant la seva viabilitat com a substitut del combustible dièsel tradicional. L'amoníac es presenta com una prometedora alternativa lliure de carboni degut a les seves zero emissions de diòxid de carboni durant la combustió. No obstant això, desafiaments com la seva alta temperatura d'ignició i baixa velocitat de flama requereixen una anàlisi i una optimització detallats.

Aquest estudi empra el programari GT-Power per a desenvolupar un model unidimensional d'un injector treballant amb amoníac, comparant el seu rendiment amb un injector treballant amb dièsel tradicional sota diverses condicions operatives. S'analitzen paràmetres clau com la pressió d'operació, la temperatura i el cabal màssic per a determinar les condicions òptimes per a la combustió de l'amoníac. Els resultats indiquen que, encara que l'amoníac pot potencialment igualar el rendiment del dièsel, són necessàries modificacions específiques en les condicions d'operació per a condicionar l'amoníac i assegurar que sempre estiga en fase líquida. Les troballes contribueixen a l'objectiu més ampli d'aconseguir solucions de transport sostenibles, proporcionant idees sobre l'aplicació pràctica de l'amoníac en motors de combustió interna.

Paraules clau: Modelització 1D, Injector d'amoníac, Motor de combustió interna, Motor d'encesa per compressió, Rendiment de la combustió, Combustibles alternatius, GT-Power

Acknowledgements

En primer lugar, quiero expresar mi más profundo agradecimiento a mi tutora, Gabriela Bracho, por confiar en mí para este proyecto, por su apoyo constante y por sus valiosos consejos, sin los cuales nada de esto habría sido posible. También al departamento y al CMT, por brindarme los recursos necesarios para el desarrollo de este trabajo, así como por el extenso conocimiento que han compartido conmigo.

A mi familia, que ha creído en mí desde el principio, incluso en los momentos en que yo no lo hacía. A mis padres, por estar siempre a mi lado, por darme todas las oportunidades que he tenido en la vida, por alimentar mi curiosidad desde pequeña y permitirme ser, con todas mis rarezas e incongruencias. Por hacerme leer. A mis abuelos, por ser ese pilar fundamental que me ha acompañado en cada paso y que siempre ha sabido sacarme una sonrisa. A mis tíos y primos, por la confianza y el cariño que siempre me han mostrado. Y a aquellos que ya no están con nosotros en las comidas de los domingos, pero que siempre formarán parte de quienes somos. Os quiero muchísimo.

A todos mis profesoras y profesores, les agradezco por haberme inspirado a lo largo de estos años y por enseñarme con dedicación y pasión. A todas aquellas personas que, quizás sin saberlo, me han impulsado a aprender cosas nuevas. Por ayudarme a descubrir y desarrollar mis capacidades. Por escucharme y por guiarme. Por compartir su conocimiento con generosidad, por hacer accesible lo complejo y por fomentar mi crecimiento personal.

Y finalmente, a mis amigas y amigos, que a lo largo de estos años me han hecho sentir que había también un huequito para mí en el mundo, que me han hecho más valiente, más confiada y más humana. En particular, un abrazo muy fuerte y apretadito a Omar, Andrea e Irene, quienes comenzaron siendo compañeros y ahora son los hermanos que siempre soñé, por estar siempre ahí y por su apoyo inestimable. También a Jana, Nati, Lucía, Ramón, Pedro, Javi(s) y Sergio, sin quienes estos años en Valencia habrían sido, sin duda, mucho más aburridos. Y a aquellos valientes que, con infinita paciencia, han logrado el título honorífico en soportar mis excentricidades desde hace años y sin embargo, aunque no termine de entender por qué, siguen acompañándome en cada paso.

Estoy tremendamente orgullosa de haber llegado hasta aquí (llegué a pensar que este día no llegaría nunca), y deseo que vosotros también lo estéis, porque este logro es, en gran medida, vuestro.

Executive Summary
Resumen ejecutivo

The student Laura Plazas García as the author, and Gabriela Bracho León as the supervisor of this Final Degree Project titled **1D Modelling of an Ammonia Injector for a Compression Ignition Engines**, prior to obtaining the degree of Bachelor in Industrial Technologies Engineering from the Universitat Politècnica de València, acknowledge and confirm that it complies with the aspects outlined in the present executive summary:

*La estudiante Laura Plazas García como autora y Gabriela Bracho León como tutora de este Trabajo Fin de Grado titulado **1D modelling of an ammonia injector for compression ignition engines** y antecedente a la obtención del título de Graduado en Ingeniería en Tecnologías Industriales por la Universitat Politècnica de València conocen y confirman que cumple con los aspectos señalados en el presente resumen ejecutivo:*

Concept **(ABET)**	**Concepto (traducción)**	**¿Cumple? (S/N)**	**¿Dónde? (págs.)**
1. *Identify:*	**1. Identificar:**	S	
1.1. *Problem statement and opportunity*	1.1. Planteamiento del problema y oportunidad	S	2-6
1.2. *Constraints (standards, codes, needs, requirements & specifications)*	1.2. Toma en consideración de los condicionantes (normas, códigos, necesidades, requisitos y especificaciones)	S	2-9
1.3. *Setting of goals*	1.3. Establecimiento de objetivos	S	6
2. *Formulate:*	**2. Formular:**	S	
2.1. *Creative solution generation (analysis)*	2.1. Generación de soluciones creativas (análisis)	S	36-48, 57-58, 59-69
2.2. *Evaluation of multiple solutions and decision-making (synthesis)*	2.2. Evaluación de múltiples soluciones y toma de decisiones (síntesis)	S	49-58, 59-71
3. *Solve:*	**3. Resolver:**	S	
3.1. *Fulfilment of goals*	3.1. Cumplimiento de objetivos	S	59-69, 72
3.2. *Overall impact and significance (contributions and practical recommendations)*	3.2. Impacto global y alcance (contribuciones y recomendaciones prácticas)	S	21-22, 23-30, 73

Contents

I Project Report 1

1 Introduction 2
1.1 Justification 2
1.1.1 Meeting the energy needs of a growing world 2
1.1.2 Pollution related to the transportation sector 3
1.1.3 Research directions and innovations 5
1.1.4 Challenges of these new technologies 6
1.2 Research Question 6
1.2.1 Problem Statement and Opportunity 6
1.2.2 Constraints 7
1.3 Objectives 7
1.3.1 Ammmonia as fuel for internal combustion engines 7
1.3.2 Sustainable Development Goals 7
1.4 State of the art 10
1.4.1 CMT institution 10
1.4.2 CMT previous research 11
1.5 Structure of the document 11

2 Background 13
2.1 Traditional Fuels 13
2.1.1 Historical Introduction 13
2.1.2 Use and development of the traditional fuels: ICE systems 14
2.1.3 Fuels and their properties 17
2.1.4 Issues and Limitations of the Use of Traditional Fuels 22
2.2 New carbon-free fuels 24
2.2.1 Hydrogen 24
2.2.2 Alternatives to Hydrogen 26
2.2.3 Ammonia 27
2.2.4 Current position of ammonia as a fuel 31
2.3 Injection system 32
2.3.1 Types of injection systems 32
2.3.2 Functions 33
2.3.3 Injector types 34
2.3.4 Parts and Components of the Injection System 34
2.3.5 Hydraulic characterization 36

3 Method 37
3.1 Modelling 37
3.1.1 Representing Fluid dynamics 37
3.1.2 One-Dimensional (1D) Modelling 38

3.2 GT-Power 38
3.2.1 Description of the software 38
3.2.2 Main characteristics of the software 39
3.2.3 Modifiable parameters 39
3.3 Model 40
3.3.1 Model Background 40
3.3.2 Describing distinct parts and components in the model 40
3.3.3 Rate of Injection 46
3.3.4 Diesel Injection 47
3.3.5 Control volume orifices 47
3.3.6 Model Validation 49

4 Model upgrade 50
4.1 Sensitivity analysis with Diesel 50
4.1.1 Repsol CEC RF-06-99 Diesel Fuel 50
4.1.2 Sensitivity study with GT-Power® 51
4.2 Notable findings 52
4.2.1 Rail Pressure 52
4.2.2 Fuel Temperature 53
4.2.3 Energizing time 54
4.2.4 OA and OZ geometries 55
4.2.5 Other parameters 58
4.3 Modelling ammonia's fuel properties 58

5 Performance analysis of ammonia in engine simulations 60
5.1 Comparative Analysis of Injection Rates 60
5.1.1 Maximum Injection Rate 61
5.1.2 Injection Duration 61
5.1.3 Injection Rate Stability 62
5.1.4 Initial Injection Response 62
5.2 Parameter adjustment 63
5.2.1 Rail Pressure 63
5.2.2 Fuel Temperature 64
5.2.3 Injection time 65
5.2.4 OZ diameter 67
5.2.5 OA diameter 69
5.3 Comparison with other fuels 70

6 Conclusions and future work 73
6.1 Conclusions 73
6.2 Future Work 74

II Annex 1
Sensitivity analysis with diesel 2
Rail pressure 2
Fuel Temperature 3
Energizing time 4
OA and OZ geometries 5
Other parameters 16

Sensitivity analysis with ammonia . . . 17
    Rail pressure . . . 17
    Fuel Temperature . . . 18
    Energizing time . . . 19
    OA and OZ geometries . . . 20
Comparison with methanol . . . 31
    Injection rate at 400 bar . . . 31
    Injected mass at 400 bar . . . 31
    Injected volume at 400 bar . . . 32
    Mass flow in OZ at 400 bar . . . 32
    Throat temperature in OZ at 400 bar . . . 33
    Throat temperature in OA at 400 bar . . . 33
    Throat pressure in OA at 400 bar . . . 34

III Specifications Document **1**

IV Budget **1**

List of Figures

1.1 Total energy supply (TES) by source, World, 1990-2021 [18] 3
1.2 Total final consumption (TFC) by source, World, 1990-2021 [18] 3
1.3 Total final consumption (TFC) by sector, World, 1990-2021 [18] 4
1.4 Transport total final consumption (TFC) by source, World, 1990-2021 [18] . 4
1.5 Electricity generation by source, World, 1990-2021 [18] 5
1.6 SDG [30] 8

2.1 4-strokes engine 15
2.2 2-strokes engine 16
2.3 Classification of most common liquid fuels [12] 17
2.4 Classification of most common gaseous fuels [12] 18
2.5 Specific energy and energy density for fuels [44] 20
2.6 Volumetric energy density of different fuels 21
2.7 The energy pathway towards a net zero carbon mobility scenario [31] 24
2.8 Low and upper flammability limits of various substance [15] 25
2.9 Hydrogen Properties and their influence on engine performance and design requirements [13] 26
2.10 Characteristics of ammonia as a fuel in internal combustion engines [13] . . 28
2.11 Schematic of the Haber-Bosch ammonia synthesis reaction [44] 28
2.12 Schematic green ammonia synthesis combined with electrolysis-based hydrogen production [8] 29
2.13 Schematic of green ammonia production [44] 30
2.14 Cost estimate for ammonia and hydrogen transportation by cargi ships, railway and road trailers [44] 31
2.15 Carbon-free ammonia production and its various end-use [8] 32
2.16 Methods to deliver fuel to the combustion chamber [42] 33
2.17 Components of a solenoid injector in a common-rail system [25] 34
2.18 Components and layout of a typical common-rail system [42] 35
2.19 Operation of common-rail injector [25] 35

3.1 Gamma Technologies logo 38
3.2 Main interface of GT-Power® 39
3.3 Complete model map in GT-POWER [34] 41
3.4 Solenoid valve of a common-rail injector [25] 42
3.5 Electrovalve model layout [34] 43
3.6 Injector Holder layout [34] 44
3.7 Needle and nozzle layout [34] 45
3.8 Experimental vs Modelled (Constant Pressure and Variable Pressure) . . . 46
3.9 Silicone mold technique for control volume geometry determination [34] . . 47

4.1 Injection rates for different rail pressures using diesel as a fuel 53

4.2 Discharge coefficients for different rail pressures using diesel as a fuel 53
4.3 Injection rates for different fuel temperatures with diesel and $ET = 1ms$ . . 54
4.4 Discharge coefficient for different fuel temperatures with diesel 54
4.5 Injection rates for different energizing times using diesel as a fuel 55
4.6 Injection Rate for OZ Diameters (ET=1 ms) 56
4.7 Injection Rate for OA Diameters (ET=1 ms) 56
4.8 Injection Rate for OZ Diameters (ET=2 ms) 56
4.9 Injection Rate for OA Diameters (ET=2 ms) 56
4.10 Microscopic internal damage in the OA orifice of an injector working with diesel (From CMT experiments) 57
4.11 Injection Rate for different chamber temperatures (ET=1 ms) 58
4.12 Injection Rate for different wall temperatures (ET=1 ms) 58

5.1 Injection rate for ammonia and diesel under the same operating conditions . 60
5.2 Injection rate for ammonia at different rail pressures 63
5.3 Discharge coefficient for ammonia at different rail pressures 64
5.4 Injection rate for ammonia at different fuel temperatures 65
5.5 Discharge coefficient for ammonia at different fuel temperatures 66
5.6 Injection rate for ammonia with different ET 67
5.7 Injection rate for ammonia with OZ diameters 67
5.8 Injection rate for ammonia with OZ diameters (ET=2) 68
5.9 Injection rate for ammonia with OA diameters 69
5.10 Injection rate comparison of different fuels 71
5.11 Injected mass comparison of different fuels 72
5.12 Injected volume comparison of different fuels 72

List of Tables

1.1 Degree of Work Relation to the Sustainable Development Goals (SDGs) . . 10

2.1 Most common fuels' densities and kinematic viscosities [12] 19
2.2 Most common fuels' flammability limits with air [12] 19
2.3 Most common fuels' Heating Values [12] 21
2.4 Ammonia's combustion characteristics compared to other fuels, 300K at 100kPa [45] 27

4.1 Repsol CEC RF-06-99 Diesel Fuel properties [35] 50
4.2 Parameter settings for diesel in the simulation 52
4.3 OA Diameters 55
4.4 OZ Diameters 55
4.5 Comparison of Ammonia and Diesel Fuel Properties 59

5.1 Simulation Parameters 61
5.2 Simulation Parameters 63
5.3 Simulation Parameters 65
5.4 Simulation Parameters 66
5.5 Simulation Parameters 68
5.6 Simulation Parameters 69
5.7 Comparison of Ammonia, Diesel, and Methanol Fuel Properties 70
5.8 Parameters set up 71

List of Abbreviations and Acronyms

ASTM - American Society for Testing and Materials

BOE - Boletín Oficial del Estado

BP - British Petroleum

CAE - Computer-Aided Engineering

CCS - Carbon Capture and Storage

CEC - Coordinating European Council

CFD - Computational Fluid Dynamics

CI - Compression-Ignition (Engine)

CMT - Clean Mobility & Thermofluids

DI - Direct Injection

E10 - Ethanol 10% (a type of fuel)

E85 - Ethanol 85% (a type of fuel)

ECU - Engine Control Unit

ETBE - Ethyl Tert-Butyl Ether

EVI - Electric Vehicle Initiative

FAME - Fatty Acid Methyl Ester

GLP - Gas Liquefied Petroleum

GT - Gamma Technologies

HHV - High Heating Value

HV - Heating Value

ICE - Internal Combustion Engine

IDI - Indirect Injection

IEA - International Energy Agency

LFL - Lower Flammable Limit

LHV - Lower Heating Value

MJ - Megajoules

MTBE - Methyl Tert-Butyl Ether

NASA - National Aeronautics and Space Administration

OECD - Organisation for Economic Co-operation and Development

ROI - Return on Investment

SCR - Selective Catalytic Reduction

SDG - Sustainable Development Goals

SI - Spark-Ignition (Engine)

STP - Standard Temperature and Pressure

TFG - Trabajo Final de Grado (Final Degree Project)

UFL - Upper Flammable Limit

UNFCCC - United Nations Framework Convention on Climate Change

UPV - Universitat Politècnica de València

VAT - Value Added Tax

Part I

Project Report

Chapter 1

Introduction

1.1 Justification

1.1.1 Meeting the energy needs of a growing world

Need and importance of energy and its supply

Energy plays a fundamental role in modern society, as many aspects of daily life depend on it. From generating electricity to illuminate homes and power electronic devices, to transporting people and goods, and to producing food and manufacturing goods, energy is an essential component of the economy and human development.

However, the indiscriminate use of certain forms of energy, especially those derived from fossil fuels, has led to serious environmental problems such as climate change and air and water pollution. Therefore, the quest for cleaner and more sustainable forms of energy is one of the most significant challenges for modern society.

Despite advances in expanding energy infrastructure, millions of people worldwide still lack access to modern energy services. Ensuring universal access to energy is crucial for reducing poverty, improving health and well-being, and promoting sustainable development.

Increase in consumption

Global energy consumption is skyrocketing due to a combination of factors: population growth and urbanization (increased demand in dense areas and expansion of infrastructure), economic development and industrialization (production processes and transportation), technological advancements and new lifestyles (rising per capita consumption), and expansion of the transportation sector (fossil fuels).

This combination drives exponential energy consumption, generating challenges in energy security, environmental sustainability, and climate change. The transition to clean and renewable sources becomes urgent to address them.

1.1.2 Pollution related to the transportation sector

Context data

The International Energy Agency (IEA) is an autonomous organization established in 1974 under the framework of the Organisation for Economic Co-operation and Development (OECD). The IEA aims to promote secure, sustainable, and affordable energy policies globally. It conducts comprehensive analyses of the global energy market, assessing trends, challenges, and opportunities in areas such as energy supply and demand, energy efficiency, emerging technologies, and environmental impact.

In Figures 1.1 and 1.2, it can be observed that the supply and total consumption of global energy from 1990 to 2020 have consistently increased. Clearly, the majority of this energy has been generated from fossil fuels such as coal, natural gas, and petroleum derivatives. Despite increases in other energy sources, those remain minor in comparison.

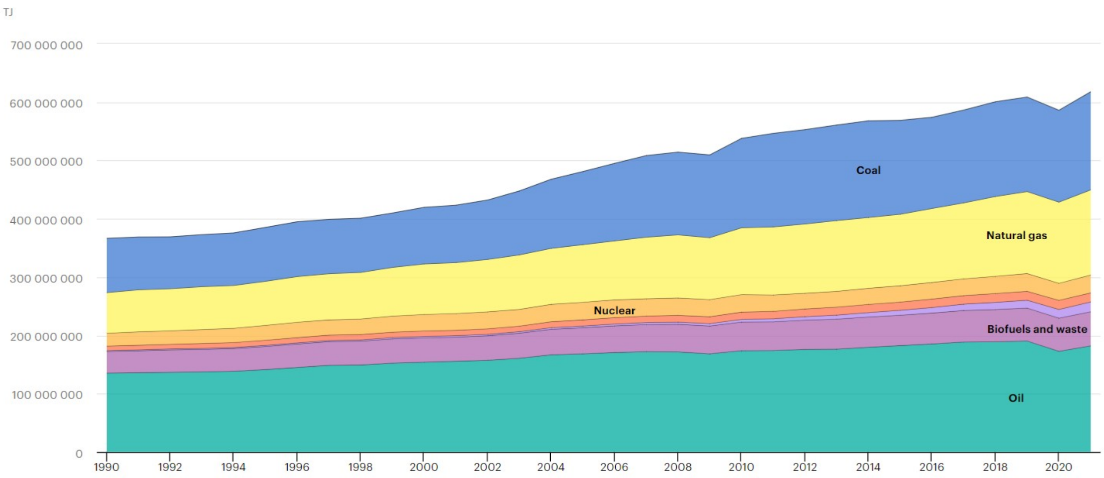


Figure 1.1: Total energy supply (TES) by source, World, 1990-2021 [18]

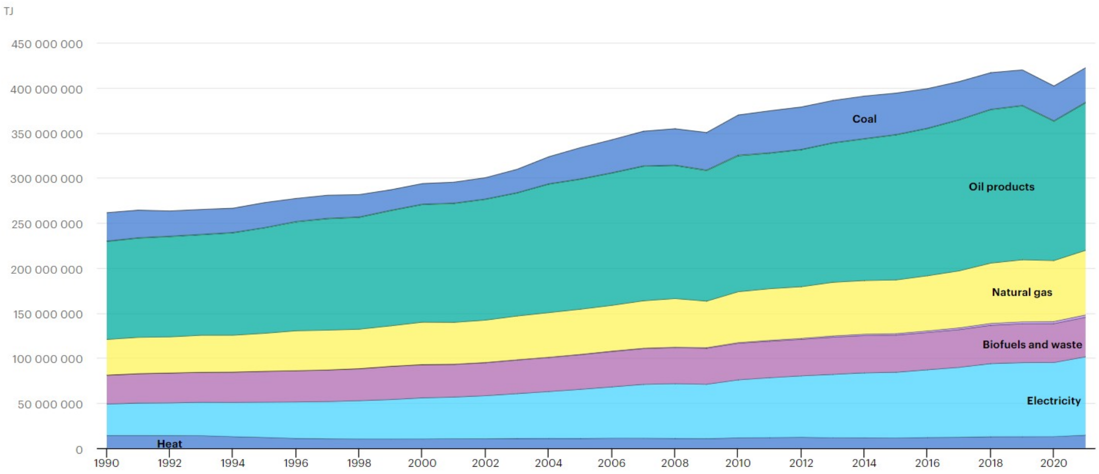


Figure 1.2: Total final consumption (TFC) by source, World, 1990-2021 [18]

Furthermore, Figure 1.3 provides the breakdown of energy consumed by sectors, where it can be clearly seen that the most energy-intensive sectors are industrial, transportation, and residential, with the primary source of this consumed energy being fossil fuels. Specifically, in the transportation sector, as depicted in Figure 1.4, it is almost entirely composed of the combustion of petroleum derivatives.

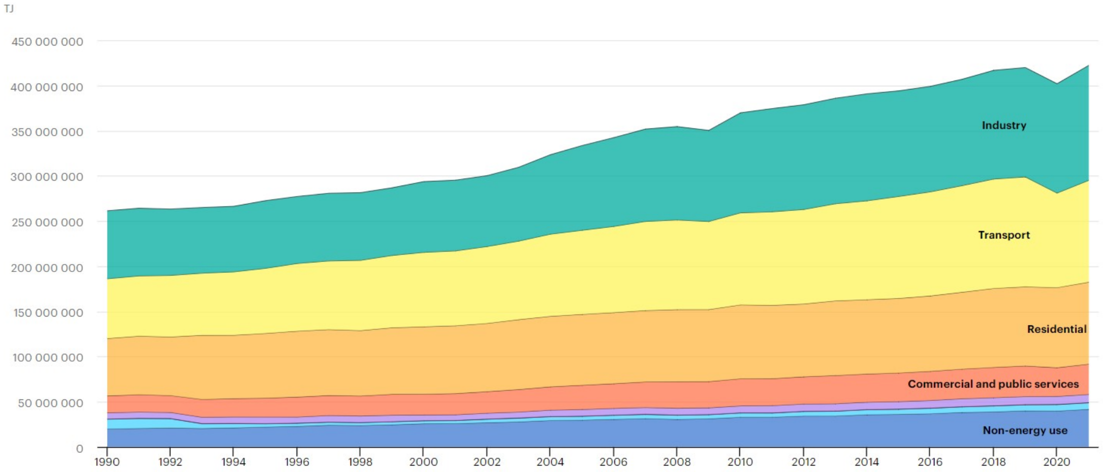


Figure 1.3: Total final consumption (TFC) by sector, World, 1990-2021 [18]

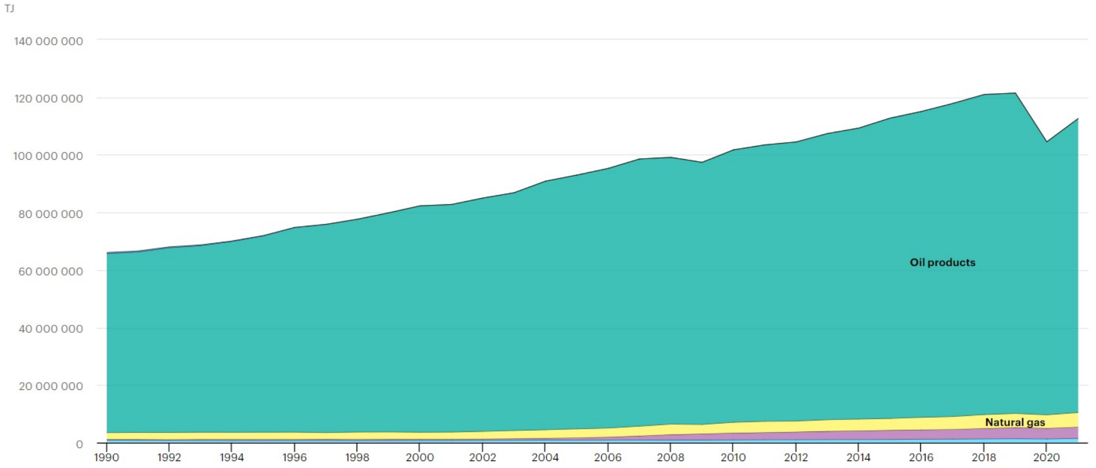


Figure 1.4: Transport total final consumption (TFC) by source, World, 1990-2021 [18]

The transportation sector

Despite the increasing use of renewable energy sources, non-renewable fossil fuels continue to dominate the global energy landscape, accounting for over 85% of the planet's energy supply. However, this dependence on fossil fuels is unsustainable, given their limited reserves and the serious environmental consequences of their combustion.

The combustion of fossil fuels significantly contributes to atmospheric carbon dioxide (CO_2) levels, surpassing 36.57 billion tons and exacerbating global warming through the greenhouse effect. It is remarkable that carbon emissions related to traffic, with road transport alone contributing to over 70% of these emissions, underscore the urgent need for sustainable energy alternatives. In response to this, low-carbon or zero-emission fuels are gaining ground as potential solutions to mitigate emissions from internal combustion engines (ICEs) [29].

Furthermore, the finite nature of fossil fuel reserves poses a challenge to the sustainability of contemporary transportation infrastructure. As **reserves diminish** and **extraction becomes increasingly costly**, the need for diversification in energy sources becomes more **urgent**. The undeniable reality of this situation demands a fundamental shift in how transportation solutions are conceived and implemented.

1.1.3 Research directions and innovations

Electric transportation

In order to avoid greenhouse gas emissions derived from the combustion of fossil fuels, two main solutions are considered. The first involves the adoption of electric motors, thus eliminating the combustion process. The second alternative consists of using fuels that do not emit CO_2 into the atmosphere. Both options have the potential to reduce emissions, improve air quality, and promote sustainable mobility.

Currently, the option of electric vehicles is the most socially accepted and is somewhat more developed at the user level. However, it still faces significant challenges that question its long-term viability. On one hand, the origin of the electricity used, which as it can be observed in Figure 1.5, despite having diversified more in recent years towards the use of renewable energies, still predominantly comes from the combustion of fossil fuels. Additionally, the driving range or autonomy of electric vehicles still does not match that of internal combustion vehicles, which can be a drawback for long trips or in areas with limited charging infrastructure. In fact, the network of charging stations for electric vehicles is still in the process of development and is not as extensive as that of gas stations. Furthermore, the batteries of electric vehicles, crucial for their operation, have a high cost and limited lifespan. Their production and recycling processes can also generate additional environmental impacts. For these reasons, it seems pertinent to lean towards the second solution, which consists of using low-carbon or carbon-free fuels to mitigate emissions from internal combustion engines.

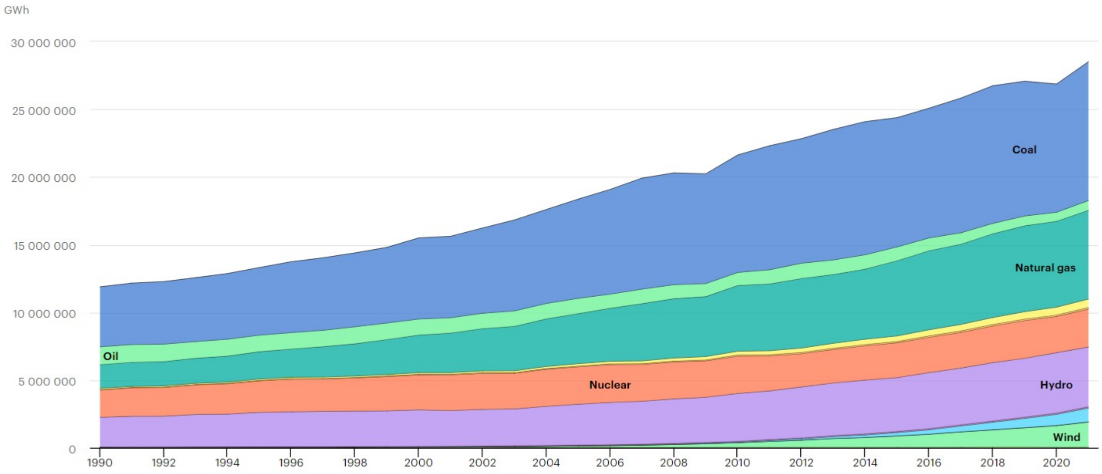


Figure 1.5: Electricity generation by source, World, 1990-2021 [18]

Carbon-free fuels

Hydrogen has emerged as a leader among these alternative fuels, recognized for its potential as a carbon-neutral energy carrier in both transportation and electric power applications. Despite its promises, the widespread adoption of hydrogen faces technological complexities and inherent drawbacks, including safety concerns, infrastructure availability, storage limitations, and performance issues in internal combustion engines [13].

Concurrently, **ammonia** has garnered attention as a viable alternative transportation fuel, offering distinct advantages over hydrogen. However, concerns about the high cost and low efficiency of both hydrogen and ammonia have raised doubts about their commercial viability and widespread adoption, as evidenced by the reduction or cessation of hydrogen vehicle production by automotive companies in Japan and South Korea [13].

Despite these advancements, there remains a lack of comprehensive studies examining the utilization of hydrogen and ammonia in specialized design modifications and adaptations for both spark ignition (SI) and compression ignition (CI) engines. Therefore, urgent efforts are needed to advance the application and technological advancements of these energy carriers.

1.1.4 Challenges of these new technologies

This bachelor's thesis undertakes a comprehensive exploration of the viability and efficacy of using ammonia as a substitute for diesel in internal combustion engines. By elucidating the synthesis, properties, and combustion characteristics of ammonia, this research endeavours to catalyse transformative change within the transportation sector. Through empirical analysis and theoretical modelling, it aims to clarify the potential of ammonia-powered internal combustion engines to inaugurate a new era of sustainable mobility, offering a beacon of hope in an otherwise uncertain landscape.

1.2 Research Question

Within the scope of this research work, the necessary modifications in a conventional diesel injection system of compression ignition internal combustion engines will be explored to adapt it to the use of ammonia as a carbon-free fuel. In this bachelor's thesis, the simulation of the internal flow of ammonia in a high-pressure fuel injector (direct injection) is proposed, to investigate the effect that the properties of this fluid (NH_3) have on the injection process. For this purpose, a 1-D model of an injector will be used, and different operating conditions will be evaluated to understand their effect on the fuel flow and system dynamics. The obtained results will be used to couple them to a global engine model.

1.2.1 Problem Statement and Opportunity

As previously mentioned, ammonia presents a promising alternative fuel for internal combustion engines, primarily due to its zero carbon dioxide emissions during combustion. Despite this advantage, its use poses significant technical challenges, particularly in optimizing the injection system for maximum efficiency and minimal emissions. This project builds on existing research by focusing on the adaptation of a diesel injection system to operate with ammonia, addressing key technological barriers and exploring opportunities for enhancing transportation sustainability.

1.2.2 Constraints

The successful implementation of ammonia injection systems must comply with established technical standards and safety regulations. This includes adapting existing diesel engine design codes, meeting performance specifications, and overcoming operational constraints like maintaining ammonia in its liquid phase during injection. These factors are crucial to ensuring that the system not only meets industry standards but also functions effectively and safely.

1.3 Objectives

1.3.1 Ammmonia as fuel for internal combustion engines

The main objective of this Bachelor's Thesis is the characterization of an ammonia injection system for compression ignition internal combustion engines. This study will begin with the implementation of a one-dimensional model of a common-rail direct injector using GT-Power software, followed by testing various operating parameters and boundary conditions. To achieve this, the following partial objectives will be addressed:

1. Determine the optimal operating pressure conditions.
2. Determine the optimal operating temperature conditions.
3. Determine the required injection ratio.

For this purpose, the results obtained with ammonia will be compared with those obtained with diesel to ensure that the performance obtained is comparable.

1.3.2 Sustainable Development Goals

Climate change is a serious threat that requires unified global action. Legislation and international agreements are essential for reducing greenhouse gas emissions and mitigating their impact on the environment. The United Nations Framework Convention on Climate Change (UNFCCC) was the starting point, followed by important agreements such as the Kyoto Protocol (1997) and the Paris Agreement (2015).

In the latter, member countries commit to limiting the increase in global temperature to 1.5°C above pre-industrial levels by the end of the century, as well as achieving net zero emissions (a balance between the amount of greenhouse gases produced and the amount removed from the atmosphere) by 2050. Additionally, for the first time, the 17 Sustainable Development Goals (SDGs) are defined, which constitute a joint action plan for the 2030 agenda.

These agreements establish binding objectives for emission reduction and are complemented by regional measures, such as those implemented by the European Union. It is crucial to highlight that these measures not only obligate countries but also encourage investment in clean technologies and innovation. The implementation of these agreements is essential for achieving the SDGs, which address urgent social, economic, and environmental issues globally, providing a clear and coherent framework for action and fostering the development of sustainable solutions by businesses and institutions to combat climate change. The 17 SGDs are depicted in Figure 1.6.

Figure 1.6: SDG [30]

This Bachelor's thesis addresses key aspects of the following SDGs:

SDG7: Ensure access to affordable, reliable, sustainable, and modern energy.

While renewable energies already account for about 30% of energy consumption in the electricity sector, their widespread adoption in heating (10.4%) and transportation (4%) sectors remains a significant challenge [30].

SDG9: Industry, innovation, and infrastructure.

Economic progress, social well-being, and combating climate change largely depend on investment in infrastructure, sustainable industrial development, and technological advancement. In a context of rapid global economic transformation and increasing inequalities, sustained growth must be accompanied by industrialization that, on the one hand, makes opportunities accessible to all people and, on the other hand, is based on innovation and resilient infrastructure.

Investment in infrastructure - transportation, irrigation, energy, and information and communication technologies - is essential for achieving sustainable development and empowering communities in many countries. To achieve Sustainable Development Goal 9 (SDG 9) by 2030, it is essential to support least developed countries (LDCs), invest in advanced technologies, reduce carbon emissions, and increase access to mobile broadband.

CO_2 emissions related to energy reached a historic high of 36.8 billion metric tons in 2020. This alarming data underscores the urgent need to adopt cleaner and more sustainable alternative energy solutions [30].

In this context, the development of ammonia as an alternative fuel emerges as a promising opportunity. Ammonia would not only enable more sustainable growth in industrial and transportation sectors but, due to its easy production and management, could also be rapidly implemented in developing countries, driving their economic and social growth.

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

Climate change, an existential threat caused by human activities, jeopardizes life on Earth as we know it. The accelerated increase in greenhouse gas emissions is driving climate change at a much faster pace than anticipated, with devastating consequences including extreme weather events, changes in climate patterns, and rising sea levels. If urgent action is not taken to address climate change, the progress made in development over the past decades will be undermined. Mass migrations, social instability, and conflicts are just some of the serious repercussions expected [30].

Scientists warn that, if left unchecked, the effects of climate change could raise the global average temperature by over 3°C, with irreversible impacts on all of the planet's ecosystems. Biodiversity will be severely affected, food systems will collapse, and living conditions in many regions will become unsustainable.

In the face of this alarming situation, the development of technologies that enable the implementation of carbon-free energy systems, such as ammonia, emerges as an urgent necessity and one of the most effective measures to combat climate change.

The development of technology to use ammonia as a fuel could be a turning point in addressing these challenges, offering several compelling advantages:

- **Emission-free combustion:** Ammonia does not produce greenhouse gas emissions or local pollutants when burned, making it a sustainable alternative to fossil fuels [13].
- **Cost-effectiveness:** Ammonia is a relatively inexpensive and abundant fuel, making it economically attractive [13].
- **Simple production, transportation, and storage:** Ammonia is easy to produce, transport, and store, using infrastructure similar to natural gas [13].
- **Adaptability to existing systems:** Implementing ammonia as a fuel would require minimal modifications to existing heating and transportation systems, reducing transition costs [22].

In essence, harnessing ammonia as a fuel presents a unique opportunity to decarbonize heating and transportation sectors, paving the way for a more sustainable and efficient energy future. The transition to clean and sustainable energy systems is crucial to mitigate the effects of climate change and ensure the survival of our planet.

In the table below (1.1) is summarized the degree of the project's alignment with the Sustainable Development Goals (SDGs).

Sustainable Development Goals	**High**	**Medium**	**Low**	**Not Applicable**
1. No poverty.				X
2. Zero hunger.				X
3. Good health and well-being.				
4. Quality education.				X
5. Gender equality.				X
6. Clean water and sanitation.			X	
7. Affordable and clean energy.	X			
8. Decent work and economic growth.		X		
9. Industry, innovation, and infrastructure.	X			
10. Reduced inequalities.				X
11. Sustainable cities and communities.		X		
12. Responsible consumption and production.		X		
13. Climate action.	X			
14. Life below water.			X	
15. Life on land.			X	
16. Peace, justice, and strong institutions.				X
17. Partnerships for the goals.		X		

Table 1.1: Degree of Work Relation to the Sustainable Development Goals (SDGs)

1.4 State of the art

1.4.1 CMT institution

The **CMT (Clean Mobility & Thermofluids)** is a research centre located in Valencia, Spain, dedicated to the study and development of technologies related to clean mobility and thermofluids [11]. Its main focus is on seeking innovative solutions to reduce pollutant emissions and improve energy efficiency in transportation. The centre conducts research in areas such as electric propulsion, biofuels, thermal engine optimization, and computational simulation of transportation systems. The CMT collaborates closely with companies, academic institutions, and government agencies to drive technological advancement in the field of sustainable mobility and contribute to mitigating climate change.

1.4.2 CMT previous research

The Clean Mobility and Thermofluids centre (CMT) at the Universitat Politècnica de València (UPV) has conducted extensive research in the field of internal combustion engines, focusing particularly on **injection systems** and alternative fuels. Their work on **diesel injection systems** encompasses both **experimental** and **modeling** [42], [34], [36] approaches. Experimentally, CMT has investigated the intricacies of diesel injection, analyzing the behavior of **fuel sprays**, **atomization**, and **combustion processes** under various conditions. This experimental data has been critical in developing and validating advanced computational models that predict the performance and emissions of diesel engines with high accuracy.

In addition to diesel injection, CMT has been at the forefront of researching **ammonia as a potential fuel** for internal combustion engines. This line of investigation is more developed experimentally [33], [41]. The research involves studying its feasibility as a fuel. The findings from these experimental studies are paving the way for the development of cleaner and more sustainable engine technologies. The combined efforts in both diesel injection and ammonia research underscore CMT's commitment to advancing engine technology and contributing to a sustainable future in the automotive sector.

1.5 Structure of the document

This bachelor thesis consists of 3 documents:

- Document I: Report
- Document II: Specifications
- Document III: Budget

In order to facilitate the understanding and follow-up of the work carried out in the report, as well as the results derived from it, the document has been divided into 6 chapters.

Once the objectives and background of the thesis are established in **Chapter 1**, **Chapter 2** will provide the background for this work. It will cover the historical use of traditional fuels in internal combustion engines, as well as their properties that make them suitable for this type of energy generation system. Their limitations will also be addressed, especially regarding pollutant emissions, transitioning towards other potentially cleaner and more sustainable alternative fuels like hydrogen. However, the large-scale implementation of hydrogen as a fuel also has several problems that ammonia aims to mitigate. Additionally, the injection systems for internal combustion engines, their parts, functions, and components will be described.

Next, **Chapter 3** describes the methodology of the work. It explains the principles of fluid dynamics modeling and its potential. Additionally, the software to be used, GT-Power by Gamma Technologies, and the model previously developed by Payri [34], from which this work will be developed, are presented.

Chapter 4 focuses on studying the model, describing the initial tests, and how it was adapted to be used with ammonia. It includes a prior sensitivity analysis with diesel and the description of the properties assigned to the "ammonia" object that will serve as the fuel in the study.

Chapter 5 will present the results obtained and the insights that can be drawn from them. Finally, **Chapter 6** will discuss the conclusions of the project and future work in this field.

The **conditions document** outlines the specific requirements, standards, and constraints that need to be adhered to throughout the project. It provides detailed descriptions of the technical specifications, operational procedures, and regulatory compliances necessary to ensure the successful execution and reliability of the study.

The **budget document** provides a detailed financial plan for the project, listing all the expected costs and resources required. It includes an itemized breakdown of expenses such as equipment, software, personnel, and other operational costs, ensuring that all aspects of the project are adequately funded and financially managed.

Chapter 2

Background

2.1 Traditional Fuels

2.1.1 Historical Introduction

Internal combustion engines (ICEs) as we know them have more than a century of history [28]. For this reason, their mechanisms and operation are widely known and studied. The first antecedents of ICEs were the **steam engines** developed during the first Industrial Revolution in the 18th century . These were the first machines capable of producing non-natural mechanical energy [12] and share a main characteristic with current ICEs: being volumetric machines [7]. That is, the working fluid is contained in a delimited volume, which allows the fluid to be metered with precision.

Steam engines were practically the only known heat engines for almost two centuries. Although they coexisted with hot air engines, these did not represent a real commercial alternative [12]. Thanks to advances in the materials and mechanical devices used, steam engines were considerably perfected. However, the nature of the processes that allowed the obtaining of mechanical energy remained a mystery until well into the 19th century, when the work of the physicist Nicolas Léonard Sadi Carnot laid the foundations of a new scientific discipline: Thermodynamics[9].

The arrival of ICEs can be placed in 1876, with the first patent of the German Nicolaus Otto known as *"Gasmotor"* [12]. These machines quickly replaced steam engines due to their **lower weight**, **cost** and **greater ease of starting and stopping** . This first patent follows the line proposed a few years earlier by Alphonse Beau de Rochas, french engineer and becomes the first modern four-stroke engine, that is, it includes a pre-compression that significantly improves the performance of the machine. This led to the German couple Karl and Bertha Benz patenting the first car equipped with an ICE following this system in 1886.

Another key point in the history of ICEs was the presentation of the patent in 1893 and the subsequent prototype in 1897 of the engine of the German engineer Rudolf Christian Karl Diesel, which would later inherit his name [20].

Since then, these engines have undergone a great technological evolution in response to the needs of society. Initially, after World War II, the industry focused on improving performance, leaving fuel consumption in the background. However, from the oil crises of the 1970s onwards, the focus shifted to reducing fuel consumption. This trend was accentuated by the problem of air pollution, leading to the aspiration to develop smaller and more efficient engines.

2.1.2 Use and development of the traditional fuels: ICE systems

This section introduces internal combustion engines (ICEs), focusing on their internal functioning, various types, and the challenges associated with reducing pollutant emissions when used with traditional fuels. First, the basic concepts of combustion and the operational mechanisms of thermal engines will be covered. Then, the two primary ICE systems, spark-ignition and compression-ignition, will be analyzed.

Introduction to Engines and Combustion

An engine is a device that transforms any type of energy into mechanical energy. A **thermal engine** obtains energy from a compressible fluid (chemical energy stored in matter). This chemical energy can be released and harnessed through an additional process such as combustion [12].

Combustion engines can be **external** combustion (occurring outside the working fluid) or **internal** combustion (where the working fluid itself undergoes the process) [12]. Often, in the latter case, the working fluid is a mixture of air and fuel.

Fundamentals of Combustion

Combustion is the core of any internal combustion engine (ICE): it is a self-sustained and exothermic reaction between a **fuel** and an **oxidizer** (usually oxygen in the air) that releases heat and light. [28] In the context of ICEs, efficient and clean combustion is crucial for optimal performance and minimizing environmental impact.

There are two main types of combustion based on how the fuel and air interact: **premixed flames** and **diffusion flames** [12]. In premixed flames, the fuel and air mix before entering the combustion chamber. Spark-ignition engines (SI engines) rely on this type of combustion. In contrast, in diffusion flames, the fuel is directly injected into the cylinder containing compressed air, and mixing occurs as the fuel burns. Compression-ignition engines (CI engines) use diffusion flames.

The **air-fuel ratio** is a crucial parameter that significantly influences the operation of both types of engines. It represents the proportion of air and fuel in the mixture. An ideal or stoichiometric ratio ensures complete combustion, converting all the fuel and oxygen into products like water vapor and carbon dioxide [28]. However, in real conditions, engines often operate with lean (excess air) or rich (excess fuel) mixtures to optimize performance or minimize specific emissions [12].

Flammability limits define the range of air-fuel ratios within which combustion can occur for each combustible substance under certain pressure and temperature conditions [28]. There are two limits: a lower flammability limit (LFL) and an upper flammability limit (UFL) between which a flame can form and propagate. If the mixture is too lean (too much air), ignition becomes difficult, or the initiated reaction cannot sustain itself, causing the flame to extinguish. Conversely, a rich mixture (too much fuel) can lead to incomplete combustion, resulting in fuel wastage and increased emissions (inefficiency).

Internal Combustion Engine's Strokes

There are two main types of ICEs based on the number of strokes (up-and-down movements) of the piston required to complete one cycle of combustion and their functioning is similar.

Four-stroke engines complete one combustion cycle in four strokes of the piston [12]. Each stroke has a distinct function 2.1:

- **Intake**: The piston moves down, drawing the fuel-air mixture into the cylinder through an open intake valve.
- **Compression**: The intake valve closes, and the piston moves up, compressing the fuel-air mixture.
- **Power**: The spark plug ignites the compressed fuel-air mixture, generating hot gases that push the piston down, creating power.
- **Exhaust**: The exhaust valve opens, and the piston moves up, pushing the spent exhaust gases out of the cylinder.

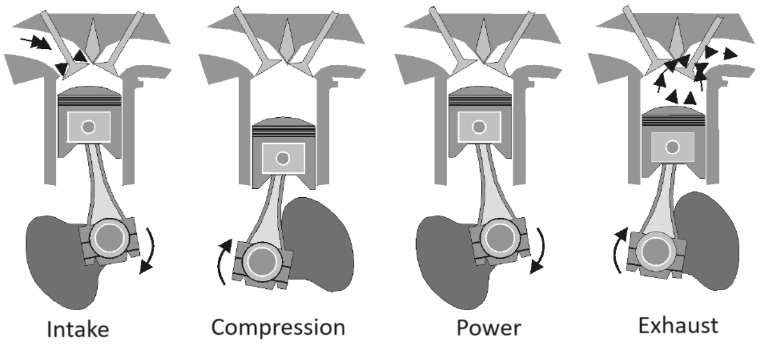


Figure 2.1: 4-strokes engine

Two-stroke engines (in figure 2.2), on the other hand, complete one combustion cycle in two strokes of the piston. During the first stroke, the intake and compression processes occur. The fuel-air mixture is drawn into the cylinder as the piston moves up, and then the mixture is compressed as the piston moves down. The second stroke involves power and exhaust processes. Ignition of the compressed fuel-air mixture generates hot gases that push the piston down, producing power. Simultaneously, the exhaust gases from the previous cycle are pushed out of the cylinder [28]. Both two-stroke and four-stroke engines have their own advantages and disadvantages, making them suitable for different applications. Two-stroke engines are generally simpler, lighter, and more powerful for their size, but they are also less fuel-efficient and produce more emissions. Four-stroke engines are more complex and heavier, but they are generally more fuel-efficient, cleaner, and quieter [28].

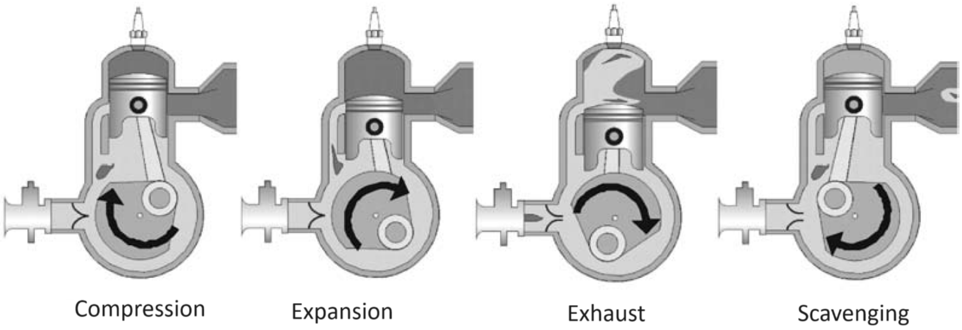


Figure 2.2: 2-strokes engine

Internal Combustion Engine Systems: Spark-Ignition Engines and Compression-Ignition Engines

An internal combustion engine (ICE) is a type of engine where the combustion of the air-fuel mixture occurs within the engine cylinder. This process generates hot gases at high pressure, which expand, moving pistons or other mechanical components, generating power.

ICEs are widely used in cars, motorcycles, aircraft, and power generation systems. They are mainly classified into two types: spark-ignition engines (SI engines), which use a spark plug to ignite the fuel, and compression-ignition engines (CI engines), which rely on the heat produced by compressed air to ignite the fuel [12].

a. Spark-Ignition Engines (SI Engines)

These engines use a spark plug to ignite a pre-mixed air-fuel mixture. They usually run on gasoline and are known for their smooth operation. However, they tend to have lower efficiency compared to compression-ignition engines. Factors such as flame propagation speed and ignition timing significantly impact the performance and emissions in SI engines [28].

b. Compression-Ignition Engines (CI Engines)

Unlike SI engines, CI engines rely on the auto-ignition of the fuel due to the high temperatures and pressures created during the compression stroke. These engines typically use diesel fuel and are known for their durability and higher efficiency [12]. However, they can be noisier and emit more pollutants compared to SI engines. CI engines require high compression ratios and precise fuel injection for optimal performance [28]. The fuel needs to be injected late in the compression process to avoid pre-ignition, and the injection system must ensure proper atomization for efficient combustion [12].

Pollutant Emissions in ICEs

The combustion process in ICEs inevitably generates pollutants such as nitrogen oxides (NO_x), hydrocarbons (HC), and carbon monoxide (CO) [12]. These pollutants contribute to air pollution and have adverse impacts on health and the environment.

To address these issues, engineers are constantly innovating and developing cleaner combustion technologies. Some strategies include:

- **Optimization of Combustion Processes:** Improving air-fuel mixing, injection techniques, and ignition timing can lead to more complete combustion, reducing unburned hydrocarbons and CO emissions [28].
- **Lean-Burn Engines:** Operating engines with leaner air-fuel mixtures can help reduce NO_x formation. However, careful optimization is needed as this can lead to other issues like higher HC emissions [28].
- **Exhaust Gas Aftertreatment Systems:** Systems such as catalytic converters and diesel particulate filters can capture and reduce pollutants in exhaust gases after combustion [12].

2.1.3 Fuels and their properties

The development of fuels has progressed alongside engines, adapting to market needs, social and economic changes, and a growing environmental awareness. Fuels are substances that react exothermically with oxygen, converting the energy of their molecular structure into thermal energy. They are classified into **solids**, **liquids**, and **gases** [12] The most usual fuels can be found in figures 2.3, 2.4. However alternative internal combustion engines (ICEs) rely on liquid or gaseous fuels because of their high reaction speed. Nonetheless, some studies suggest that solid fuels could be used if they are finely pulverized [38].

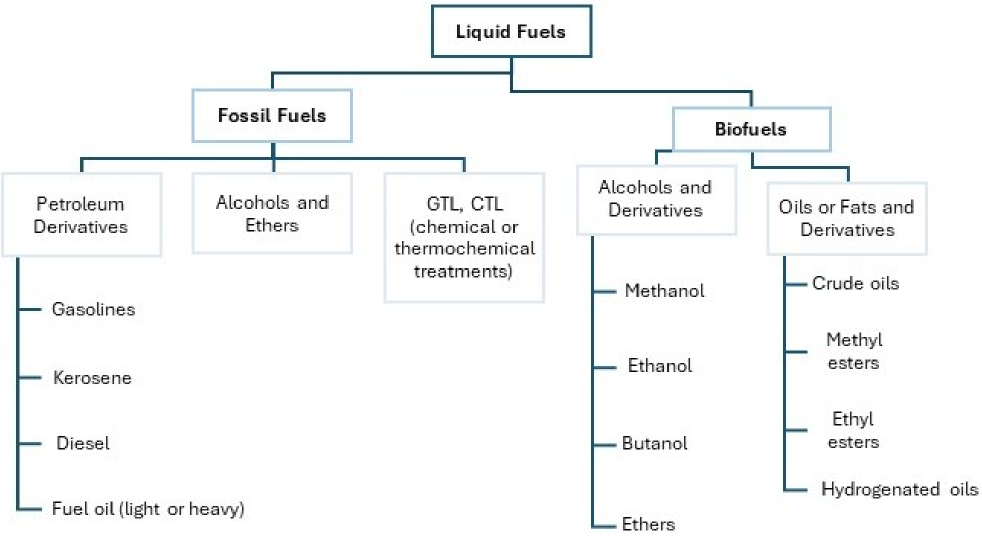


Figure 2.3: Classification of most common liquid fuels [12]

Physicochemical Properties

The fuels commonly used in alternative engines are liquid fuels, which are easier to store, and derived from petroleum, thus being fossil fuels. Gasoline, used in spark-ignition engines (SI), and diesel, used in compression-ignition engines (CI), are the main refined products from oil companies. Their **ease of storage** under ambient conditions and **high**

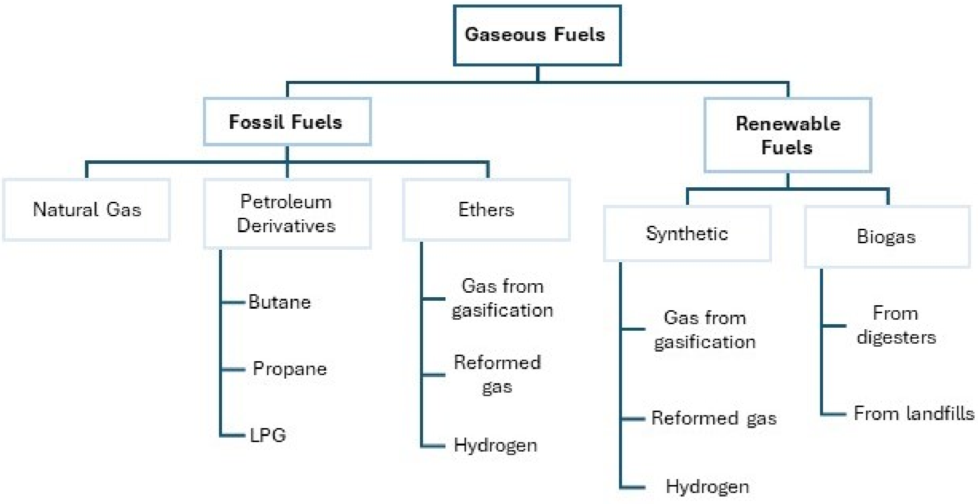


Figure 2.4: Classification of most common gaseous fuels [12]

energy density provide engines with great autonomy and simplicity in their fuel systems, but require systems that facilitate their evaporation and mixing with the oxidant, as **combustion takes place in the gaseous phase**. Gaseous fuels, although they mix homogeneously and burn with lower emissions, have a high specific volume that makes storage difficult and reduces autonomy, generally ruling them out for long-distance transportation [28].

Looking to the future, hydrogen is considered a potential energy vector, although its technological and industrial implementation is still far off, as already discussed [29]. Meanwhile, biofuels, despite being subject to strict quality and sustainability limitations, are gradually gaining prominence [4], but they do not yet represent a strong competition against traditional petroleum-derived fuels [12]. For this reason, ammonia presents itself as a potential candidate to replace these fuels [8].

a. Density

Density is the magnitude that expresses the relationship between the mass and volume of a substance [39]. It varies with pressure and temperature. The density of the fuel is an important factor in internal combustion engines because it determines the amount of energy that can be stored in a given volume of fuel. A denser fuel contains more energy per unit volume, meaning less fuel is needed to generate the same amount of energy. However, a denser fuel can be more difficult to atomize, affecting injection, which can impact dosing and, in many cases, have a higher boiling point, making vaporization and thus combustion more difficult. European density specifications are between **720 and 775 kg/m^3 for gasoline**, **820 and 845 kg/m^3 for diesel**, and **860 and 900 kg/m^3 for biodiesel**, limiting gasoline-ethanol and diesel-biodiesel blends [12].

b. Viscosity

Viscosity is the property of fluids that characterizes their resistance to flow due to friction between their molecules [39]. Dynamic viscosity refers to the resistance of a fluid to flow when an external force is applied and is measured in pascal-seconds ($Pa \cdot s$) and kinematic viscosity is calculated by dividing the dynamic viscosity by the density of the fluid and is expressed in square meters per second (m/s) [47]. The latter should be low to avoid pressure losses, but in fuels like diesel and fuel oil, it must be sufficient to meet lubrication requirements [12]. Some of the most common fuel's densities and viscosities are presented in figure 2.1.

Table 2.1: Most common fuels' densities and kinematic viscosities [12]

Fuel	**ρ (kg/m^3) at 15°C**	**ν (cSt) at 40°C**	**Fuel**	**ρ (kg/m^3) at 15°C**	**ν (cSt) at 40°C**
Methanol	791.3	0.58	Kerosene	775-840	1.8*
Ethanol	789.4	1.13	Diesel	820-845	2-4.5
Butanol	809.7	2.22	Fuel oil	920-950	100-1000
MTBE	745	0.48	BioDiesel (FAME)	860-900	3.5-5
ETBE	747	0.54	Fischer-Tropsch Diesel	770-800	2-4.5
Gasoline	720-775	0.65	n-Dodecane	750	0.36
Hydrogen (liquid)	70.85	0.0161	Hydrogen (gas)	0.08988	0.0089
Ammonia (liquid)	682	0.326	Ammonia (gas)	0.73	0.25

**Typical value (ASTM D1655 standard requires < 8 cSt at -20°C)*

c. Flammability

Fuel flammability plays a fundamental role in the efficient, clean, and safe operation of internal combustion engines. This property determines the ease with which the fuel ignites and the combustion rate, directly influencing engine performance and efficiency. Some of the parameters used to characterize it are **flammability limits** (already mentioned), **flash point**, **autoignition temperature**, **octane number (ON)**, **methane number (MN)**, and **cetane number (CN)**.

Adequate flammability is essential for initiating and maintaining combustion within the engine cylinder. However, incomplete combustion due to poor flammability can generate unburned residues, such as soot and carbon monoxide, reducing engine efficiency and increasing pollutant emissions. It is also important to consider fuel flammability in terms of safety. An overly flammable fuel can pose fire and explosion risks, especially in the event of leaks or spills [28] (See figure 2.8).

Table 2.2: Most common fuels' flammability limits with air [12]

Fuel	**Li**	**Stequiometric**	**Ls**
Methane	34.4	17.3	10.3
Methanol	12.6	6.5	1.6
Ethanol	18.5	9.0	2.7
Propane	30.7	15.7	5.9
Gasoline	18.2	14.6	3.1
Hydrogen	348.0	34.5	4.8
Ammonia	9.64	6.1	4.7

d.Volatility

Volatility is a property that allows substances to change from liquid to gas and disperse into the environment. It is determined by the distillation curve. Volatility influences cold starts and the formation of pollutants [12]. In engines' cold starts, a highly volatile fuel evaporates easily at low temperatures, allowing for an adequate air-fuel mixture to initiate combustion and start the engine without difficulty.

Volatility also affects fuel atomization and mixing within the engine cylinder. A highly volatile fuel atomizes easily into small droplets, promoting a homogeneous mixture with air and efficient combustion. However, a highly volatile fuel can also increase losses during storage, tank filling, and engine operation, especially in hot climates. This can generate emissions of unburned hydrocarbons and affect the economic efficiency of the engine or be dangerous by generating flammable vapours that increase the risk of fires and explosions [28].

e. Stability

Stability is the resistance to degradation during storage, crucial for fuel quality [12]. An unstable fuel can degrade over time, forming deposits, gums, and sediments that can clog injectors, filters, and other parts of the fuel system. This can affect fuel atomization, air-fuel mixture, combustion, and safety, ultimately reducing engine power and efficiency. Fuel stability and flammability are also linked to its **impurity content**, which can include sulfur, water, free fatty acids, glycerin, metals, and solid particles, with the risks already described [12].

f. Energy density

Energy density, specific energy, and volumetric energy density are key metrics used to evaluate the performance of fuels. **Energy density** refers to the amount of energy stored in a given system or region of space per unit volume [32]. It is a measure of how much energy can be stored in a fuel within a specific volume and is often expressed in megajoules per liter (MJ/L). **Specific energy**, also known as gravimetric energy density, is the amount of energy per unit mass of the fuel, typically expressed in megajoules per kilogram (MJ/kg) [32]. This metric indicates how much energy can be obtained from a fuel per unit of weight, making it crucial for applications where weight is a critical factor, such as portable energy sources (see figure 2.5).

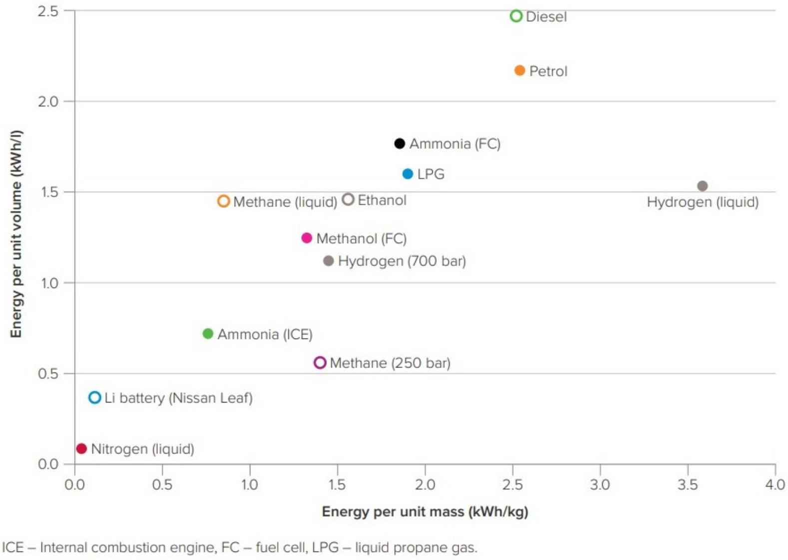


Figure 2.5: Specific energy and energy density for fuels [44]

Volumetric energy density combines these two concepts by evaluating how much energy can be stored per unit volume and per unit mass (see figure 2.6), providing a comprehensive assessment of a fuel's energy efficiency and storage requirements [32]. These metrics are essential for comparing different fuels and determining their suitability for various applications, taking into account factors such as storage space, weight limitations, and energy output.

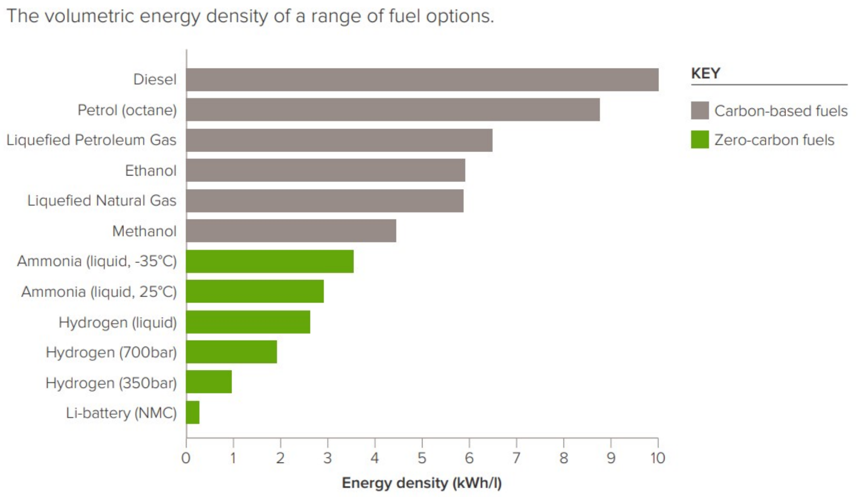


Figure 2.6: Volumetric energy density of different fuels

Thermochemistry of Combustion

Understanding the combustion process involves assessing various fundamental concepts, including Calorific Value, Air-to-Fuel ratio, Intake Pressure, and the relationship between Power and Efficiency in different engine types.

a. Heating Value

The Heat of Combustion or Heating Value (HV) of a fuel is defined as the heat energy released during the **stoichiometric combustion** of a unit mass of fuel, maintaining the burned products under the same temperature and pressure conditions as the initial reactants [12]. It's important to distinguish between the **High Heating Value (HHV)** and **Lower Heating Value (LHV)** (see figure 2.3). HHV is obtained when products and reactants are in standard conditions, with condensed water and its latent heat of vaporization released, while LHV considers water in the products in vapor phase. The choice between these values depends on the context and the need for a more accurate measurement of the fuel's energy content [28].

Table 2.3: Most common fuels' Heating Values [12]

Fuel	HHV (kJ/kg)	LHV (kJ/kg)	Fuel	HHV (kJ/kg)	LHV (kJ/kg)
Ammonia	22 500	18 600	Diesel	45 000	42 400
Methanol	22 884	20 094	Gasoline	46 500	43 400
Ethanol	29 847	26 952	Butane	49 210	45 277
Butanol	36 020	33 090	GLP	50 152	46 607
MTBE	37 957	35 108	Propane	50 325	46 334
ETBE	39 247	36 315	Methane	55 522	50 032
BioDiesel (FAME)	40 170	37 530	Hydrogen	1 421 180	120 210

b. Air-fuel ratio

Stoichiometry is essential in determining the quantitative relationships between reactants and products in combustion [12]. In an ideal process, with sufficient oxygen available, fuel components can be completely oxidized into carbon dioxide and water. Studying stoichiometric air-to-fuel ratio, concerning stoichiometric combustion process with air, allows understanding the efficiency and the amount of fuel required for complete combustion.

c. Power and Efficiency
Power in an engine refers to the amount of work it can perform in a specific time period, commonly expressed in watts (W). Power is a measure of the engine's capacity to convert the chemical energy of fuel into useful mechanical work. Efficiency, on the other hand, refers to the efficiency with which the engine converts the chemical energy of fuel into useful mechanical work. It's calculated as the ratio between the useful power produced by the engine and the total energy contained in the consumed fuel; typically expressed as a percentage.

The distinctive characteristics in the mixture formation (i.e., how fuel and air are mixed before ignition) between spark ignition engines (SI) and compression ignition engines (CI) present particular challenges specific to each engine type. SI engines can burn more fuel with the same mass of admitted air by mixing before entering the combustion chamber, allowing them to produce more work per cycle, translating into higher specific power. Additionally, the flexibility in mixture formation allows SI engines to operate at higher speeds than CI engines, contributing to their ability to generate more power. On the other hand, in terms of efficiency, CI engines tend to have higher performance by compressing the air before fuel injection according to the amount of injected fuel [12]. Therefore, although both concepts are linked, they are not equivalent.

2.1.4 Issues and Limitations of the Use of Traditional Fuels

Emissions from Internal Combustion Engines (ICEs)

Swedish Nobel laureate Svante Arrhenius was a pioneer in theorizing the impact of carbon dioxide (CO_2) on Earth's climate back in 1896 [5]. However, these ideas faced initial criticism and faded from public consciousness until the 1950s.

Growing environmental concerns and advancements in analytical methods rekindled interest in greenhouse gases after the 1950s. While initially pursued by isolated research groups, a growing body of studies emerged, pointing towards a link between global warming and human-caused (anthropogenic) emissions of greenhouse gases [37].

Internal combustion engines (ICEs) are a significant source of high emissions due to the combustion of fossil fuels. Every combustion process is associated with an environmental pollution problem and the combustion process in ICEs involves burning a mixture of fuel and air, which leads to the formation of various pollutants that will be depicted next. As the demand for automotive transportation has increased, so has the emission of these pollutants, contributing to a variety of environmental issues [6].

While all energy sources emit greenhouse gases, fossil fuels are the biggest culprits. Their high emission rates, combined with our heavy reliance on them (86% of our energy comes from fossil fuels), are a major driver of rampant CO_2 emissions [17].

The surge in automobile usage gave rise to a new type of air pollution, characterized by the presence of unburned or partially burned hydrocarbons (HC) and nitrogen oxides

(NO_x) emitted from vehicle exhaust fumes. These pollutants, when exposed to sunlight, undergo photochemical reactions, generating tropospheric ozone and peroxyacetyl nitrates. These compounds, along with nitrogen dioxide (NO_2), form a yellowish-brown cloud that irritates the eyes and respiratory tract, commonly known as photochemical smog [12]. This phenomenon became prevalent in cities like Los Angeles during the 1950s, sparking public concern about the pollutants emitted by combustion systems. Today, a significant portion of industrial budgets is dedicated to mitigating environmental impact, driven by both product regulations and inspections of industrial facilities [37].

Fossil Fuels: Non-Renewable and Depleting

One of the critical issues with traditional fuels is that they are non-renewable. Fossil fuels, such as oil, coal, and natural gas, are finite resources formed over millions of years. Oil's finite nature and the difficulty of accurately assessing reserves raise concerns about its long-term availability, as shown by production limitations in any given area [3]. Their continued use not only depletes these resources but also poses significant environmental and economic risks.

Oil reigns supreme as the modern world's energy source, supplying roughly 40% of global needs and fueling nearly all transportation systems (oil consumption increased by 5.3 million barrels per day (b/d) in 2021)[6]. Notably, the transportation sector alone consumes around 60% of this oil: a majority of the consumption growth came from gasoline (1.8 million b/d) and diesel/gasoil (1.3 million b/d)[6]. While a diverse range of alternative transport fuels exist, many haven't reached widespread adoption [3].

The term "**energy transition**" refers to a fundamental change in how we approach energy. It involves moving away from fossil fuels and embracing renewable energy sources. This shift is driven by the need for a sustainable energy system that is both environmentally friendly and economically viable [27]. Mitigating CO_2 emissions is a central pillar of the energy transition [21]. This broader goal encompasses several key objectives:

- **Developing sustainable energy systems**: This involves building infrastructure and technologies that rely on clean and renewable energy sources.
- **Ensuring access to clean energy**: Everyone should have access to reliable and affordable clean energy.
- **Enhancing energy security**: A diversified energy mix reduces reliance on any single fuel source, improving overall energy security.
- **Combating climate change**: Reducing greenhouse gas emissions is crucial to mitigate the effects of climate change (cite: sustainablefuture).
- **Protecting food chain systems**: Climate change can disrupt food production and distribution, making a sustainable energy system vital for food security.

Several countries have implemented or promoted the use of alternatives like natural gas-based fuels, biofuels, ethanol, and methanol. However, these can still contribute to climate change, and further technological advancements are needed to mitigate their negative environmental impacts. Electric, solar, and hydrogen hold promise for powering vehicles, but the upfront costs of these fuels or their associated technologies remain a significant barrier.

Biodiesel holds promise as a renewable fuel source that can reduce dependence on fossil

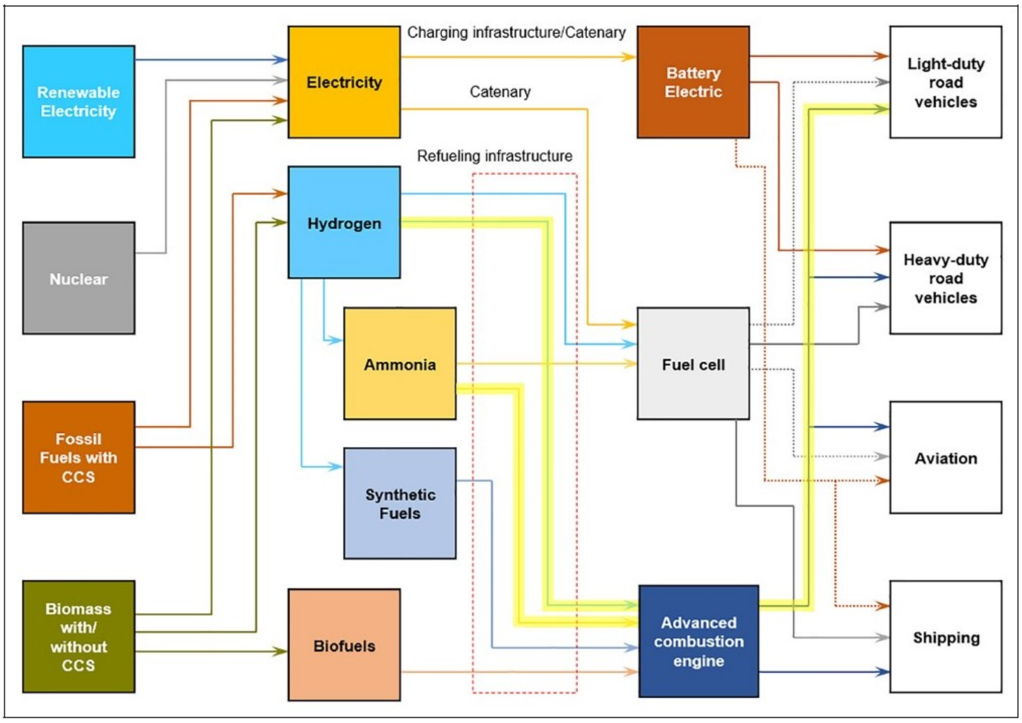


Figure 2.7: The energy pathway towards a net zero carbon mobility scenario [31]

fuels. However, its environmental impact is complex. While it may reduce greenhouse gas emissions from vehicles, its production can strain resources like water and land. In some cases, clearing land for biodiesel crops can even worsen emissions by releasing stored carbon. Additionally, competition between food and fuel crops for land can raise food prices. Therefore, careful consideration is needed to ensure biodiesel production is truly sustainable [24].

The potential of hydrogen as a viable long-term transport has been explored [14] but establishing a hydrogen economy presents sizable scientific and technological hurdles across production, delivery, storage, conversion, and end-use [29].

To address the limitations of traditional fuels, a transition to carbon-free alternatives such as hydrogen and ammonia emerges as the most sensible option (see figure 2.7. These fuels do not contain carbon and therefore do not produce CO2, CO, or HCs when burned.

2.2 New carbon-free fuels

2.2.1 Hydrogen

Characteristics and Properties

Hydrogen, the most abundant element in the universe, exhibits several key characteristics that make it a **promising carbon-neutral fuel** (see figure 2.9). To begin with, its **high diffusivity** [8] allows hydrogen molecules to spread and mix quickly with air, facilitating more uniform and efficient combustion. This property is crucial for ensuring that the fuel **burns completely** and **reduces the formation of harmful emissions**. Additionally, hydrogen's **broad flammability range** (as it can be seen in the figure2.8 below) [13], spanning 4-75% by volume, enables it to ignite and sustain combustion across a wide variety of air-fuel mixtures, enhancing its suitability for different engine designs and operating conditions. Moreover, hydrogen has a **high flame speed** [13], meaning it burns quickly once ignited. This rapid combustion can improve engine efficiency by ensuring that the fuel is burned completely, which is particularly beneficial in high-performance applications. On top of that, hydrogen boasts a **high energy content per unit mass**, at 120.1 MJ/kg [31], significantly higher than other fuels. This high energy density means that hydrogen can provide more energy for a given weight, enhancing the efficiency and performance of fuel systems that utilize it.

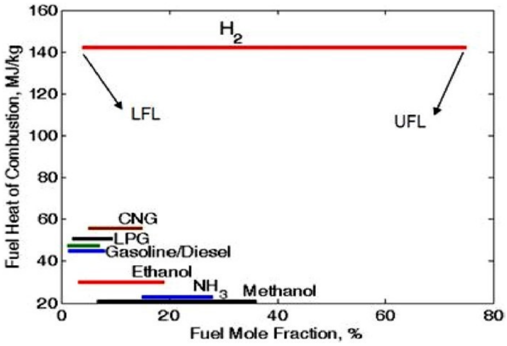


Figure 2.8: Low and upper flammability limits of various substance [15]

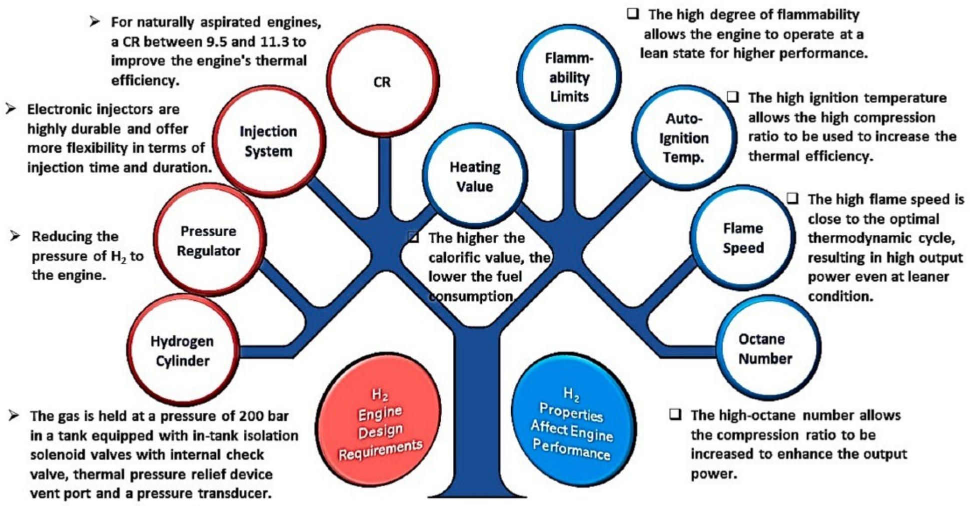
Furthermore, hydrogen's **high octane number** of 130 [13] indicates its resistance to knocking, which is the premature ignition of the fuel-air mixture in the engine. A higher octane number allows engines to operate at higher compression ratios, improving thermal efficiency and overall engine performance. One of hydrogen's most significant advantages as a fuel is that, **when burned, it produces no carbon emissions**, only water vapor. This characteristic is critically important in the context of reducing greenhouse gas emissions and combating climate change.

Additionally, hydrogen has a **lower ignition energy** of 0.02 MJ [13] compared to conventional fuels, which implies that hydrogen can ignite more easily and at lower energy inputs. This enhances the efficiency of the combustion process and reduces the production of nitrogen oxides (NO_x) generated at high temperatures.

Limitations

Hydrogen, despite its promising characteristics, presents several limitations that complicate its widespread adoption as a fuel. One significant challenge is its **fast burn rate**, which can lead to issues such as **pre-ignition**, **backfire**, and **knocking** [13]. **Pre-ignition** occurs when the hydrogen-air mixture ignites before the intended ignition point, while **backfire** refers to the ignition of the mixture outside the combustion chamber. **Knocking** is the result of uncontrolled ignition within the engine. These phenomena can cause severe damage to engine components, reduce performance, and pose significant challenges for maintaining combustion stability.

Additionally, hydrogen **storage** is both complex and costly. Hydrogen must be stored either under high-pressure conditions (350-700 bar) [13] or at cryogenic temperatures (below



- For naturally aspirated engines, a CR between 9.5 and 11.3 to improve the engine's thermal efficiency.
- Electronic injectors are highly durable and offer more flexibility in terms of injection time and duration.
- Reducing the pressure of H_2 to the engine.
- The gas is held at a pressure of 200 bar in a tank equipped with in-tank isolation solenoid valves with internal check valve, thermal pressure relief device vent port and a pressure transducer.

☐ The higher the calorific value, the lower the fuel consumption.

☐ The high degree of flammability allows the engine to operate at a lean state for higher performance.

☐ The high ignition temperature allows the high compression ratio to be used to increase the thermal efficiency.

☐ The high flame speed is close to the optimal thermodynamic cycle, resulting in high output power even at leaner condition.

☐ The high-octane number allows the compression ratio to be increased to enhance the output power.

Figure 2.9: Hydrogen Properties and their influence on engine performance and design requirements [13]

-252.9°C [31] to achieve a practical energy density. High-pressure storage requires robust and expensive containment systems to withstand the pressure, while cryogenic storage demands sophisticated insulation and refrigeration systems to maintain the extremely low temperatures. Both methods present significant technical and economic hurdles, making storage a major challenge for hydrogen fuel adoption [8].

Safety concerns are also paramount with hydrogen. Due to its highly flammable nature, hydrogen requires stringent safety measures during handling and storage to prevent accidents [13]. Even small leaks can lead to explosive mixtures when hydrogen mixes with air, and its small molecular size makes it prone to leakage through materials that might contain other gases more effectively. These safety considerations necessitate careful design and monitoring of hydrogen storage and distribution systems.

Moreover, the **production of hydrogen**, particularly through water electrolysis, is **energy-intensive** and **expensive** [13]. Electrolysis involves splitting water into hydrogen and oxygen using electricity, often derived from renewable sources. While this method produces green hydrogen with no direct emissions, it requires a substantial amount of energy, making it less economically feasible for large-scale production compared to other energy carriers. This high energy demand also contributes to the overall cost, limiting the feasibility of hydrogen as a large-scale solution for meeting global energy needs.

To address these limitations, hydrogen is often utilized in a **dual-fuel configuration**, where it is blended with diesel or other fuels. [8].

2.2.2 Alternatives to Hydrogen

Other alternative fuels such as **methanol**, **ethanol**, and **biodiesel** [24] offer various benefits, including reducing greenhouse gas emissions and improving engine performance. Methanol and ethanol, both alcohol-based fuels, for instance, have higher octane ratings than conventional gasoline [46] , [23] (allowing higher compression ratios and more efficient combustion) while **biodiesel** contributes to a reduction in lifecycle greenhouse gas emissions since the carbon dioxide released during combustion is offset by the CO2 absorbed by the plants used to produce the oil feedstock [10].

Methanol (CH_3OH) is a simple alcohol that can be produced from natural gas, coal, renewable resources like biomass or even from CO_2 and renewable hydrogen. It burns cleaner than gasoline, producing fewer emissions of harmful pollutants such as NO_x, particulate matter, and volatile organic compounds (VOCs) [46],[23] . **Ethanol** (C_2H_5OH) is commonly produced from biomass, including corn, sugarcane, and cellulosic materials. Ethanol-blended fuels, such as E10 (10% ethanol) and E85 (85% ethanol), are widely used and help reduce greenhouse gas emissions by displacing a portion of the fossil fuels with renewable content. Additionally, ethanol's combustion properties lead to cleaner exhaust emissions, contributing to better air quality [23].

2.2.3 Ammonia

Characteristics and Properties

Table 2.4: Ammonia's combustion characteristics compared to other fuels, 300K at 100kPa [45]

Property	**Methane (CH_4)**	**Hydrogen (H_2)**	**Methanol (CH_3OH)**	**Ammonia (NH_3)**
Density (kg/m^3)	0.66	0.08	786	0.73
Dynamic viscosity $\times 10^{-5}$ (P)	11.0	8.80	594	9.90
Low heating value (MJ/kg)	50.05	120.00	19.92	18.80
Laminar burning velocity (m/s) - close to stoich.	0.38	3.51	0.36	0.07
Minimum ignition energy (mJ)	0.280	0.011	0.140	8.000
Auto-ignition temperature (K)	859	773-850	712	930
Octane number	120	-	119	130
Adiabatic flame temperature (with air) (K)	2223	2483	1910	1850
Heat capacity ratio, γ	1.32	1.41	1.20	1.32
Gravimetric Hydrogen density (wt%)	25.0	100.0	12.5	17.8

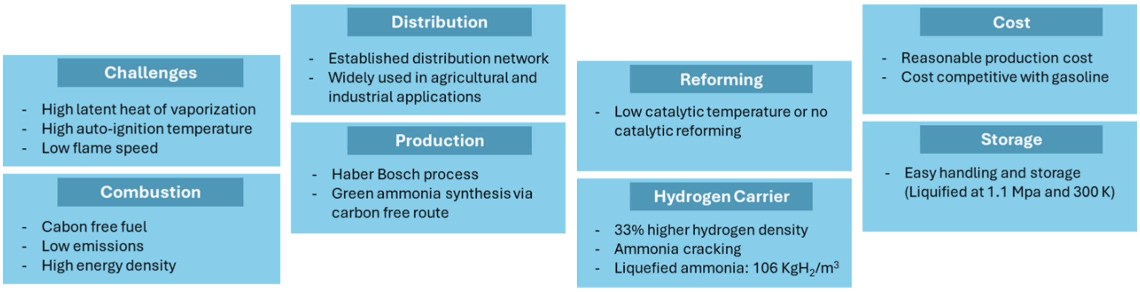
Ammonia (NH_3) is a colourless gas [8], increasingly recognized for its potential as an alternative fuel (see figure 2.4 below). It has a **density** of approximately **0.73 kg/m^3** at standard temperature and pressure (STP) [13], making it **less dense than air**. Its **boiling point is -33.59°C** [26], meaning it readily evaporates at room temperature. Additionally, its **low viscosity** [40] allows ammonia to flow easily through pipelines and injectors, facilitating its transport and distribution.

Ammonia has an **energy density of 18.6 MJ/kg and 11.2 MJ/L in liquid form** [31]. This energy density is higher than that of hydrogen but lower than conventional hydrocarbon fuels such as gasoline and diesel. The **higher energy density compared to hydrogen** [13] makes ammonia a more efficient fuel in terms of storage and transportation. It can store more energy per unit volume, which is advantageous for applications where space and weight are critical factors. The main characteristics of ammonia as a fuel in ICEs are summarized in figure 2.10.

Limitations

i. Combustion Properties

Ammonia has a **high auto-ignition temperature of 651°C** [31] (ammonia requires more energy to ignite compared to conventional fuels) and a **low flame speed** [13] (slower and less efficient combustion, which can lead to incomplete burning), ranging from 0.32 to 0.40 m/s [7]. These characteristics make it **difficult to achieve stable and efficient combustion**. To overcome these challenges, advanced combustion strategies are required, such as **optimizing the air-fuel mixture** and **improving ignition systems**.



Challenges
- High latent heat of vaporization
- High auto-ignition temperature
- Low flame speed

Combustion
- Cabon free fuel
- Low emissions
- High energy density

Distribution
- Established distribution network
- Widely used in agricultural and industrial applications

Production
- Haber Bosch process
- Green ammonia synthesis via carbon free route

Reforming
- Low catalytic temperature or no catalytic reforming

Hydrogen Carrier
- 33% higher hydrogen density
- Ammonia cracking
- Liquefied ammonia: 106 KgH_2/m^3

Cost
- Reasonable production cost
- Cost competitive with gasoline

Storage
- Easy handling and storage (Liquified at 1.1 Mpa and 300 K)

Figure 2.10: Characteristics of ammonia as a fuel in internal combustion engines [13]

ii. Storage and safety

Storing ammonia is more straightforward than storing hydrogen, as it can be kept **in liquid form at relatively low pressures around 10 bar** [13]. However, ammonia is **highly toxic** and **corrosive** [23], which necessitates specially designed storage tanks and handling protocols. These tanks must be constructed from materials that can resist ammonia's corrosive effects to prevent leaks and maintain structural integrity over time.

The **toxicity** of ammonia is a significant concern, as exposure to concentrations above **150-300 parts per million (ppm)** can cause severe health issues, including respiratory problems and chemical burns [13]. Ammonia's pungent odor acts as an effective early warning for leaks, as it is detectable at very low concentrations. However, this is not sufficient to mitigate the risks associated with its use [19].

iii. Production

The predominant method for producing ammonia is the **Haber-Bosch process** (see figure 2.11 below) [19], which involves the **catalytic reaction of hydrogen and nitrogen at high temperature and pressure**. This process, known as **brown ammonia production** [44], is highly energy-intensive, consuming 8 MWh of energy per tonne of ammonia. Most of this energy consumption, and approximately 90% of the associated carbon emissions, are attributed to hydrogen production. Hydrogen is typically generated via steam reforming of natural gas, coal, heavy fuel oil, or naphtha, all of which contribute significantly to the carbon footprint of ammonia production [19].

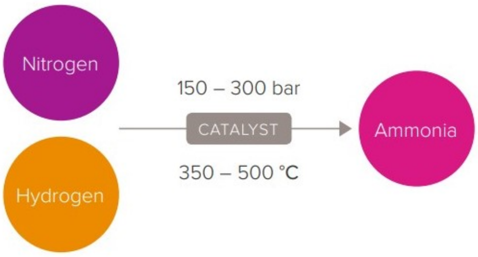


Figure 2.11: Schematic of the Haber-Bosch ammonia synthesis reaction [44]

To mitigate the environmental impact, **blue ammonia production** employs the same Haber-Bosch process but incorporates carbon capture and storage (CCS) to reduce emissions. Steam methane reforming with CCS can capture up to 90% of carbon dioxide emissions [44], though overall lifecycle emission reductions are limited to 60-85% [44] due to upstream emissions from natural gas extraction.

Green ammonia production represents the most sustainable approach [44, 19], using renewable electricity to power the electrolysis of water, thereby generating hydrogen without carbon emissions. This hydrogen is then combined with nitrogen in the Haber-Bosch process, as shown in scheme 2.13. The main challenge for green ammonia lies in the cost [19], particularly the high cost of electricity. However, regions with abundant renewable energy resources can potentially achieve cost-competitive green ammonia production [44]. Ongoing research aims to improve the efficiency and reduce the costs of green ammonia production through the development of more active catalysts for the Haber-Bosch process, enhanced ammonia separation methods, and exploration of novel production techniques such as biological nitrogen fixation, electrochemical production, and chemical looping processes [44].

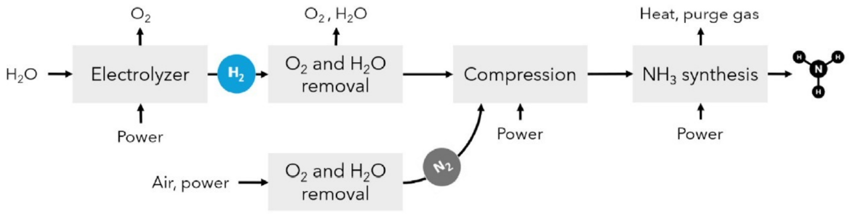


Figure 2.12: Schematic green ammonia synthesis combined with electrolysis-based hydrogen production [8]

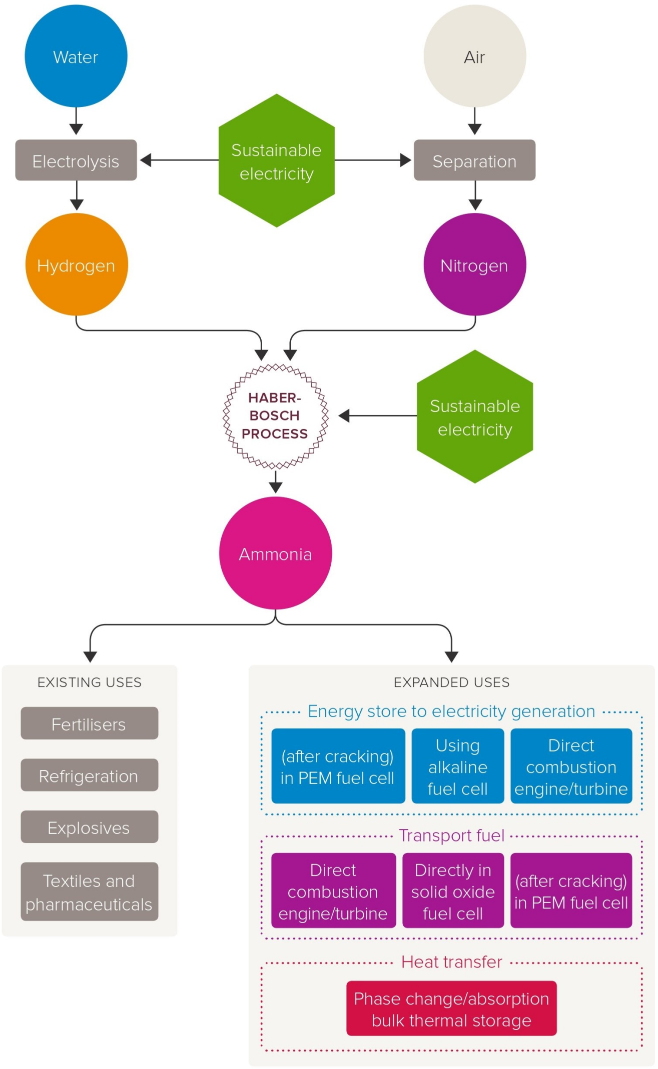


Figure 2.13: Schematic of green ammonia production [44]

iv. Transportation

Ammonia transportation leverages **a well-established infrastructure** [44] originally developed for industrial uses, facilitating its efficient distribution from production sites to end-users. This infrastructure includes various transportation methods, each designed to handle the specific challenges posed by ammonia's properties (see figure 2.14).

Ammonia is transported in **pressurized tanks** that maintain it in liquid form at relatively low temperatures [44]. Typically, the tanks are made from materials like stainless steel or other alloys that can withstand ammonia's corrosive effects. The tanks are also equipped with safety features such as pressure relief valves to manage any unexpected increases in pressure and prevent tank rupture. This method of transportation is commonly used for both short-distance and long-distance shipments, ensuring that ammonia remains in its liquid state during transit [44].

Dedicated **pipelines** [44] are used to transport large quantities of ammonia over long distances. These pipelines are constructed from materials such as specially coated steels and corrosion-resistant alloys. Pipelines provide a cost-effective and efficient means of transporting ammonia, particularly when it needs to be moved from production facilities to storage terminals or industrial users.

Ammonia is also transported by **rail and road** [44] using specially designed tanker cars and trucks. These vehicles are equipped with robust safety features to handle accidental releases and protect against the hazards of ammonia transport. This mode of transportation provides flexibility and access to regions not served by pipelines, making it an essential component of the ammonia supply chain.

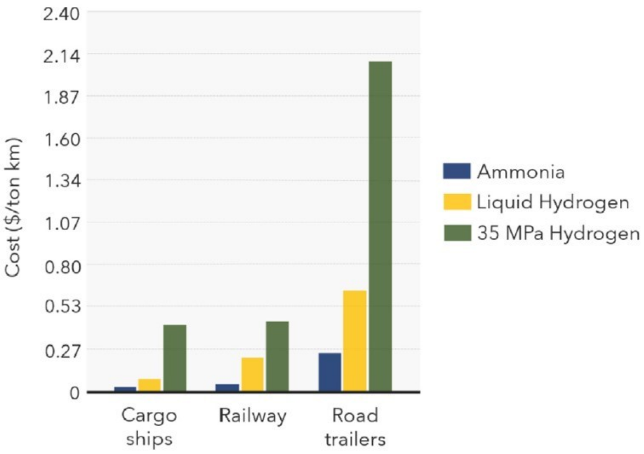


Figure 2.14: Cost estimate for ammonia and hydrogen transportation by cargi ships, railway and road trailers [44]

2.2.4 Current position of ammonia as a fuel

Comparison of NH3 and Other Fuels

As seen, Ammonia (NH_3) stands out among alternative fuels due to its unique properties and potential for carbon neutrality. Compared to hydrogen, **ammonia is easier to store and transport**, as it can be **liquefied** under **moderate pressure** and **does not require cryogenic temperatures**. This makes ammonia a more practical choice for large-scale energy storage and long-distance transportation.

In contrast with conventional hydrocarbon fuels like gasoline and diesel, ammonia has a **lower energy density**, with **18.6 MJ/kg** compared to **gasoline's 44 MJ/kg** [13]. However, ammonia's advantage lies in its potential to be produced from renewable energy sources [44], offering a pathway to reducing greenhouse gas emissions, as shown by Cardoso [8] in figure 2.15. Additionally, ammonia does not produce CO2 during combustion, which is a significant environmental benefit over fossil fuels.

Ammonia in ICE Systems

Ammonia is blended with hydrogen or diesel to improve overall engine **performance**. Blending **ammonia with hydrogen** can significantly improve flame speed (which is relatively low for ammonia) and **combustion stability** [40]. By adding hydrogen (has a higher flame speed and broader flammability range) these issues can be mitigated. Its

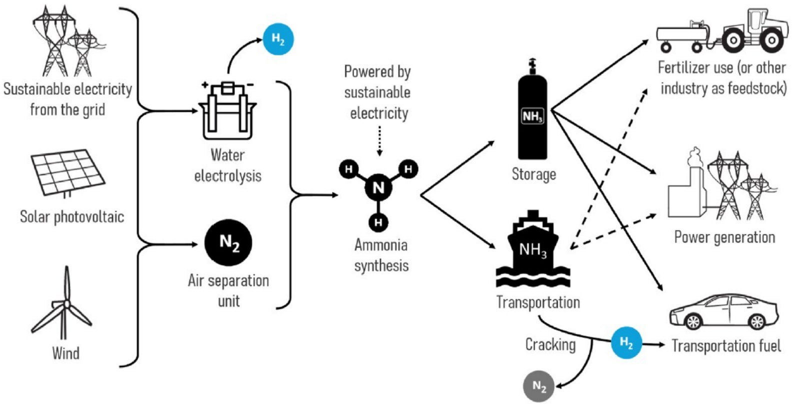


Figure 2.15: Carbon-free ammonia production and its various end-use [8]

presence helps to sustain the combustion process, leading to more efficient and stable engine operation. This blend is particularly beneficial in spark ignition (SI) engines.

In compression ignition (CI) engines, ammonia can be blended with **diesel** to **reduce carbon dioxide** (CO_2) emissions [31]. Diesel has a higher energy density and better ignition properties compared to ammonia, which makes it a suitable partner for blending. The addition of diesel helps to initiate the combustion process more effectively, while the ammonia reduces the overall carbon footprint of the fuel mix. However, this blend requires careful management of nitrogen oxides (NO_x) emissions, which can increase due to the presence of ammonia. Advanced combustion strategies and after-treatment systems, such as selective catalytic reduction (SCR), are necessary to control NO_x emissions and ensure compliance with environmental regulations [31].

2.3 Injection system

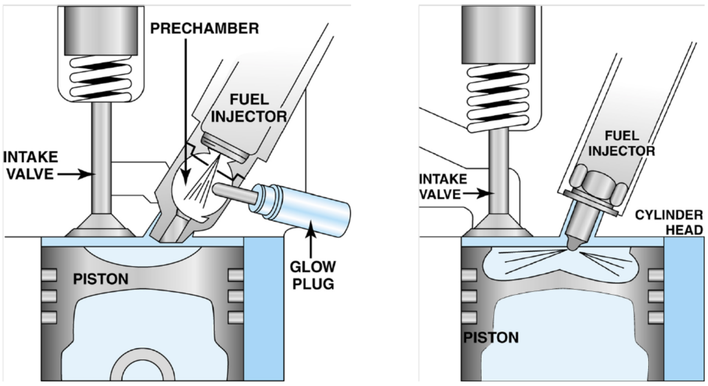
The injection system is the set of elements responsible for supplying fuel to the engine appropriately at each moment. Understanding the various aspects of injection systems in compression ignition engines is crucial for developing and optimizing engine models. This section delves into the fundamental components and functions of injection systems, types of injection mechanisms, and their hydraulic characteristics. By comprehensively studying and characterizing the injection system, we can simulate its behaviour under different operating conditions, analyse the effects of various parameters, and ultimately enhance engine performance and efficiency.

2.3.1 Types of injection systems

In compression ignition (CI) engines, the evolution of injection systems has been paramount in enhancing fuel efficiency and reducing emissions. The primary types of injection systems are direct injection (DI) and indirect injection (IDI) [12].

Direct injection systems

Direct injection systems inject fuel directly into the combustion chamber, so the mixing process depends mainly on the injection system's performance (the high injection pressure and the fineness of atomization): the combustion chamber is machined into the piston,



(a) IDI injection system (b) DI injection system

Figure 2.16: Methods to deliver fuel to the combustion chamber [42]

and the injector is centrally located in the cylinder head (see figure 2.16 b.) above, injecting fuel through multiple small orifices (100-200 µm) at high pressures (300-2000 bar) [12].

This injection system type allows lower flow, pressure and thermal losses compared to IDI and therefore higher engine efficiency, but its operation is noisier and the mixing process is poorer allowing lower engine speeds [12].

Indirect injection systems

Indirect injection systems, on the other hand, inject fuel into a pre-combustion chamber ((see figure 2.16 a.) at relatively low pressure (200-400 bar for diesel), promoting better mixing and smoother combustion. In indirect injection systems, the air movement (a high-speed turbulence is created during the compression stroke) plays the most crucial role in generating the necessary diffusive and convective fields for the mixing process [12].

This system main advantages are its better fuel dispersion (better air-fuel mixture), the simplicity of the injection system (its role is secondary) and its smoother and quitter operation. Also, since it achieves lower temperature and pressure peaks (due to the high-quality mixture), the NO_x emissions are reduced. But, on the other hand, its thermal efficiency is also reduced due to a larger thermal exchange surface due to the additional chamber and higher pressure drops [12].

2.3.2 Functions

The injection system in CI engines performs several critical functions to ensure efficient and clean engine operation. One of the primary functions is **fuel delivery**, where the system precisely meters and delivers the correct amount of fuel to the combustion chamber. This ensures that the engine operates efficiently under various loads and speeds. **Atomization** is another crucial function, where the injector breaks fuel into fine droplets, facilitating efficient **mixing** with air and complete combustion. **Timing control** is essential for injecting fuel at the optimal point in the engine cycle, maximizing power output and minimizing emissions [12].

2.3.3 Injector types

There are two types of injectors: solenoid-type (first generation) and piezoelectric (second generation).

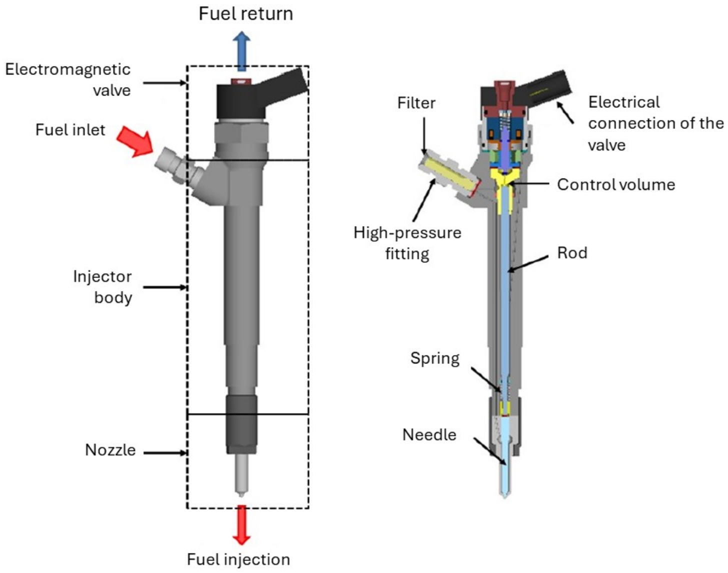


Figure 2.17: Components of a solenoid injector in a common-rail system [25]

Solenoid injectors (figure reffig:components)), a significant advancement in modern diesel engine technology, use an electromagnetic solenoid to control fuel injection. An electric current creates a magnetic field that moves the injector needle, allowing precise control of the fuel injection process. These injectors are known for their high precision and capability of multiple injections per engine cycle, which helps reduce emissions and engine noise while enhancing overall performance [12, 25]. **Piezoelectric injectors** represent the second generation of advanced fuel injection technology, offering several notable improvements over traditional solenoid-type injectors. These injectors utilize piezoelectric elements, which are materials that change shape when an electric current is applied. This change in shape allows for precise control over the injector needle, resulting in faster and more accurate fuel injection [12].

2.3.4 Parts and Components of the Injection System

A typical solenoid injector consists of several key components that work together to ensure efficient fuel delivery and optimal engine performance. First, the **injector body** houses all internal components and connects to the fuel rail. The **solenoid valve**, controlled by electrical signals from the **engine control unit (ECU)**, actuates the injector **needle**, which opens and closes to allow fuel flow into the combustion chamber. The **nozzle** is responsible for **atomizing** the fuel into a fine spray, ensuring efficient mixing with air and complete combustion. Additionally, a **spring** ensures that the needle returns to its closed position after each injection, and an electrical connector links the injector to the ECU. These components collectively ensure precise control over the injection process, optimizing engine performance and emissions [12].

Beyond the solenoid injector itself, the main components of the entire solenoid injector system include the **fuel pump**, **common rail**, **ECU**, **pressure sensor**, and **fuel filter**.

The common-rail system (see figure 2.18) is named for the single rail that distributes fuel to all injectors (instead of having an independent rail for each injector). It provides better control of injection timing and duration, maintains high injection pressure independent of engine speed, and ensures practically constant injection pressure throughout the injection process. Additionally, it allows for multiple injections per cycle [12].

The **fuel pump** delivers fuel at high pressure to the common rail (see figure 2.19), which distributes it evenly to each injector at a consistent pressure. The **ECU** plays a critical role in controlling the timing and duration of fuel injection based on real-time engine parameters, ensuring optimal combustion. **Pressure sensors** monitor the fuel pressure within the rail, providing feedback to the ECU for precise control. The **fuel filter** removes impurities from the fuel before it reaches the injectors, protecting the system from potential damage and ensuring clean combustion [12].

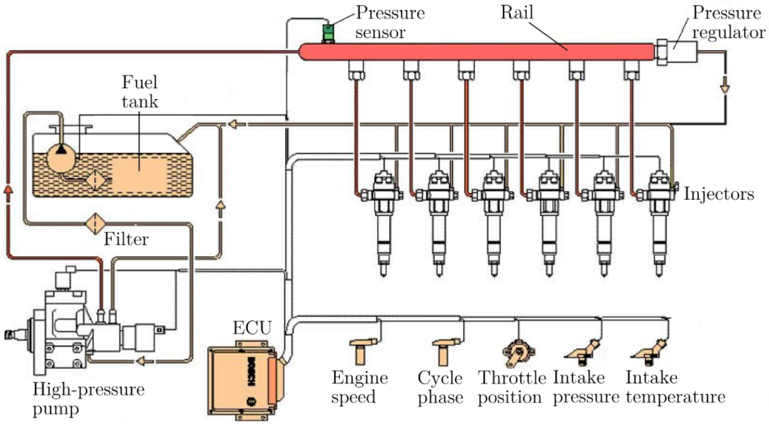


Figure 2.18: Components and layout of a typical common-rail system [42]

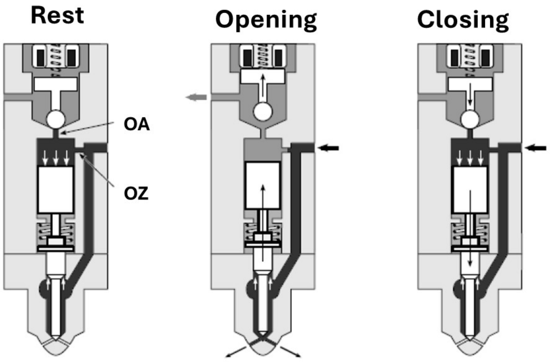


Figure 2.19: Operation of common-rail injector [25]

2.3.5 Hydraulic characterization

- Hydraulic characterization of the injection system involves a detailed analysis of the fluid dynamics within the injector. Key aspects of this characterization include **flow rate** measurement, **pressure drop**, **discharge coefficient**, and **cavitation** analysis [12].
- The **flow rate** determines the amount of fuel delivered by the injector per unit time, which is crucial for understanding the injector's performance under various conditions.
- **Pressure drop** assessment involves evaluating the loss of pressure as fuel flows through different components of the injector, affecting overall efficiency.
- The **discharge coefficient** measures the injector's efficiency in converting fuel pressure into flow rate.
- **Cavitation**, the formation of vapor bubbles in the fuel, can significantly impact injection performance and durability.

To simulate and analyse the injector's behaviour under different operating conditions an **advanced modelling software (GT-SUITE)** will be used.

Chapter 3

Method

3.1 Modelling

3.1.1 Representing Fluid dynamics

Fluid mechanics is the branch of physics that studies the behaviour of fluids and their behaviour when forces are applied on them. **Computational Fluid Dynamics (CFD)** is the branch that uses numerical analysis and algorithms to solve and analyse problems involving fluid flows [47] . In CFD, different representation models are used to simplify and solve complex fluid dynamics problems. The choice of model depends on the nature of the problem, the desired accuracy, and computational resources.

Zero-dimensional (0D) models are the simplest form of representation where the system is treated as a single point without spatial variation [16]. These models are typically used for systems where the changes in properties are purely time-dependent. They are useful for initial approximations and understanding the overall behaviour of a system without detailed spatial resolution.

One-dimensional (1D) models consider variations in only one spatial dimension [47]. These models are used when the flow properties vary significantly along a single axis and changes in the perpendicular directions are negligible. 1D models strike a balance between simplicity and detail, making them suitable for a variety of engineering and that it is why they'll be used in this project to give a first understanding of the subject matter.

Two-dimensional (2D) models extend the analysis to two spatial dimensions, providing more detail than 1D models. They are used when variations in the flow properties are significant in two directions, while the third dimension can be assumed uniform or negligible.

And three-dimensional (3D) models provide the most comprehensive representation, considering variations in all three spatial dimensions [47]. 3D modelling considers variations in all three spatial dimensions, providing a comprehensive and detailed representation of the physical system. The primary advantage of 3D models is their accuracy and ability to simulate real-world scenarios with high fidelity. However, this comes at the cost of increased computational requirements and complexity. 3D models are resource-intensive and often require advanced numerical methods and significant computational power.

In computational modelling, the representation of physical phenomena can vary significantly depending on the dimensionality chosen for the model. The two primary forms of representation are one-dimensional (1D) and three-dimensional (3D) models.

3.1.2 One-Dimensional (1D) Modelling

1D modelling simplifies the representation of physical systems by **considering variations in only one spatial dimension**. This approach is particularly useful for problems where changes in the other two dimensions are either negligible or can be averaged out. Common applications of 1D modelling include fluid flow in pipes, heat transfer in rods, and wave propagation in strings. The governing equations for 1D models often derive from conservation laws such as mass, momentum, and energy, tailored to one-dimensional analysis.

The primary advantages of 1D models are their **computational efficiency** and **simplicity**. They require fewer computational resources and are easier to solve compared to higher-dimensional models. However, they cannot accurately capture phenomena that inherently require multi-dimensional analysis, such as turbulence and complex geometries.

3.2 GT-Power

3.2.1 Description of the software

GT-Power® is a leading engine simulation software developed by **Gamma Technologies** (see Figure). It is extensively used in the automotive industry for the design and analysis of internal combustion engines and related systems. The software allows engineers to simulate the performance and behaviour of engine components, enabling optimization and innovation in engine development [43]. GT-Power® allows for the **simulation of complete engine systems and virtual complex prototypes** (reducing the need for expensive and time-consuming physical prototypes), including intake and exhaust systems, fuel injection systems, turbochargers, after-treatment systems, among others [43]. This approach enables users to understand how different components interact and affect overall engine performance.

Figure 3.1: Gamma Technologies logo

The software employs sophisticated algorithms to predict the behaviour of engines under various operating conditions which helps in anticipating engine performance and identifying potential issues before physical prototyping. This includes **simulations of combustion processes**, **heat transfer**, **fluid flow**, and **emissions formation**.

The software includes robust tools for data **analysis** and **visualization**: reports, charts, and graphs can be generated to analyse simulation results. This helps in identifying trends, understanding performance characteristics, and making informed design decisions.

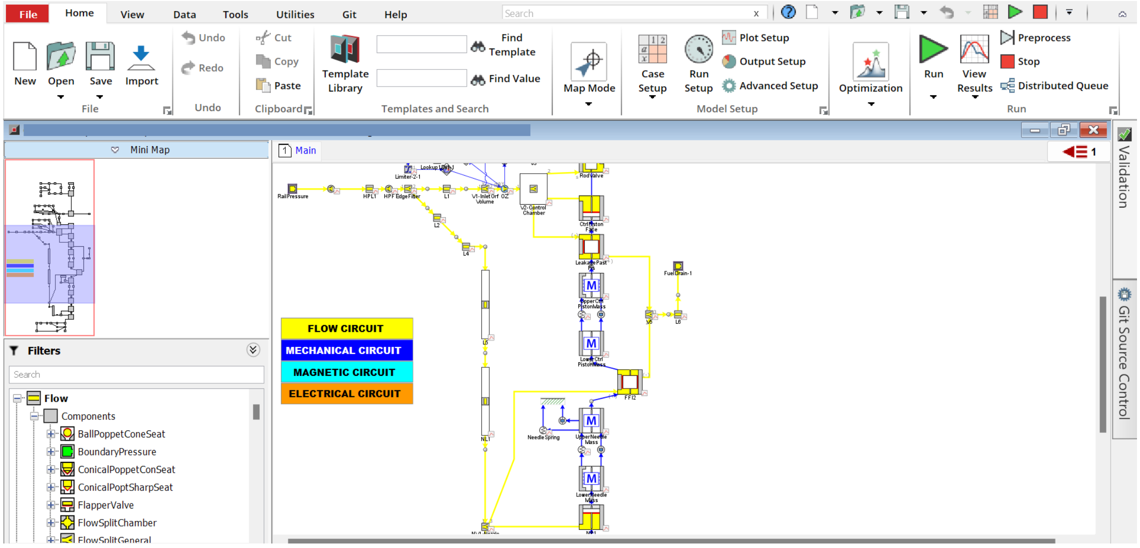


Figure 3.2: Main interface of GT-Power®

3.2.2 Main characteristics of the software

GT-Power® offers a comprehensive suite of features that make it an indispensable tool for engine simulation and a suitable tool for this project:

- includes **extensive libraries of engine components** such as cylinders, turbochargers, intercoolers, and exhaust systems [43].
- employs **advanced algorithms** to simulate the complex thermodynamic and fluid dynamic processes within the engine [43].
- **integrates with other Computer-Aided Engineering (CAE) tools and software**, facilitating a streamlined workflow in the engine development process [43].
- provides an **intuitive graphical user interface**, making it accessible to both novice and experienced users [43].

3.2.3 Modifiable parameters

GT-Power® allows users to modify a wide range of parameters to tailor the simulation to specific requirements. Some of the key modifiable parameters that will be effectively utilized in the project include:

- **Engine Geometry**: Users can define the geometric parameters of the engine components, such as bore, stroke, and compression ratio.
- **Material Properties**: The software allows for the customization of material properties for different engine components to simulate realistic behaviour under various conditions.
- **Fluid properties**: Users can modify fluid properties, such as viscosity, density, specific heat, and thermal conductivity, to accurately represent different fluids like air, fuel, and coolant within the engine system.
- **Operating Conditions**: Users can set and vary operating conditions such as ambient temperature, pressure, and fuel composition.

- **Boundary Conditions**: Users can specify boundary conditions, including inlet and outlet conditions, to accurately reflect real-world scenarios.

3.3 Model

3.3.1 Model Background

The R.Payri study [34] focuses on the development and validation of a one-dimensional (1D) model for a solenoid common-rail injector. This model aims to understand the hydraulic interactions between close-coupled injection events, which are critical for optimizing diesel engine performance. The 1D model was developed using the GT-SUITE® software, incorporating detailed geometrical and hydraulic characteristics of the injector obtained through experimental measurements. The primary goal is to simulate and analyse the dynamic behaviour of the injector under various operating conditions to enhance fuel efficiency and reduce emissions. The document focuses on a general description of the solenoid common-rail injector and its modelling without specifying a particular model or brand.

3.3.2 Describing distinct parts and components in the model

The 1D model of the injector includes several key components and encompasses electrical, electromagnetic, and hydraulic systems to accurately simulate the behaviour of a solenoid common-rail injector.

Parts of the model

- **The electrical system** (in orange) provides the energy required for injector operation and influences the speed and precision of the electromagnetic response. It is composed of the **electrical circuit** (including a current source, resistance, and coil) and the **electromagnetic valve** (the coil is part of the electromagnetic valve, influencing the armature movement). Each element has a crucial function: the **current source** supplies the necessary electrical energy to the **coil**, and when the current flows through it, it generates a magnetic field, which is essential for the operation of the electromagnetic system. The **resistance** controls the current flow and contributes to the overall electrical characteristics of the circuit.
- The **electromagnetic circuit** (in blue) converts electrical energy into mechanical movement. It is responsible for simulating the generation of the magnetic field (created by the coil) and creating a force on the armature, causing its movement (opening and closing the control valve). The elements included are the **magnetic path** (magnetic objects (MF1–MF4) and the AirGap object), a **control valve mass** (CtrlValveMass) representing the moving elements in the control valve, FluidPiston objects, simulating the **fluid-dynamic forces** acting on the armature surfaces and Flapper-valve template, which models the interaction between the armature and the control volume OA.
- The **hydraulic system** (in yellow) manages the actual fuel delivery process, ensuring that the correct amount of fuel is injected at the right time and pressure for optimal combustion. The internal pressure is regulated trough **OZ and OA orifices** (by controlling the fuel flow into and out of the control volume), influencing the injector's dynamic response. The **needle** and **nozzle** components control the

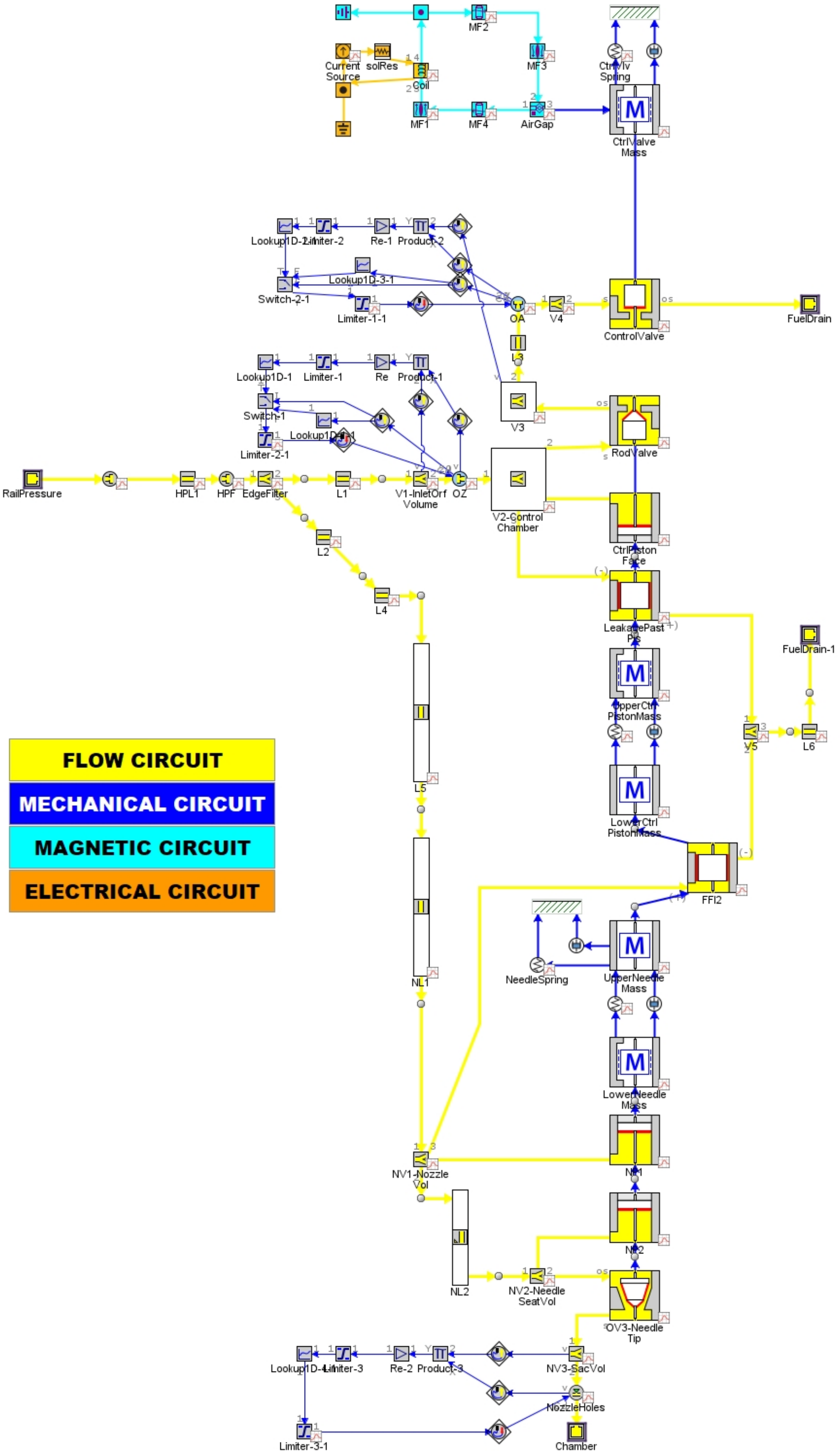


Figure 3.3: Complete model map in GT-POWER [34]

timing and quantity of fuel injection, ensuring optimal combustion (they simulate needle lift and flow through nozzle orifices). The injector holder includes the fuel inlet line, control volume, piston rod mass, and a Rate of Injection (ROI) meter to measure the injection rate and calibrate the injector's dynamic behavior.

By **integrating these three systems**, the model can accurately simulate the complex interactions and dynamics of a solenoid common-rail injector, providing valuable insights for optimization and performance improvement. The electrical and electromagnetic systems are integrated through the coil, as the electrical system supplies current to it, generating a magnetic field that moves the armature. The electromagnetic and hydraulic systems are connected through the movement of the armature (controlled by the magnetic field), which opens or closes the control valve, thereby controlling fuel flow into the control volume. The hydraulic system is integrated into the injection process as it regulates the fuel flow and pressure in the control volume, driving the needle lift and fuel injection through the nozzle orifices, determining the injection rate and pattern.

Main components of the model

The key components of the model are each modelled to replicate its real-world behaviour accurately.

- **Electromagnetic Valve** (figure 3.5): This component controls the opening and closing of the injector. The model includes elements representing the electrical circuit, magnetic forces, and fluid dynamics acting on the armature surfaces. It is composed of:

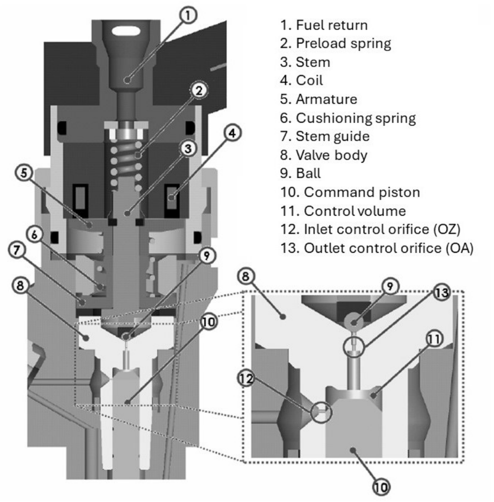


Figure 3.4: Solenoid valve of a common-rail injector [25]

  - **Electrical circuit** (in orange): current source, resistance, and coil
  - **MF1–MF4 magnetic objects**: create a defined path for the magnetic flux generated by the coil; this path ensures that the magnetic field is concentrated and directed towards the armature efficiently (by creating a well-defined path, magnetic losses are minimized ensuring that the maximum possible magnetic force is applied to the armature: this optimization is crucial for achieving precise

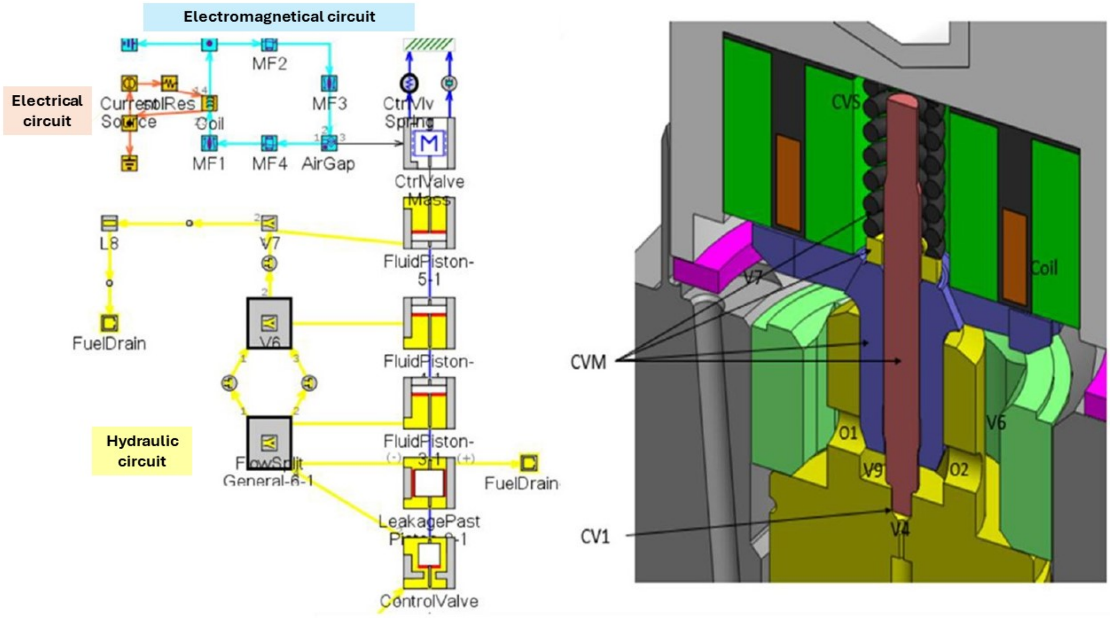


Figure 3.5: Electrovalve model layout [34]

control over the armature movement). The response is therefore rapid and precise.

- **AirGap object**: represents the physical gap between the magnetic elements and the armature, where the magnetic field exerts force to move the armature. The magnetic path ensures that the magnetic flux density is sufficient in the AirGap object.
- **Control Valve Mass** (CtrlValveMass): represents the combined mass of all moving elements in the control valve, primarily the armature, and accounts for their inertia and dynamic behaviour. This accurate mass representation is essential for simulating the armature's movement under magnetic force, affecting the timing and precision of the fuel injection process. Heavier masses respond more slowly due to greater inertia, while lighter masses respond more quickly, influencing injector opening and closing timing and, consequently, the fuel injection duration and quantity. Additionally, the CtrlValveMass balances the magnetic force generated by the coil with the mechanical forces from the spring and fluid dynamics, ensuring reliable valve operation.
- **FluidPiston** objects: represent the forces exerted by the fuel as it moves through the injector (ensure that all forces acting on the armature are accounted for). These forces are applied to the armature and other moving components and they can either assist or resist the movement, depending on the direction and magnitude of the fuel flow.
- **Flapper-valve** template: used to simulate the interaction between the armature and the control volume. It models how the armature moves to open or close the control valve, allowing or restricting fuel flow into the control volume. The flapper-valve template also helps in balancing the forces such as the electromagnetic force from the coil, the mechanical force from the spring, and the fluid-dynamic forces from the fuel. **The control valve system** includes the

flapper valve as a critical component. The flapper valve's movement is what directly controls the fuel flow, but it is the control valve system (including the armature and electromagnetic elements) that determines when and how the flapper valve moves.

- **Fuel drain** elements: refer to components or pathways that allows excess or unused fuel to be returned from the injector back to the fuel tank

- **Injector Holder** (figure 3.6): Manages the fuel pressure and flow into the control volume, controlling fuel flow dynamics and simulates the mechanical deformation of the piston rod due to pressure forces (ineludible when making multiple injections) It is composed of:

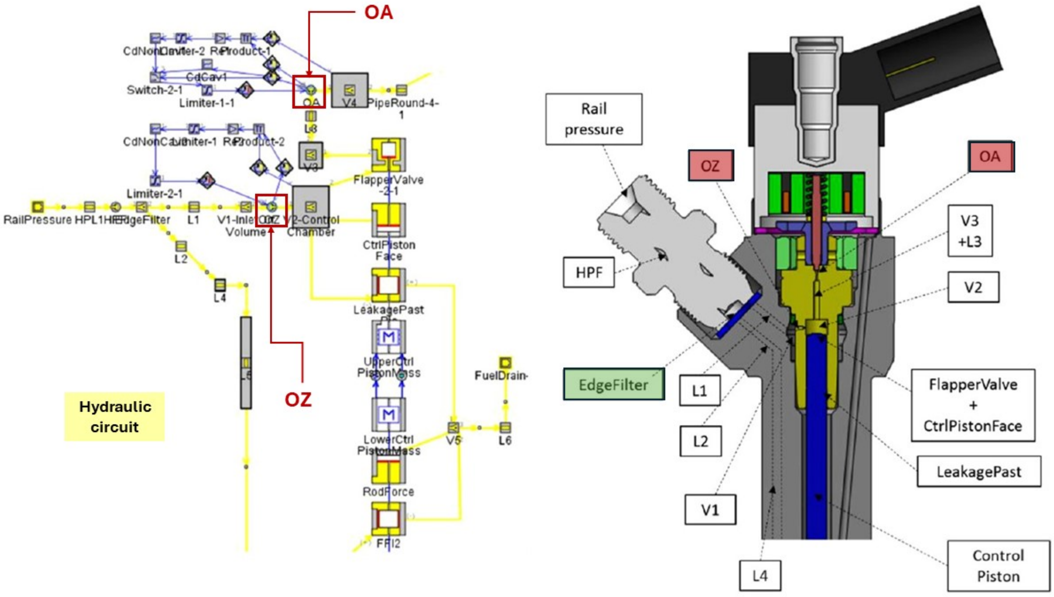


Figure 3.6: Injector Holder layout [34]

- **Fuel inlet line**: its primary function is to supply high-pressure fuel to the injector. It connects the injector to the common rail or fuel pump, ensuring a steady and reliable flow of fuel necessary for the injection process. It is also designed to withstand the high pressures and maintain them and must ensure that the fuel entering the injector is free from contaminants (Filter in green). The fuel inlet line object represents the physical properties of the actual fuel inlet line, such as its length, diameter, material properties, and pressure resistance.

- **Control volume**: acts as a chamber where fuel pressure is controlled before it is delivered to the nozzle for injection. Proper characterization of the control volume and its orifices helps avoid cavitation, a phenomenon that can cause damage and inefficiency in the fuel injection system.

- Piston rod mass: represents the combined mass of the piston rod and any associated moving components within the injector.

- **RailPressure boundary condition**: represents the high-pressure fuel supply coming from the common rail.

  - **OZ and OA orifices**, in red, (with discharge coefficient control logic): are critical components that manage the flow of fuel into and out of the control volume. The discharge coefficient control logic associated with these orifices is used to accurately simulate the fuel dynamics and pressure conditions within the injector. The characteristics of this orifices will be detailed later in section 3.3.5.
  - Spring, dampener compounds, FluidPiston and Flapper valve objects are used similarly as before to describe more accurately the forces actuating in the system.

- **Needle and Nozzle** (figure3.7): Simulates the needle lift which regulates the flow of fuel through the nozzle orifices to the combustion chamber (in green). The model includes:

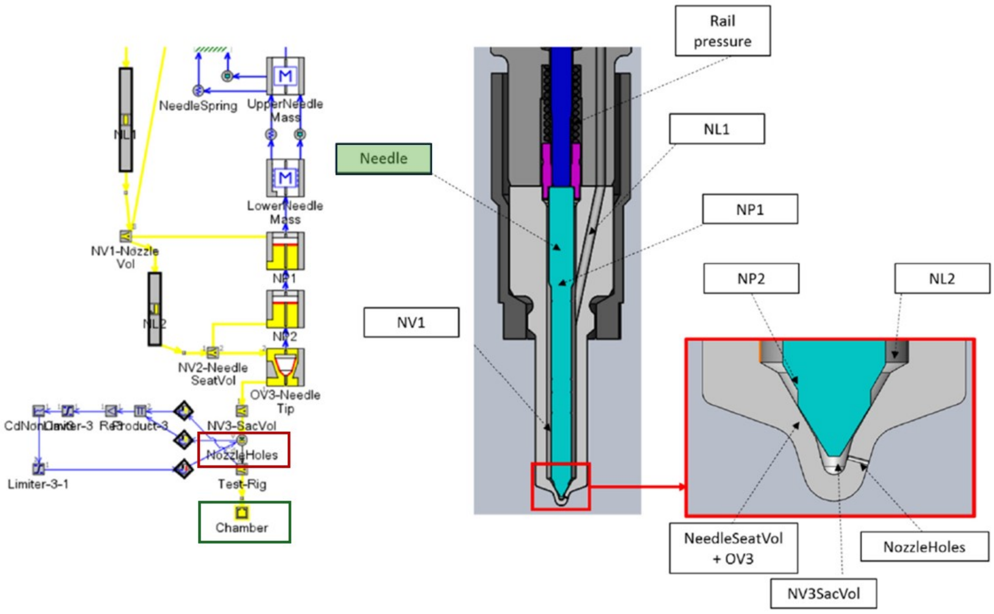


Figure 3.7: Needle and nozzle layout [34]

  - **Needle mass**: represents the mass of the injector needle (in green). The position of the needle determines the size of the flow passage through the nozzle, thereby controlling the start, duration, and end of the fuel injection event.
  - **Intermediate Spring and Dampener**: provides the necessary force to return the needle to its closed position when the injector is not activated. This ensures that the injector closes quickly and reliably after each injection event. The dampener helps to absorb and reduce oscillations or vibrations of the needle, providing smoother operation and reducing wear (improves the precision and repeatability of the injection events).
  - **Flow passages** from nozzle inlet to sac volume (**NL1, NV1, NL2**): direct the fuel from the nozzle inlet through various sections to the sac volume just before the nozzle holes. They are critical in shaping the fuel's flow path and influencing the pressure dynamics within the injector.

- **ConicalPoppetConSeat** template: represents the seating area where the needle meets the nozzle body. This conical seat ensures a tight seal when the needle is in the closed position, preventing fuel leakage.
- **NozzleHoles** object (in red): the final exit points for the fuel as it is injected into the combustion chamber. They play a critical role in atomizing the fuel into fine droplets, which is essential for efficient mixing with air and proper combustion.

3.3.3 Rate of Injection

The **rate of injection (ROI)** measures the fuel delivery rate over time during an injection event. It is a critical parameter in internal combustion engines because it significantly influences engine performance, efficiency, emissions, and overall combustion characteristics.

The ROI was **experimentally measured** in the R. Payri paper [34] using an Electronic Valve Injection (EVI) rate of injection meter based on the Bosch long-tube methodology. These measurements captured the dynamic pressure increase caused by fuel injection, providing data to calibrate the 1D model (see figure).

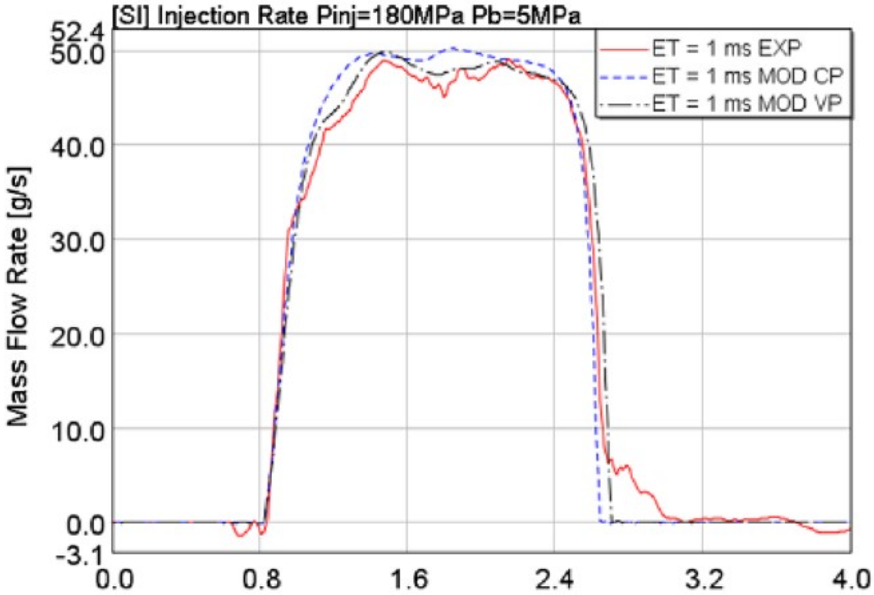


Figure 3.8: Experimental vs Modelled (Constant Pressure and Variable Pressure)

First, the rate at which fuel is injected determines **how well it mixes with air** in the combustion chamber and it also affects the **timing and location of fuel ignition**, which is crucial for **efficient combustion** (reducing fuel consumption), achieving the desired **power output** (related to the amount of fuel injected) and **reducing the formation of pollutants** such as soot (particulate matter) and nitrogen oxides (NO_x).

Furthermore, controlling the injection rate helps in maintaining the **optimal combustion temperature and pressure**, thereby improving the **thermal efficiency** of the engine which influences engine's **longevity** (managing the thermal load on components reduces the risk of thermal stress and failure)

3.3.4 Diesel Injection

The model specifically addresses the diesel injection process, which involves **high-pressure fuel delivery** into the combustion chamber. Key aspects of diesel injection modelled include:

- **Injection Pressure**: Simulated at various levels (e.g., 30 MPa, 50 MPa, 100 MPa, and 180 MPa) to evaluate its effect on injection dynamics.
- **Energizing Time (EI)**: The duration of the electrical signal controlling the injector, varied to study its impact on the injection rate and mass flow.
- **Ignition Delay**: The time between the start of injection and the start of combustion. An optimal injection rate can shorten the ignition delay, leading to smoother combustion.
- **Premixed Combustion Phase**: Rapid mixing of fuel and air leads to a brief but intense combustion phase. The injection rate affects this phase, impacting noise and emissions.
- **Diffusion Combustion Phase**: Fuel burns as it mixes with air. The rate at which fuel is injected affects this phase, influencing the completeness of combustion and emissions.

3.3.5 Control volume orifices

The OZ and OA orifices in the injector model are critical components that manage the flow of fuel into and out of the control volume. Their pressure control is essential for the precise operation of the injector (optimizing fuel flow, reducing pressure losses, and ensuring consistent injection events), affecting the timing and quantity of fuel injection. This leads to better fuel atomization and combustion, improving engine performance and reducing emissions. Accurate modelling of these orifices is necessary to predict and control the injector's behaviour during different phases of operation. This figure below (3.9) shows

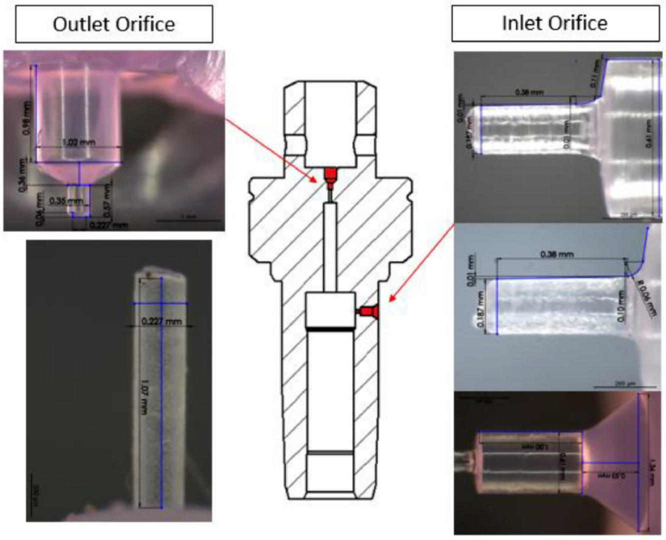


Figure 3.9: Silicone mold technique for control volume geometry determination [34]

how the orifices where measured using the silicone mold technique and their measures later on implemented in the model.

The **OZ (Inlet Orifice)** allows fuel to enter the control volume of the injector. It is designed to manage the flow rate and minimize cavitation, ensuring that fuel enters at the correct pressure (and it is maintained) and flow rate. The geometry of the OZ orifice, such as its diameter and shape, is optimized to control the fuel flow characteristics and avoid cavitation. These characteristics vary according to the fuel used, and in the model considered, they are chose to be optimal for diesel.

The **OA (Outlet Orifice)** allows fuel to exit the control volume. It plays a key role in regulating the pressure within the control volume by controlling the outflow of fuel. The design considerations are similar to OZ; the OA orifice's design is critical for managing flow rates and preventing cavitation.

The model implements **discharge coefficient control logic**, that dynamically adjusts the discharge coefficient (defined below) based on real-time operating conditions. This logic ensures that the simulated fuel flow through the OZ and OA orifices accurately reflects the behaviour under varying pressures and flow rates.

It takes into account various factors such as Reynolds number and cavitation number to determine the flow characteristics. This logic helps in understanding how changes in operating conditions, such as pressure and flow rate, affect the performance of the orifices.

- The **Discharge Coefficient (C_d)** is a dimensionless number that characterizes the flow efficiency of an orifice. It is influenced by the orifice geometry and the flow conditions.
- The **Reynolds Number (Re)** is used to characterize the flow regime (laminar or turbulent) and its impact on the discharge coefficient. The discharge coefficient is often a function of the Reynolds number under non-cavitating conditions.
- The **Cavitation Number (K)** is used to assess the likelihood of cavitation occurring at the orifice. When cavitation occurs, it significantly affects the discharge coefficient and flow characteristics.

Non-Cavitating Flow
For non-cavitating conditions, the discharge coefficient can be expressed as an asymptotic function of the Reynolds number:

$$Cd = Cd_{\max} - \frac{A}{\sqrt{Re}} \tag{3.1}$$

where $Cd_{\max}$ and A are constants determined by the orifice geometry.

Cavitating Flow
When cavitation occurs, the discharge coefficient depends on the cavitation number:

$$Cd = C_c\sqrt{K} \tag{3.2}$$

where C_c is the contraction coefficient, and K is the cavitation number:

$$K = \frac{P_{\text{inj}} - P_v}{P_{\text{inj}} - P_b} \tag{3.3}$$

where P_{inj} is the injection pressure, $P_v$is the vapor pressure of the fuel, and P_b is the backpressure.

3.3.6 Model Validation

The 1D model was **validated through extensive comparison with experimental data** obtained from injection rate measurements. Validation involved:

- **Single Injections**: Simulating single injection events at different pressures and energizing times to ensure the model accurately reproduced the main features of the injection rate profile.
- **Statistical Analysis**: Assessing the model's accuracy in predicting total injected mass and injection timing through statistical measures like the coefficient of determination (R^2).

Overall, the 1D model demonstrated a high degree of accuracy in replicating experimental injection profiles, providing valuable insights for optimizing diesel injection systems and it will be the starting point of the development of this bachelor thesis.

Chapter 4

Model upgrade

4.1 Sensitivity analysis with Diesel

In the 1D model, tests will be conducted using **ammonia**. However, to correctly interpret these results, it is necessary to understand the system with the fuel for which it was originally designed, which in this case is diesel [34]. The diesel fuel used is **Repsol CEC RF-06-991**, for which all thermodynamic properties are characterized over a wide range of pressure and temperature conditions, including those typical of internal combustion engines. Preliminary **sensitivity studies** are conducted to determine which model parameters depend on which variables. This allows for a comparison of the obtained data to understand which results are influenced by the type of fuel used and which are independent of it. Also, since the model is designed for diesel, it will be the benchmark to which the results obtained with ammonia can be compared.

4.1.1 Repsol CEC RF-06-99 Diesel Fuel

Table 4.1: Repsol CEC RF-06-99 Diesel Fuel properties [35]

Test	**Unit**	**Result**	**Uncertainty**
Density at 15°C	kg/m^3	843	±0.2
Viscosity at 40°C	mm^2/s	2.847	±0.42
Volatility			
65% distilled at	°C	294.5	±3.7
85% distilled at	°C	329.2	±3.7
95% distilled at	°C	357.0	±3.7
Cetane Number		51.52	±2.5
Cetane Index		49.6	±0.51
Calorific Value			
Higher Calorific Value	MJ/kg	45.58	
Lower Calorific Value	MJ/kg	42.78	
Fuel molecular composition		$C_{13}H_{28}$	

Repsol CEC RF-06-99 is a reference diesel fuel commonly used in various **experimental** and **computational** studies to analyse diesel engine performance, injection characteristics, and spray behaviour. Below are some key properties and relevant applications (properties in table 4.1).

In **experimental studies**, this diesel fuel is employed to investigate the effects of nozzle geometry on direct injection diesel engine combustion. Researchers use it to analyse how different fuel properties influence the internal flow within diesel injector nozzles, helping to improve the understanding of fuel dynamics and optimizing injector designs.

In **computational modelling**, the properties of Repsol CEC RF-06-991, such as density and viscosity, are crucial. These properties are used in computational fluid dynamics (CFD) simulations to study diesel spray and cavitation effects. The fuel's characteristics are essential for validating models that simulate injector performance and fuel spray behaviour, ensuring the accuracy and reliability of simulation results.

For **injector technology testing**, Repsol CEC RF-06-991 is used to compare the performance of various injector technologies, including solenoid and piezoelectric injectors, under different operating conditions. This application helps in determining the suitability and efficiency of different injector designs, contributing to the development of more effective fuel injection systems.

4.1.2 Sensitivity study with GT-Power®

A sensitivity test is an analysis used to evaluate **how variations in the input parameters of a model affect its outputs**. This type of test is crucial for identifying which variables have the greatest impact on system behaviour and for understanding the robustness of the model against changes in the parameters.

Utility of GT-Power® in Sensitivity Analysis:
GT-Power® is a very useful tool for performing sensitivity analyses because it **allows multiple tests or cases to be executed simultaneously**. In these analyses, ideally, only one parameter is modified at a time to evaluate its impact on the system. This allows for a direct comparison of how each parameter individually affects the model's results. Also, GT-Power® facilitates the generation of graphs of various measurements in different components of the system. This is essential for visualizing and analysing the effects of parameter changes.

Parameters Analysed in this Study
In this specific case, although the main and most representative parameter of injection is the injection rate, other relevant parameters are also analysed in 3 crucial elements:

- **Nozzle Holes**
  - **Injection rate**: measures the amount of fuel injected per unit of time.
  - **Discharge coefficient**: indicates the efficiency of the flow through the orifices. A higher coefficient means less pressure loss and better fuel atomization.
  - **Cavitation number**: evaluates the tendency of the flow to form vapor bubbles. Cavitation can damage components and reduce injection efficiency.
- **Inlet orifice (OZ) and outlet orifice (OA)**
  - **Mass flow rate**: measures the mass of fuel passing through the orifice per unit of time.
  - **Discharge coefficient**: measures the flow efficiency in the inlet orifice.

- **Cavitation number**: also measured in the inlet orifice to assess potential cavitation issues.
- **Pressure drop**: indicates the fuel pressure loss as it passes through the orifice. A lower pressure drop is preferable to maintain system efficiency.
- **Throat temperature and pressure**: measures temperature and pressure at the narrowest point of the orifice, which can affect fuel density and viscosity, influencing flow behavior.

These measurements will be taken under the normal operating conditions shown in the attached table 4.2. Each parameter will be modified individually while keeping the remaining parameters constant at their specified values in the table. This approach ensures that the results are representative of real-world operating conditions.

Parameter	**Description**	**Case 1: Diesel**	**Unit**
RailPressure	Rail Pressure (Absolute)	600	bar
FuelTemp	Fuel Temperature	50	C
Fuel	Composition	Repsol_CEC_RF-06-100	-
WallTemp	Wall Temperature	50	C
DrainPressure	Drain Pressure (Absolute)	1	bar
chamberPressure	Pressure (Absolute) at Injector Outlet	50	bar
chamberTemp	Temperature at Injector Outlet	41.5	C
chamberComp	Composition at Injector Outlet	Repsol_CEC_RF-06-100	-
simDur	Maximum Simulation Duration (Time)	4.5	ms
D_OZ	Hole Diameter	0.205	mm
D_OA	Hole Diameter	0.26	mm
SOI	Start of Injection (Time)	0.25	ms
ET	Energizing Time (Time)	1	ms
PeakCurrent	Peak of Electrical Signal	28	A
SteadyStateCurrent	Steady State Value of Electrical Signal	20	A
targetInjMass	Injected Mass to Target	1.5	-
Current	Current	Current_ET1000	A

Table 4.2: Parameter settings for diesel in the simulation

4.2 Notable findings

4.2.1 Rail Pressure

In modern diesel engines, **rail pressure** generally ranges from 500 to 2200 bar, depending on their use. In **heavy-duty** or load-bearing engines, lower pressures, ranging from 500 to 1500 bar, are sufficient. Although high pressures are generally better for fuel atomization, as they allow the fuel to break into finer particles, heavy-duty engines are designed to operate efficiently with larger fuel particles. These engines work with large volumes of fuel at lower operating speeds compared to light-duty diesel engines, and their robust design allows them to function effectively without extremely high pressures. Thus, while high pressures optimize atomization for most engines, the lower pressures in heavy-duty engines still ensure an appropriate air-fuel mixture and optimal combustion, guaranteeing reliable and durable performance under demanding working conditions.

In the 1D model considered in this study, pressures within this range will be utilized. Consequently, the injector employed is of the **heavy-duty** type, and the study aims to extrapolate the results to marine engines in the future. This approach is of interest because marine engines operate under demanding conditions and require robust and efficient fuel injection systems and understanding the injector's performance under these conditions with diesel fuel can provide valuable insights for its potential use with ammonia.

The limitation on pressures is imposed by the properties of ammonia, the intended final fuel. For ammonia to be injected correctly, it must remain in a liquid state. Experimental studies have shown that above these pressure levels, ammonia changes state[33], making the conventional commercial injector unusable. Therefore, the tests performed using diesel will be done at these rail pressure levels (600 bar).

The **drain pressure** is the pressure within the return line of a fuel injection system, where excess fuel is routed back to the fuel tank. It is maintained at **atmospheric** levels in all tests, ensuring consistent and reliable operation of the fuel injection system and preventing any backpressure that could affect the injector performance and fuel flow dynamics.

To evaluate the effect of rail pressure on the injection rate, tests were conducted at three different pressures: 300, 450, and 600 bar, with an energizing time of 1 millisecond (ms).

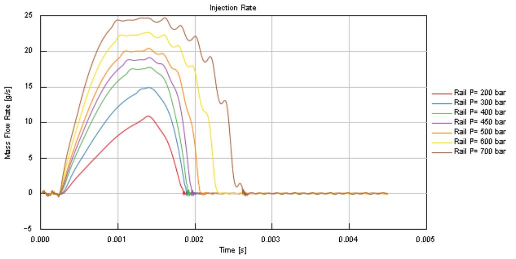


Figure 4.1: Injection rates for different rail pressures using diesel as a fuel

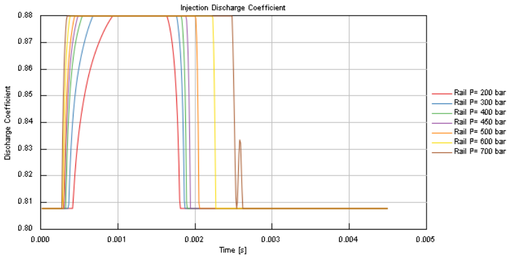


Figure 4.2: Discharge coefficients for different rail pressures using diesel as a fuel

The results showed that **increasing the pressure increases the injection rate** (see figure 4.1): rail pressure directly affects the amount of fuel injected per unit of time. Higher rail pressure results in a greater amount of fuel being injected because the fuel is forced through the injectors at a higher speed, leading to better atomization. However, it also increases the instability of the injection, as oscillations can be observed. In fact, increasing the pressure too much can lead to difficulties in controlling the flow and closing the exit valve, resulting in longer injections. This is reflected in the discharge coefficient in the nozzle hole plot (Figure 4.2). An appropriate pressure should achieve a balance between these conflicting effects.

4.2.2 Fuel Temperature

In the tests conducted, different fuel temperatures were used under specific conditions: a rail pressure of **600 bar** and an energizing time (ET) of 1 millisecond. The fuel temperatures tested were 10, 25, 50, and 70 ºC.

The injection rate graph can be divided into three main stages: **opening**, **steady state**, and **closing**. Opening is the initial phase where the injector starts to release fuel: the injection rate increases rapidly until it reaches a peak value. Then, the the intermediate phase or steady state is where the injection rate remains constant and reflects the amount of fuel injected continuously and uniformly. And during the closing, final phase, the injector stops releasing fuel so the injection rate decreases until it reaches zero. These three phases can be distinguished in figure 4.3.

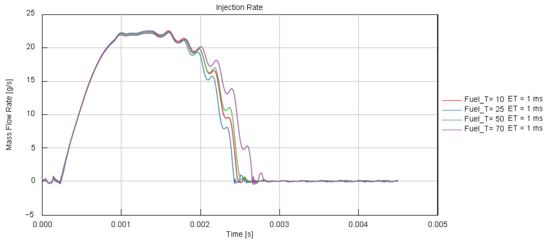


Figure 4.3: Injection rates for different fuel temperatures with diesel and ET = 1ms

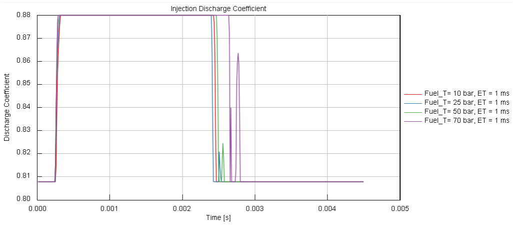


Figure 4.4: Discharge coefficient for different fuel temperatures with diesel

As it can be seen in the figure, **fuel temperature affects the injection rate mainly during the closing stage**. The opening and steady-state stages are similar across different fuel temperatures, but significant differences are observed during the closing stage:

- At lower temperatures (25 ºC): the closing is faster.
- At higher temperatures (70 ºC): the closing is slower and exhibits oscillatory behavior (also reflected in figure 4.4).

This differences may be due to first, fuel **viscosity**. In fact, at higher temperatures, the viscosity of the fuel decreases, which can affect the flow dynamics and the injector's ability to close quickly. On the other hand, the **density** of the fuel also decreases with temperature, which can alter the amount of fuel injected.

The system is specifically designed so that the pressures, dimensions, and timings are calibrated to the fuel temperature during injection, ensuring it operates at peak efficiency. In this case, **the real operating temperature in an engine is around 90ºC**, but in the experimental test rig (for rate of injection measurement) the temperature is around 50ºC. Deviating from this design temperature can lead to suboptimal performance. Relatively low temperatures have been tested because, from previous experimental trials, it is known that ammonia remains in a liquid state at low temperatures.

4.2.3 Energizing time

The energizing time (ET) is the period during which the fuel injector receives an electrical signal to open and allow fuel to flow into the combustion chamber. This duration determines how long the injector stays open, directly influencing the fuel injection process as seen in figure 4.5.

To evaluate the effects of different energizing times on the injection rate, tests were conducted with energizing times of 0.5 ms, 1 ms, 1.5 ms, 2 ms, and 3 ms. The energizing time significantly affects the injection rate mainly impacting the amount of fuel injected; a longer energizing time means the injector remains open for a more extended period, allowing more fuel to enter the combustion chamber. Additionally, a shorter energizing time may not allow the fuel flow to reach its maximum rate. Lastly, it affects the closing

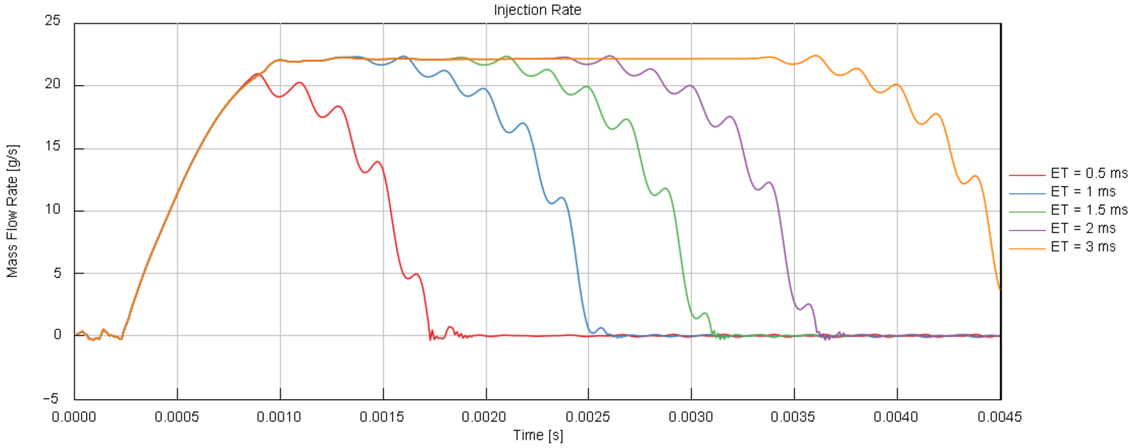


Figure 4.5: Injection rates for different energizing times using diesel as a fuel

phase of the injector. Once again, a value that balances these effects should be chosen, and in this case, ET=1ms meets the objectives.

4.2.4 OA and OZ geometries

As previously mentioned, the geometry of the control volume orifices (OA and OZ) also affects fuel injection. Various diameters of these orifices were tested to understand their impact, and tests were conducted for two energizing times, 1 ms and 2 ms. The values tested are shown in the tables 4.3 and 4.4, including their percentage variation.

Increasing or decreasing the diameter of each orifice impacts the injection rate in different ways:

Table 4.3: OA Diameters

OA	Diameter (mm)
100%	0.26
95%	0.247
105%	0.273
110%	0.286
115%	0.299
120%	0.312

Table 4.4: OZ Diameters

OZ	Diameter (mm)
100%	0.205
95%	0.19475
105%	0.21525
110%	0.2255
115%	0.23575
120%	0.246

- **OZ Orifice:**
  Increasing the diameter of the OZ orifice results in a decreased injection rate as seen in figure 4.6. This occurs because the pressure drops, leading to less fuel being injected. A **narrower opening** facilitates **quicker opening times** but makes the **closing process more difficult**. Beyond a certain diameter reduction, the opening may not even occur due to insufficient pressure. When the energizing time is increased for the same diameters (figure 4.7, the amount of fuel injected increases and the transient process becomes longer. However, the opening and closing processes remain largely unaffected.
- **OA Orifice:**
  When the diameter of the OA orifice is increased, the flow area becomes larger, which

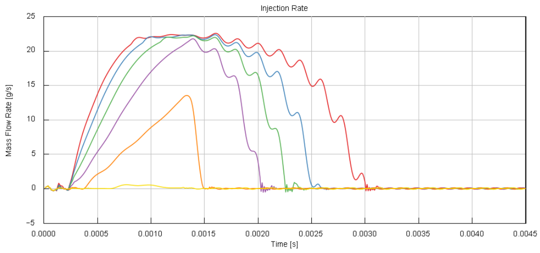


Figure 4.6: Injection Rate for OZ Diameters (ET=1 ms)

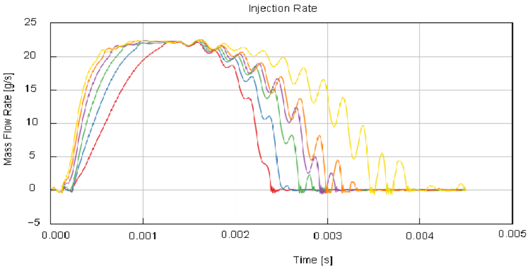


Figure 4.7: Injection Rate for OA Diameters (ET=1 ms)

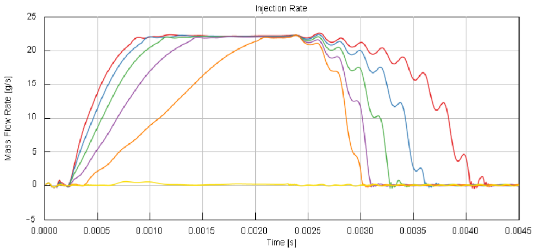


Figure 4.8: Injection Rate for OZ Diameters (ET=2 ms)

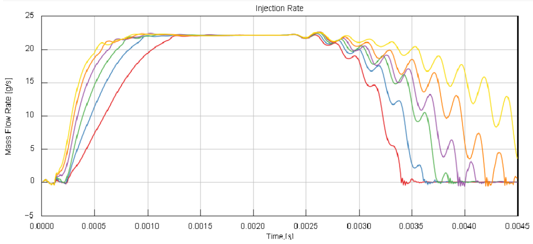


Figure 4.9: Injection Rate for OA Diameters (ET=2 ms)

can lead to a **higher mass flow rate**, allowing more fuel to pass through, as seen in figure 4.17. However, an excessively large diameter can **reduce control over the fuel flow, resulting in less precise injection.** Similar effects are observed when increasing the energizing time for the OA orifice as for the OZ orifice (figure 4.18).

For the considered operating conditions, the a slightly larger OZ and slightly narrower OA could improve the engine performance.

Effects of OZ's diameter in the control volume

To better understand the effect of OZ's dimensions in the system, the effects of it in the control volume can be helpful. First, as can be seen in figure 4.8, **a larger diameter implies a larger mass flow trough OZ** but also, a **lower pressure drop peak** (figure 4.9). (In this figure, should only be taken into account the values during the injection timing). But also, the cavitation number is affected: a larger opening, implies lower pressure levels and therefore the cavitation number increases meaning that the risk of bubbles appearing, destabilizing and wearing out the system.

The dimensions of OZ (the inlet orifice) also affect how the fluid behaves when passing through OA (the outlet orifice). In figures 4.13 and 4.14 it can be seen how **for higher diameters of OZ, OA takes longer to close**. This is due to the lowest pressure in the control volume encouraged by maintaining OA opened during most of the injection time. Also, the pressure and temperature throat stresses increase (figures 4.15 and 4.16), wearing the region.

Effects of OA's diameter in the control volume

The other way around, OA's dimensions also affect flow through OZ. **Increasing OA's diameter results in a decrease in the mass flow rate through OZ** (figure 4.19) and a **decrease in the pressure drop** (figure 4.20). Also, this results in an increase in the throat pressure and temperature in OZ, wearing out the orifice (as shown in figure 4.10).

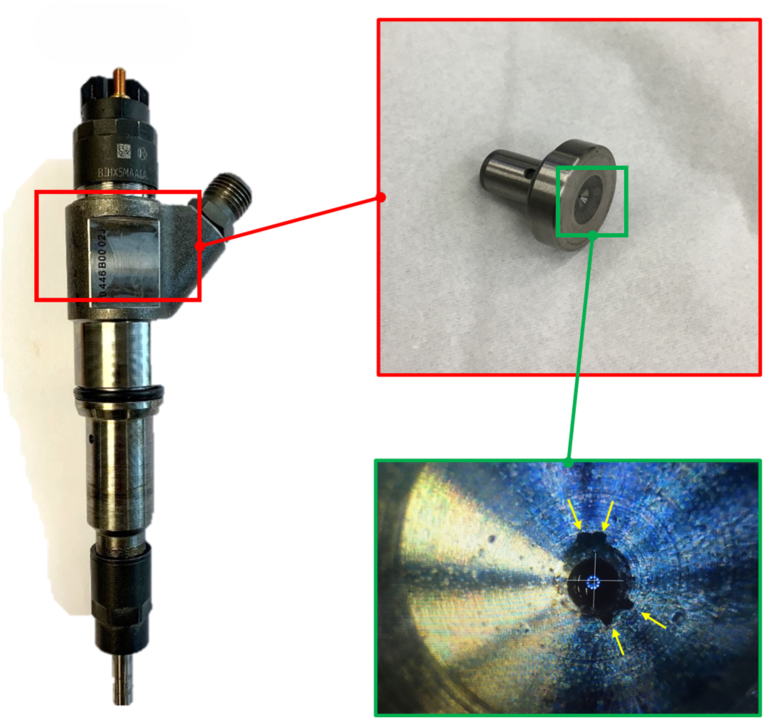


Figure 4.10: Microscopic internal damage in the OA orifice of an injector working with diesel (From CMT experiments)

On the other hand, the **increase in OA's diameter results in a higher mass flow rate through the orifice** and a **lower pressure drop** and the throat pressure and temperature gradients increase too. Elevated temperature gradients can cause **thermal stress** on the injector materials, potentially leading to wear and tear or even failure over time. This could reduce the injector's lifespan and increase maintenance needs. In addition to this, higher pressure gradients, especially in combination with these higher temperatures, can increase the risk of cavitation, which can cause pitting and erosion of the injector's internal surfaces, leading to a degradation in performance and reliability and managing the injector's operation with higher pressure and temperature gradients may be more challenging, requiring more precise control systems to ensure consistent performance.

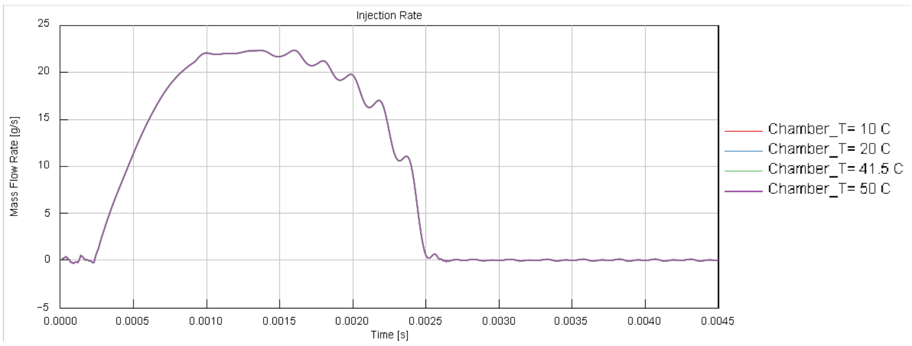


Figure 4.11: Injection Rate for different chamber temperatures (ET=1 ms)

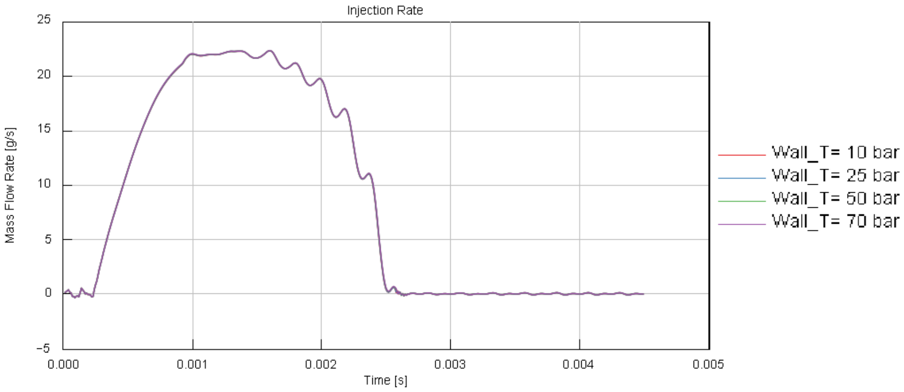


Figure 4.12: Injection Rate for different wall temperatures (ET=1 ms)

4.2.5 Other parameters

Other parameters such as **chamber temperature** (figure 4.27) and **wall temperature** (figure 4.28) have been tested and showed no influence on the injection ratio. This can be explained by the fact that these temperatures are related to elements that are outside the injector, not affecting significantly the dynamics of its elements. As a result, they do not affect the dynamics of fuel injection, which are primarily influenced by pressure, orifice geometry, and energizing time.

4.3 Modelling ammonia's fuel properties

Initially, an attempt was made to replicate the procedure performed with diesel, that is, simply replacing the type of fuel to see what would happen and conducting sensitivity tests to select the appropriate measurements for each parameter. However, the study began by testing two predefined fuels in the GT-Power® databases, named "ammonia" and "NH3-NASA". During these tests, no injection occurred; the injector had a really hard time opening despite the high pressures applied, and other parameters, such as the cavitation number, showed unrealistic values. Additionally, pressure drops were observed in certain elements that did not occur with diesel, indicating that these were not model errors.

After several tests, it was concluded that the equations that replicate the properties of the ammonia as a function of P and T were defined for a different range of operation, not covering the real operation range in direct injection systems (relatively high pressure

Table 4.5: Comparison of Ammonia and Diesel Fuel Properties

Property	**Ammonia**	**Diesel**
Chemical formula	NH_3	$C_{12}H_{23}$
Energy density (MJ/kg)	18.6	42.8
Energy density (MJ/L)	11.2^{*} 12.5^{**}	35.8
Autoignition temperature (°C)	651	210
Flame speed (m/s)	0.32–0.40	0.25–0.3
Density (kg/m^3)	0.771^{*} 600^{**}	850
Minimum ignition energy (mJ)	0.22–0.36	0.3–0.6
Dynamic viscosity (Pa·s) at 25°C	0.00013^{***}	0.0021
Low heating value (MJ/kg)	18.80	43.4
Octane number	130	8-15
Boiling point (K)	239.80	453
Freezing point (K)	195.50	180
Latent heat of vaporization (kJ/kg)	1371	300

* Gaseous form under atmospheric pressure and 20°C
** Liquefied at 0.99 MPa temperature of 25°C
*** Liquefied at 1 MPa

levels and temperature conditions). The reason for this is that they were intended for refrigerant applications, necessitating the manual redefinition of these in GT-Power.

A contribution of this work is an exhaustive search in fluid characterization libraries, such as OpenFOAM®, Converge®, and CoolProp, was conducted to obtain the thermodynamic properties of ammonia. These properties were compared with the results obtained in the laboratory under the same operating conditions. The data were treated and organized using Excel®, which facilitated their handling and analysis. This thorough process allowed the creation of an ”ammonia” object in GT-Power that corresponded to what could be achieved in the laboratory.

Chapter 5

Performance analysis of ammonia in engine simulations

5.1 Comparative Analysis of Injection Rates

To understand the behavior of ammonia as a fuel in comparison to diesel, test are carried on on to identify any observed differences due to the intrinsic properties of the fuels rather than external factors. Following the replication of these conditions, a sensitivity analysis is performed to identify the optimal operating parameters for ammonia. This analysis aims to fine-tune the parameters to achieve the best possible performance when using ammonia as a fuel. The parameters under investigation include rail pressure, fuel temperature, wall temperature, drain pressure, chamber pressure, and injector's orifices dimensions among others, all critical in determining the efficiency and effectiveness of fuel injection and combustion processes. The specific values used in the simulation for both ammonia and diesel are detailed in Table 5.1 below.

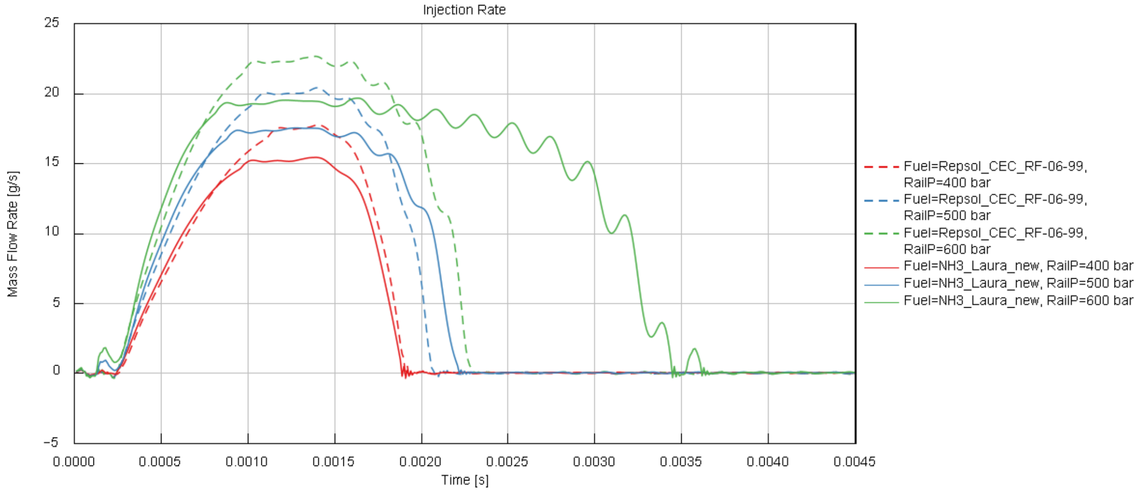


Figure 5.1: Injection rate for ammonia and diesel under the same operating conditions

Parameter	**Description**	**Case 1**	**Case 2**	**Unit**
RailPressure	Rail Pressure (Absolute)	600	600	bar
FuelTemp	Fuel Temperature	10	10	ºC
Fuel	Composition	NH3_Laura	Repsol_CEC_RF-06-99	
WallTemp	Wall Temperature	10	10	ºC
DrainPressure	Drain Pressure (Absolute)	8	8	bar
chamberPressure	Pressure (Absolute) at Injector	50	50	bar
chamberTemp	Temperature at Injector	10	10	ºC
chamberComp	Composition at Injector	NH3_Laura	Repsol_CEC_RF-06-99	
simDur	Maximum Simulation Duration	4.5	4.5	ms
dx	Discretization Length of...	0.1	0.1	mm
hpfDiam	Equivalent Diameter of E...	0.75	0.75	mm
D_OZ	Hole Diameter	0.205	0.205	mm
D_OA	Hole Diameter	0.26	0.26	mm
ET	Energizing Time	1	1	ms

Table 5.1: Simulation Parameters

The parameters for the simulations are chosen to reflect realistic operating conditions for ammonia and diesel. Figure 5.1 illustrates the injection rates for both ammonia and diesel under identical operating conditions.

The results from these simulations and sensitivity analyses will guide the optimization of ammonia as a viable alternative fuel, ensuring that it meets the performance standards required for modern engines. The behavior of diesel (in blue) serves as the benchmark, as the injector is specifically designed for it.

5.1.1 Maximum Injection Rate

The maximum injection rate for ammonia reaches approximately 20 g/s, while for diesel, it reaches around 22 g/s. This means that **diesel exhibits a slightly higher maximum injection rate compared to ammonia**. This is because diesel has a higher density than NH3. The mass flow rate is directly proportional to the density:

$$m = \rho \cdot u \cdot A \tag{5.1}$$

The injector can therefore deliver a larger amount of fuel in a short period.

A **higher maximum injection rate** can improve fuel **atomization**, resulting in a better air-fuel mixture within the combustion chamber and also allows for more fuel to be introduced in less time. A homogeneous air-fuel mixture is crucial for **efficient combustion**, which enhances engine performance and reduces pollutant emissions. However, although ammonia has a slightly lower maximum injection rate, it can still be sufficient to achieve efficient combustion, especially if other engine parameters are optimized through adjustments in injector design and engine management to achieve performance levels similar to those of diesel. The necessary adjustments are what we will aim to characterize.

5.1.2 Injection Duration

The **injection duration for ammonia is longer**, ending after the diesel injection, with a more abrupt (more stable) start and end. The longer injection period of ammonia compared to diesel can influence the overall combustion process and efficiency and is likely related to the physical properties of ammonia, such as its lower density and viscosity, which affect the fuel flow dynamics through the injector.

In theory, a longer injection duration can lead to more complete combustion of the fuel, as it has more time to mix with air inside the combustion chamber. However, a prolonged injection can also cause stability issues in combustion, especially at high engine speeds where rapid and precise injection is required, making it important to reach a balance.

The opening phase for both fuels is quite similar and fast. This is important because a **rapid and controlled injection is required for a good performance**.

5.1.3 Injection Rate Stability

The **ammonia** injection rate shows **more fluctuations and oscillations**, especially after reaching the peak, while **the diesel injection rate is more stable and consistent**. This stability is beneficial for **smooth engine operation** and **combustion stability**. Fluctuations in the injection rate can lead to inconsistent power delivery and reduced engine response, which is something that we will aim to improve.

Moreover, fluctuations in the injection rate can increase injector **wear**, as variations in pressure and flow can cause **additional stress on its components**, **reducing its lifespan** and increasing maintenance costs.

5.1.4 Initial Injection Response

The **initial injection response** refers to the time it takes for the injector to start supplying fuel after receiving the signal to do so. A quick initial response means that the fuel is injected immediately, while a slow initial response implies a delay in fuel delivery (between the time the signal to inject fuel is given and the time the fuel actually begins to enter the combustion chamber).

Since fuel combustion in an internal combustion engine depends on precise timing between fuel injection and piston position, **a delay in injection can cause the fuel to not be adequately mixed with air when compression occurs** (desynchronizing events), which delays the effective start of combustion (making it suboptimal). This means that under high load conditions (with a slower initial response), the engine's ability to quickly reach the required power is limited.

According to [33], ammonia exhibits a **slower penetration rate** (refers to the speed at which the fuel spray advances into the combustion chamber after being injected. A higher penetration rate means the fuel spreads quickly, enhancing mixing with air, while a lower penetration rate indicates slower fuel spray movement, which may lead to less efficient mixing and combustion) when injected compared to diesel. This slower penetration rate suggests a **lower momentum of the ammonia spray** (refers to the product of the mass and velocity of the fuel droplets as they are injected into the combustion chamber. Higher momentum means the spray has more force behind it, helping it to penetrate deeper into the combustion chamber and mix more thoroughly with the air. Lower momentum indicates less force, resulting in shallower penetration and potentially less efficient mixing), which is influenced by the internal flow dynamics and operational characteristics of the injector. High fuel viscosity of ammonia leads to increased friction within the sac, resulting in a slower needle lift. Consequently, this could be a explanation of why it takes longer for the injection process to commence after the energizing signal is given when using ammonia as a fuel.

5.2 Parameter adjustment

5.2.1 Rail Pressure

The initial parameter to be tested, as for diesel, is the **rail pressure**. Various rail pressure values will be examined (300 bar (red), 400 bar (blue), 600 bar (green), and 700 bar (magenta)), with the diesel plot also maintained for comparison.

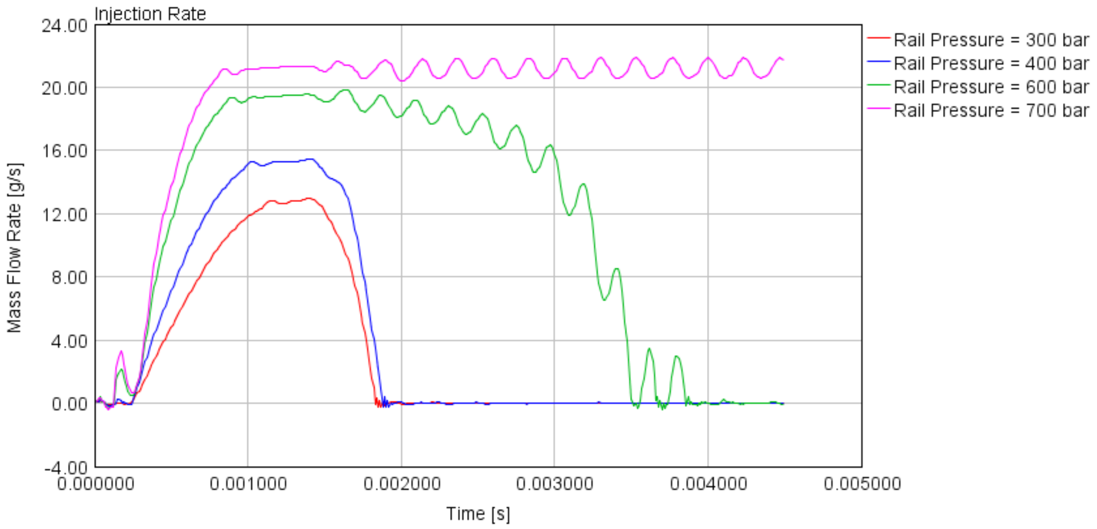


Figure 5.2: Injection rate for ammonia at different rail pressures

Parameter	Description	Cases	Unit
RailPressure	Rail Pressure (Absolute)	300, 400, 600, 800	bar
FuelTemp	Fuel Temperature	10	°C
Fuel	Composition	NH3_Laura	
WallTemp	Wall Temperature	10	°C
DrainPressure	Drain Pressure (Absolute)	8	bar
chamberPressure	Pressure (Absolute) at Injector	50	bar
chamberTemp	Temperature at Injector	10	°C
chamberComp	Composition at Injector	NH3_Laura	
D_OZ	Hole Diameter	0.205	mm
D_OA	Hole Diameter	0.26	mm
ET	Energizing Time	1	ms

Table 5.2: Simulation Parameters

As the rail pressure increases, the maximum injection rate also increases. However, it is observed that beyond 600 bar, the rate becomes very unstable and struggles to close the system.

For the 300 and 400 bar curves, the injection is relatively brief, ending around 2 ms, similar to diesel at 400 bar. For these lower pressure values, the rate is also more stable, but the maximum rate is lower. Higher rail pressure results in a faster initial response. However, it also presents initial instability.

This analysis highlights the importance of finding a balance between rail pressure and injection rate stability to maximize engine efficiency and injection system durability.

Of the values analyzed, working at **400 bar** seems to be the most pertinent to avoid instabilities, possibly slightly higher (500 or 600 bar) to get closer to the target curve, which would be the diesel curve. It should also be noted that the pressure limits ensuring proper opening and closing and thus correct injection were tested. Beyond 800 bar, closing did not occur.

This can also be contrasted with the values of the **discharge coefficient** throughout the simulation (seen in figure 5.3). The discharge coefficient is a measure of how efficiently the injector allows fuel to pass through its orifice. For lower pressures, it is necessary to optimize the injector design and possibly the injection strategy to reduce fluctuations and improve the stability of the discharge coefficient. Its fluctuations and drops must be minimized to ensure a more efficient and stable fuel injection, thus improving the overall engine performance.

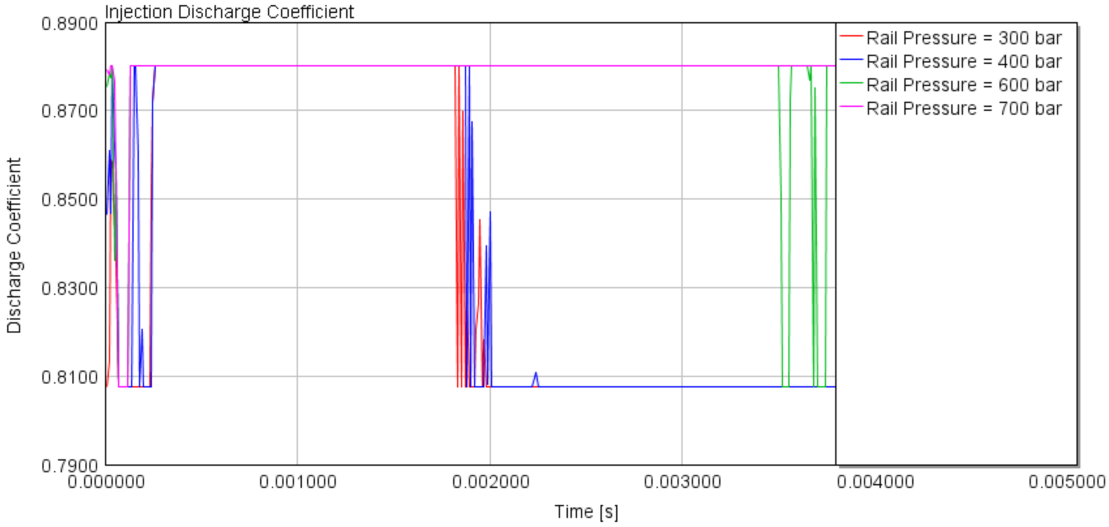


Figure 5.3: Discharge coefficient for ammonia at different rail pressures

It was observed that the model failed starting at 800 bar. These problems were also seen in the experimental trials. This is due to phase change (from liquid to vapor in the injector). This can also be seen in the model with the cavitation number **??**

5.2.2 Fuel Temperature

Different fuel temperatures were tested: 10°C (magenta), -5°C (blue), 0°C (green), 20°C (red), and 30°C (cyan), and the injection rate was measured in each case to study its effect. The rest of the operating parameters are constant and specified in table 5.3.

First, no significant difference is observed in the injection duration with respect to the fuel temperature. **The stability of the injection does not appear to be significantly affected by the fuel temperature** (figure 5.5).

The **maximum injection rate value** is influenced by the fuel temperature. This is because, at lower temperatures, the fuel's density increases. A denser fuel can contain more mass per unit volume, leading to a higher injection rate.

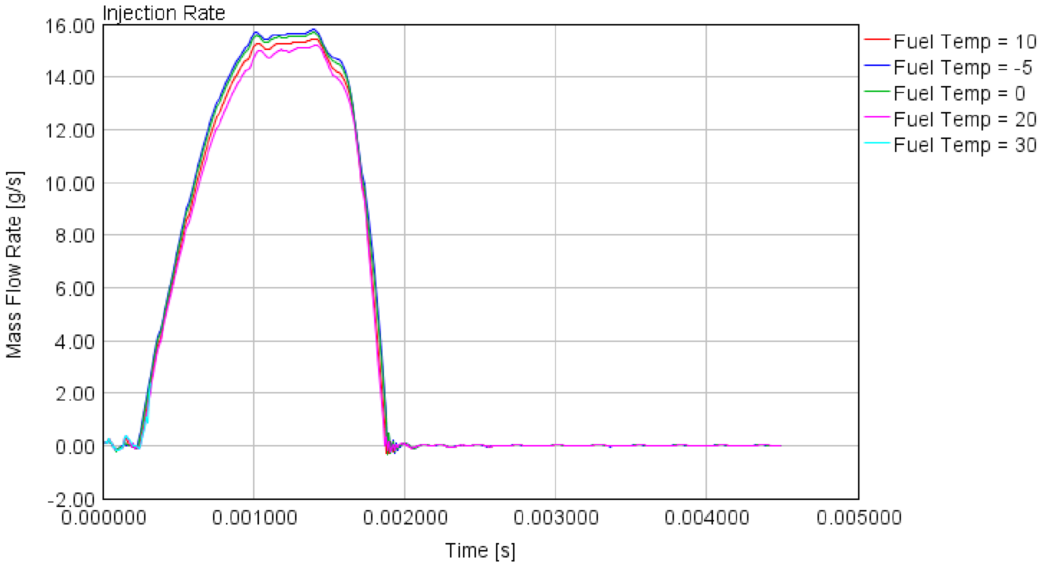


Figure 5.4: Injection rate for ammonia at different fuel temperatures

Parameter	**Description**	**Cases**	**Unit**
RailPressure	Rail Pressure (Absolute)	400	bar
FuelTemp	Fuel Temperature	**-5, 0, 10, 20, 30**	°C
Fuel	Composition	NH3_Laura	
WallTemp	Wall Temperature	10	°C
DrainPressure	Drain Pressure (Absolute)	8	bar
chamberPressure	Pressure (Absolute) at Injector	50	bar
chamberTemp	Temperature at Injector	10	°C
chamberComp	Composition at Injector	NH3_Laura	
D_OZ	Hole Diameter	0.205	mm
D_OA	Hole Diameter	0.26	mm
ET	Energizing Time	1	ms

Table 5.3: Simulation Parameters

Through iterations, it was determined that the **maximum temperature** at which the system operates is **28°C**. Ideally, the **temperature should be kept as low as possible**, although this can be challenging since, as explained in section 4.2.2, during operation, the fuel temperature can easily raise up to 70ºC.

Therefore, keeping the fuel temperature as low as possible is one of the main obstacles that the system will face when adapting it for ammonia. In experimental conditions, for specific tests, low temperatures can be maintained with the help of cooling systems.

5.2.3 Injection time

Next, different energizing times were tested. The graph shows the injection rate of ammonia for each of them: 0.5 ms (blue), 1 ms (red), 1.5 ms (green), and 2 ms (magenta). The rest of the operating parameters are constant and specified in table 5.4. The maximum injection rate is quite similar in all cases. However, **for very short energizing times (ET), the maximum value is not reached**. This suggests that, although the injection rate is generally constant, longer injection times allow for higher maximum values.

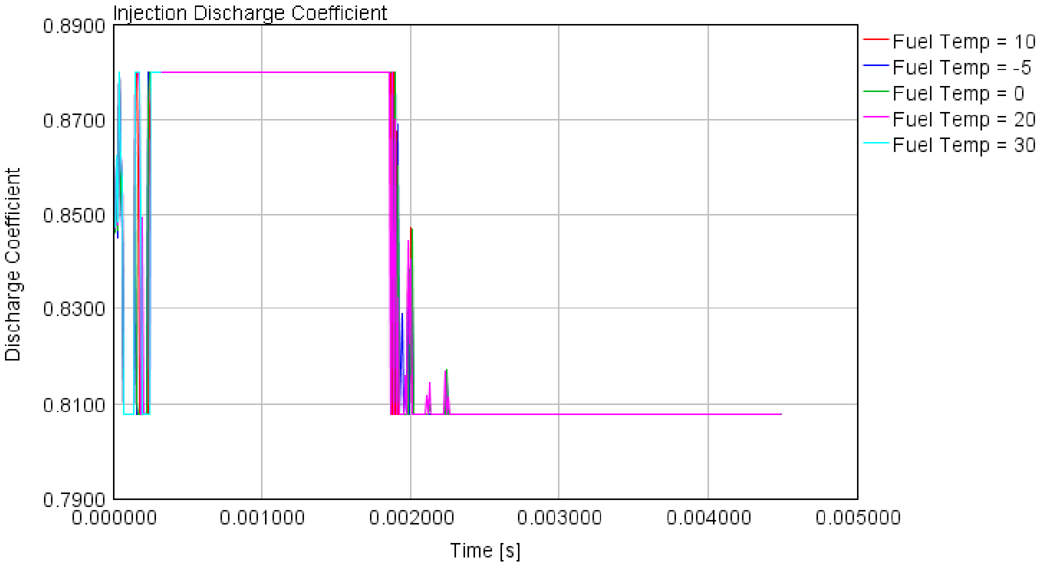


Figure 5.5: Discharge coefficient for ammonia at different fuel temperatures

Parameter	**Description**	**Cases**	**Unit**
RailPressure	Rail Pressure (Absolute)	400	bar
FuelTemp	Fuel Temperature	10	°C
Fuel	Composition	NH3_Laura	
WallTemp	Wall Temperature	10	°C
DrainPressure	Drain Pressure (Absolute)	8	bar
chamberPressure	Pressure (Absolute) at Injector	50	bar
chamberTemp	Temperature at Injector	10	°C
chamberComp	Composition at Injector	NH3_Laura	
D_OZ	Hole Diameter	0.205	mm
D_OA	Hole Diameter	0.26	mm
ET	Energizing Time	**0.5, 1, 1.5, 2**	ms

Table 5.4: Simulation Parameters

As the ET increases, so does the **duration of the injection**. This is evident in the curves, where it is observed that longer injection times result in a more prolonged injection. The curves are all quite stable, indicating that the injection system maintains a constant injection rate during the injection period. This **stability** is crucial for smooth engine operation.

All the curves exhibit the same rapid initial response, with an abrupt increase in the injection rate at the start of the injection period. The high stability of the injection rate, especially for shorter injection times, indicates that **the injection system is capable of maintaining a constant and controlled fuel flow**, which is essential for efficient engine operation.

This analysis highlights the importance of adjusting the energizing time (ET) to optimize the injection rate and combustion efficiency in compression engines using ammonia, while ensuring the stability of the injection system. To achieve a curve similar to that of diesel, the most suitable ET is **1 ms**.

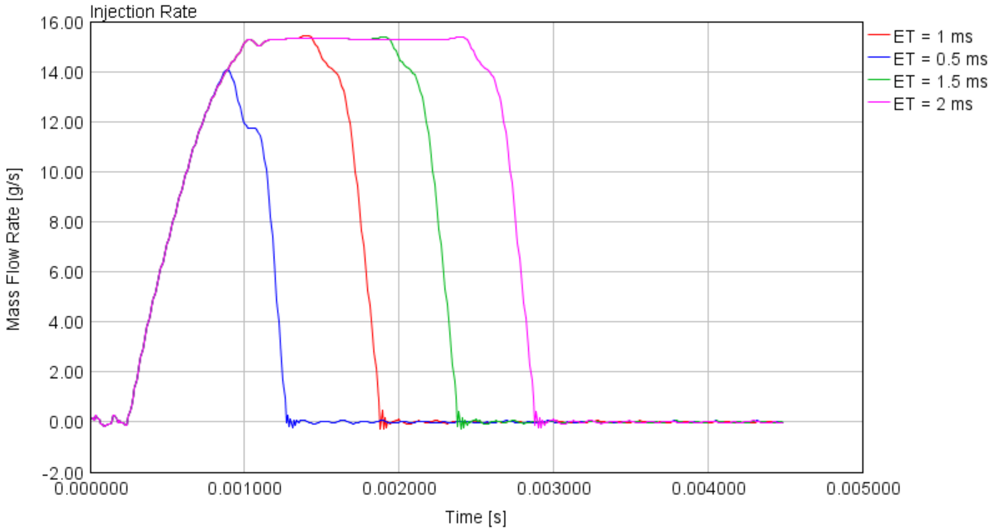


Figure 5.6: Injection rate for ammonia with different ET

5.2.4 OZ diameter

In this subsection, different values of the OZ diameter (inlet orifice) close to the reference value will be tested (conditions of the test in table 5.6) to study the impact of these variations on the fluid behavior during injection and within the control volume. This study will help identify the sensitivity to the diameter to ensure efficient and stable performance of the injection system.

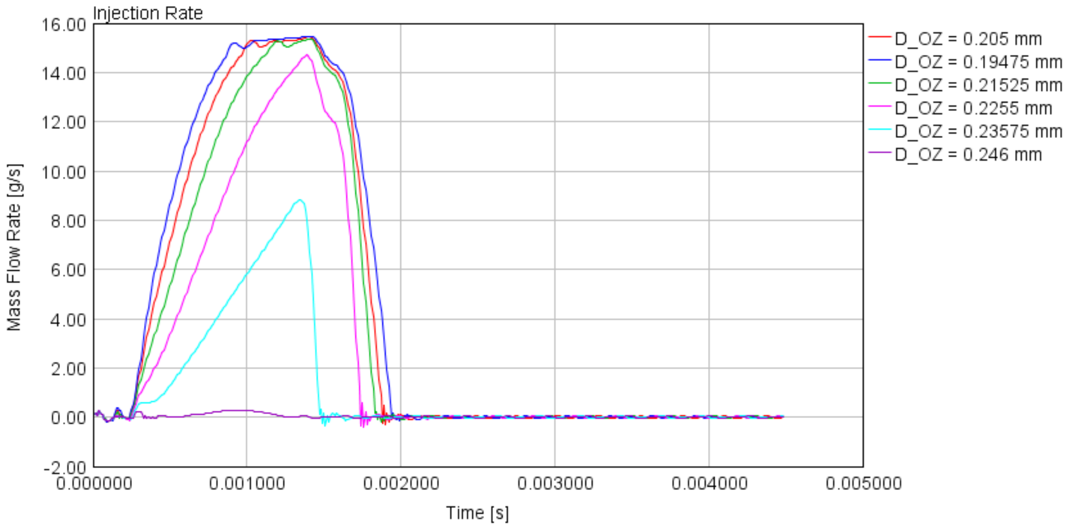


Figure 5.7: Injection rate for ammonia with OZ diameters

These results are very similar to the ones obtained for diesel. **An increase in the diameter of the OZ orifice leads to a reduced injection rate**(figure 5.6). This reduction is due to a drop in pressure, which results in less fuel being injected. A **smaller opening** allows for **faster opening times** but complicates the **closing process**. If the diameter is reduced too much, opening may not occur because the pressure is insufficient.

When the energizing time is increased for the same diameters (Figure 5.7), the amount of

Parameter	**Description**	**Cases**	**Unit**
RailPressure	Rail Pressure (Absolute)	400	bar
FuelTemp	Fuel Temperature	10	°C
Fuel	Composition	NH3_Laura	
WallTemp	Wall Temperature	10	°C
DrainPressure	Drain Pressure (Absolute)	8	bar
chamberPressure	Pressure (Absolute) at Injector	50	bar
chamberTemp	Temperature at Injector	10	°C
chamberComp	Composition at Injector	NH3_Laura	
D_OZ	Hole Diameter	**0.195, 0.205, 0.215, 0.226, 0.236, 0.246**	mm
D_OA	Hole Diameter	0.26	mm
ET	Energizing Time	1	ms

Table 5.5: Simulation Parameters

fuel injected rises and the transient process is prolonged. Nevertheless, the opening and closing processes are mostly unaffected.

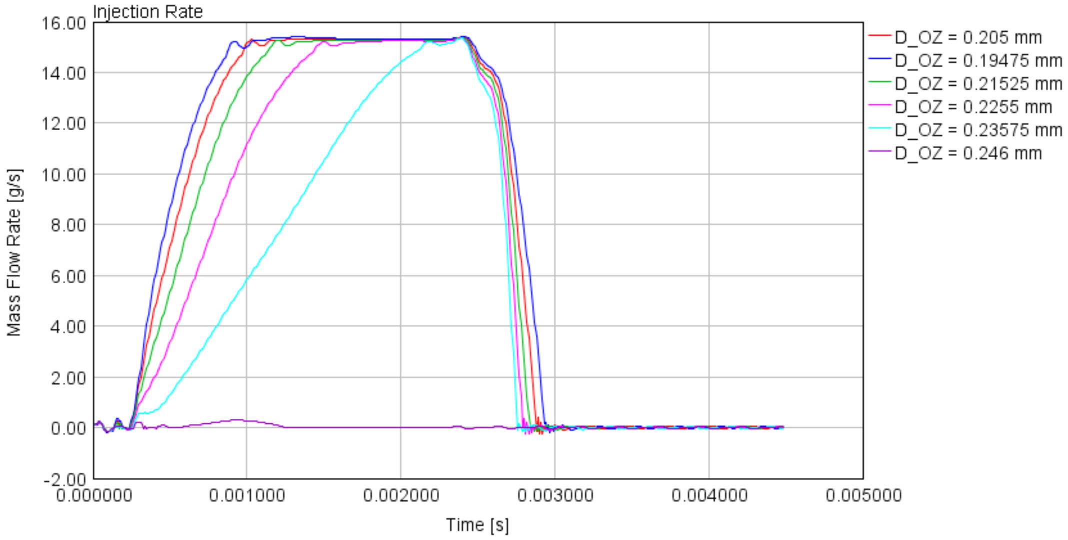


Figure 5.8: Injection rate for ammonia with OZ diameters (ET=2)

Effects of OZ's diameter in the control volume

To better understand the effect of OZ's dimensions in the system, analyzing their impact on the control volume is helpful. First, as seen in figure 5.8, **a larger diameter implies a larger mass flow through OZ**, but also, **a lower pressure drop peak** (figure 5.9). Additionally, a larger opening results in lower pressure levels, increasing the cavitation number (5.10) and thus the risk of bubble formation, which destabilizes and wears out the system.

The dimensions of OZ (the inlet orifice) also affect the fluid behavior when traversing OA (the outlet orifice). As shown in figures 5.13 and 5.14, **for larger diameters of OZ, OA takes longer to close**. This is due to lower pressure in the control volume, encouraged by keeping OA open during most of the injection time. Furthermore, increased throat pressure and temperature stresses (figures 5.15 and 5.15) contribute to wear.

These results are similar to those observed when analyzing diesel, demonstrating that both fuels exhibit comparable behaviors in terms of injection dynamics and the effects of orifice dimensions on the system.

5.2.5 OA diameter

Now, various values of the OA diameter (outlet orifice) near the reference value will be examined to assess their impact on fluid behavior during injection and within the control volume aiming to determine the ideal diameter for achieving optimal and consistent performance of the injection system. Te values considered and the other parameters' values are listed in table 5.6.

Parameter	**Description**	**Cases**	**Unit**
RailPressure	Rail Pressure (Absolute)	400	bar
FuelTemp	Fuel Temperature	10	°C
Fuel	Composition	NH3_Laura	
WallTemp	Wall Temperature	10	°C
DrainPressure	Drain Pressure (Absolute)	8	bar
chamberPressure	Pressure (Absolute) at Injector	50	bar
chamberTemp	Temperature at Injector	10	°C
chamberComp	Composition at Injector	NH3_Laura	
D_OZ	Hole Diameter	0.205	mm
D_OA	Hole Diameter	**0.247, 0.26, 0.273, 0.286, 0.299, 0.312**	mm
ET	Energizing Time	1	ms

Table 5.6: Simulation Parameters

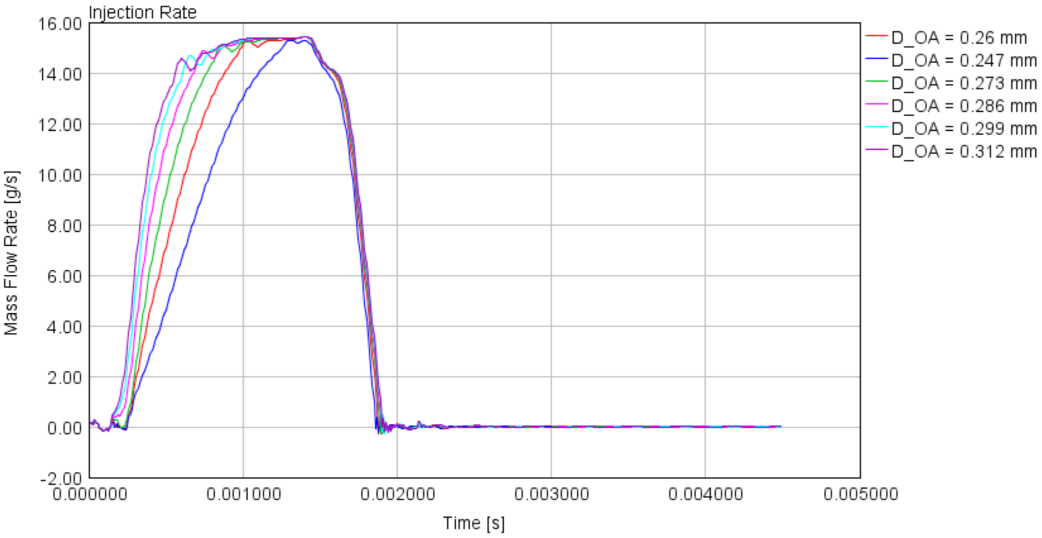


Figure 5.9: Injection rate for ammonia with OA diameters

The results are, again, similar to those obtained with diesel. Increasing the diameter of the OA orifice enlarges the flow area, which can result in a higher mass flow rate (allows more fuel to pass through) as shown in Figure 5.18.

Effects of OA's diameter in the control volume

Conversely, OA's dimensions also affect the flow through OZ. **Increasing OA's diameter results in a decrease in the mass flow rate through OZ** (figure 5.19) and a **decrease in the pressure drop** (figure 5.20). Additionally, this leads to an increase in the throat pressure and temperature in OZ, causing wear on the orifice.

On the other hand, **increasing OA's diameter results in a higher mass flow rate through the orifice** (figure 5.23) and a **lower pressure drop** (figure 5.24). The throat pressure and temperature gradients also increase (figures 5.26, 5.25) causing thermal stress on the injector, potentially leading to wear.

5.3 Comparison with other fuels

Table 5.7: Comparison of Ammonia, Diesel, and Methanol Fuel Properties

Property	**Ammonia**	**Diesel**	**Methanol**
Chemical formula	NH_3	$C_{12}H_{23}$	CH_3OH
Energy density (MJ/kg)	18.6	42.8	19.92
Energy density (MJ/L)	11.2* 12.5**	35.8	15.6
Autoignition temperature (°C)	651	210	464
Flame speed (m/s)	0.32–0.40	0.25–0.3	0.36
Density (kg/m^3)	0.771* 600**	850	786
Minimum ignition energy (mJ)	0.22–0.36	0.3–0.6	0.14
Dynamic viscosity (Pa·s) at 25°C	0.00013***	0.0021	0.00055***
Low heating value (MJ/kg)	18.80	43.4	20.09
Octane number	130	8-15	112
Boiling point (K)	239.80	453	338
Freezing point (K)	195.50	180	175
Latent heat of vaporization (kJ/kg)	1371	300	1104

* Gaseous form under atmospheric pressure and 20°C
** Liquefied at 0.99 MPa temperature of 25°C
*** Liquefied at 1 MPa

To compare the model responses with another fuel, tests were also conducted with **methanol**. The table 5.8 shows the parameters tested to compare the three fuels: diesel, ammonia, and methanol.

Ammonia and methanol have comparable characteristics when used as fuels. However, methanol contains carbon, which means that its combustion generates CO_2 and potentially other incomplete combustion products like CO, which is what using ammonia or other carbon-free fuels aims to avoid. Additionally, methanol is highly flammable, and its vapors can form explosive mixtures with air, presenting significant safety risks. In contrast, ammonia is not flammable in its liquid form and has a narrower flammability limit compared to methanol, which can reduce certain explosion risks.

Methanol is an alcohol and can also be used as a fuel. Compared to diesel and ammonia, methanol has several properties that are worth highlighting. Its energy density is 19.92 MJ/kg slightly higher than that of ammonia (18.6 MJ/kg). Regarding density, methanol has a density of 791 kg/m^3, which is considerably higher than that of gaseous ammonia (see table 5.7). This affects the storage and handling of the fuel: methanol can be stored at room temperature in a liquid state. Unlike ammonia, methanol remains in a liquid state at normal atmospheric temperature and pressure.

Parameter	**Description**	**Cases**	**Unit**
RailPressure	Rail Pressure (Absolute)	400	bar
FuelTemp	Fuel Temperature	10	°C
Fuel	Composition	Diesel, Ammonia, Methanol	
WallTemp	Wall Temperature	10	°C
DrainPressure	Drain Pressure (Absolute)	8	bar
chamberPressure	Pressure (Absolute) at Injector Outlet	50	bar
chamberTemp	Temperature at Injector Outlet	10	°C
chamberComp	Composition at Injector Outlet	Diesel, Ammonia, Methanol	
D_OZ	Hole Diameter	0.205	mm
D_OA	Hole Diameter	0.26	mm

Table 5.8: Parameters set up

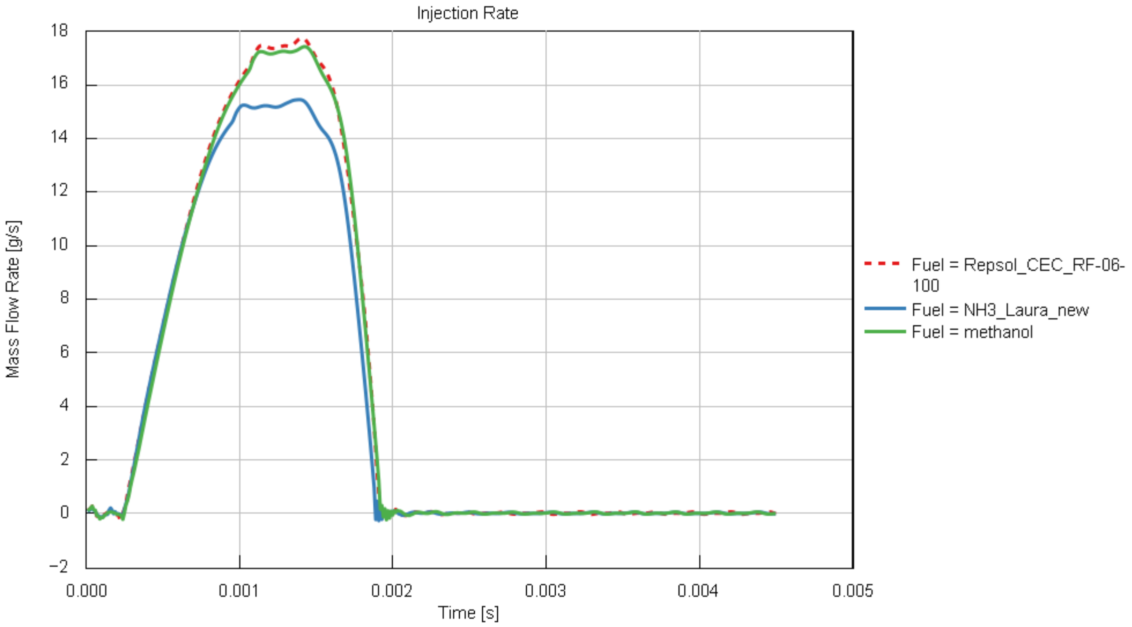


Figure 5.10: Injection rate comparison of different fuels

From the tests conducted , it can be observed that **ammonia shows a higher volumetric flow rate** (figure 5.12) but a **lower mass flow rate** (figure 5.11) compared to diesel and methanol. This is due to its lower density, which is a key property of ammonia. On the other hand, **methanol has a volumetric and mass flow rate comparable to diesel** (and therefore a similar injection rate in figure 5.10, but exhibits improved stability in its curves (probably related to its lower viscosity). Having an intermediate density between diesel and ammonia, methanol can maintain an efficient mass flow rate without the lower density issues of ammonia.

These observations indicate that the injection system needs to be adapted to the type of fuel used. However, this adaptation can be carried out without too many problems. The use of ammonia, methanol, and diesel in appropriately adjusted injection systems can result in efficient and safe operation, taking advantage of the unique properties of each fuel to optimize engine performance and energy efficiency.

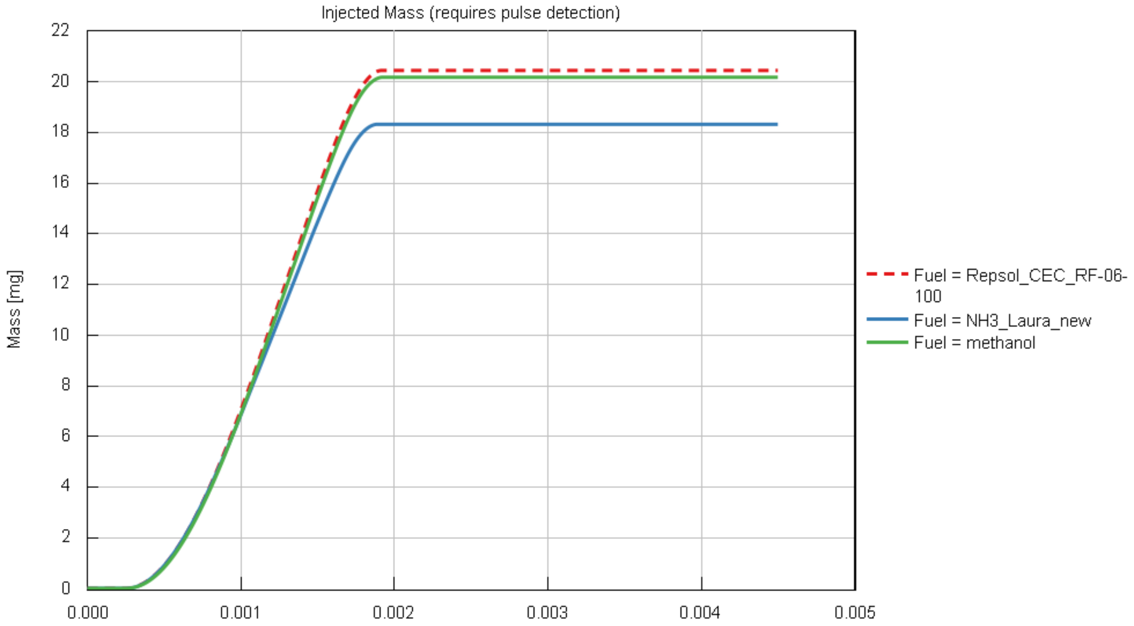


Figure 5.11: Injected mass comparison of different fuels

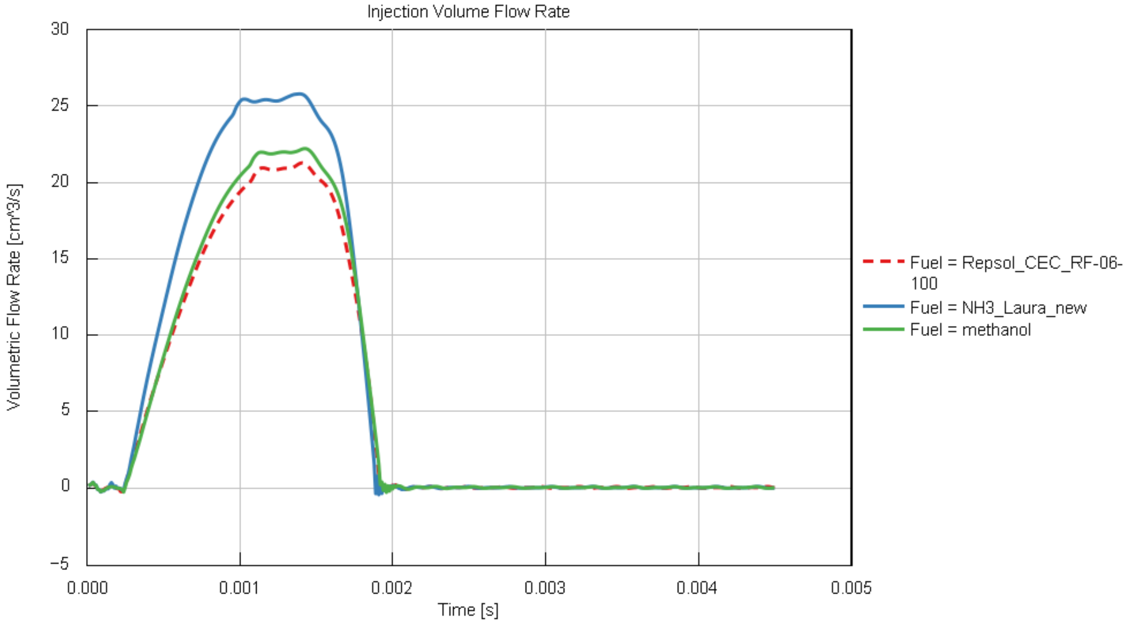


Figure 5.12: Injected volume comparison of different fuels

Chapter 6

Conclusions and future work

6.1 Conclusions

The research presented in this thesis has explored the potential of using ammonia as a viable alternative to traditional diesel fuel in compression ignition engines. The 1D modelling of the ammonia injector using GT-Power software has provided valuable insights into the operational parameters and modifications necessary to optimize ammonia combustion.

Ammonia, despite its high ignition temperature and low flame speed, can potentially match the performance of diesel when specific modifications are made to the injection system. This finding suggests that with appropriate tuning, ammonia could serve as an effective alternative fuel, providing similar power outputs and efficiencies as diesel. The modifications required to achieve this include **optimizing the injection pressure and timing to compensate for ammonia's lower reactivity and slower combustion rate**.

The study identified the optimal operating pressures and temperatures required for efficient ammonia combustion. It was found that **increasing the rail pressure and adjusting the fuel temperature** can significantly improve injection rates and combustion stability. Higher rail pressures help to overcome ammonia's high autoignition temperature, ensuring that the fuel ignites reliably within the engine. Similarly, maintaining at low temperatures the ammonia fuel can enhance atomization and mixing, leading to a more stable and complete combustion process.

Adjusting the **energizing time** was crucial to achieving the desired injection characteristics. Longer energizing times were shown to increase the amount of fuel injected, although this also necessitates careful control to avoid instability. Precise control of injection timing is essential to ensure that ammonia is delivered at the correct moment in the combustion cycle, maximizing power output and minimizing emissions. This involves fine-tuning the injector opening duration and synchronizing it with the engine's operating cycle to optimize performance.

The geometries of the inlet (OZ) and outlet (OA) orifices were shown to have a substantial impact on fluid behavior and injection performance. Optimal diameters were determined to balance the trade-offs between injection rate and control. Fine-tuning these geometric parameters is critical to ensure that the ammonia fuel is injected in a manner that promotes efficient mixing with air, complete combustion, and minimal pollutant formation.

The tests conducted in this study provide hope that ammonia could be used in applications that do not require high engine speeds, such as power generation stations or heavy-duty engines (in trucks, tractors or ships). Implementing ammonia in faster engines would still require further refinements and considerations, particularly in terms of safety. For power generation installations, ammonia could be a clean alternative, provided that its synthesis is also performed in an environmentally friendly manner.

6.2 Future Work

This project establishes a basis for further research on ammonia injection and its potential applications and implementation in internal combustion engines.

First, experimental validation is crucial for the findings of this study, which has primarily relied on 1D modelling. Conducting physical experiments with ammonia injectors under various conditions is essential to verify the accuracy of the model and provide real-world data. Such experiments will help to confirm the theoretical predictions and ensure the practical applicability of the proposed injection system.

Furthermore, future work should incorporate more advanced modelling techniques to enhance the accuracy of ammonia combustion simulations. Utilizing 3D Computational Fluid Dynamics (CFD) will allow researchers to capture the complexities of ammonia combustion more precisely, providing a deeper understanding of the underlying processes and improving the reliability of the predictions.

Additionally, investigating the compatibility of injector materials with ammonia is crucial due to ammonia's corrosive nature. Ensuring the durability of injector components is vital for practical applications. Intuitively, this material compatibility could be one of the main limitations of using ammonia in these systems. This aspect is not addressed by the current model, but it has been explored in another studies ([41]). Understanding and mitigating material degradation will be essential for the successful implementation of ammonia as a fuel.

Further studies should focus on integrating the ammonia injector model into a complete engine system. This includes assessing the performance of ammonia in a full-scale engine and understanding the implications for engine design and modifications.

The environmental impact of using ammonia as a fuel should be still studied. This includes assessing the lifecycle emissions and potential benefits over traditional fossil fuels. Additionally, research should address the necessary safety measures for handling and storing ammonia. Given ammonia's toxicity and potential health hazards, it is imperative to develop and implement rigorous safety protocols to protect personnel and the environment.

And finally, conducting an economic analysis of ammonia production, storage, and distribution will help determine the feasibility of large-scale implementation. This should include a comparison with other alternative fuels such as hydrogen and biofuels.

By addressing these areas, future research can further solidify the case for ammonia as a sustainable and efficient fuel for compression ignition engines, contributing to the broader goal of reducing carbon emissions and promoting sustainable energy solutions.

Bibliography

[1] Real decreto 486/1997, de 14 de abril, por el que se establecen las disposiciones mínimas de seguridad y salud en los lugares de trabajo. `https://www.boe.es/buscar/act.php?id=BOE-A-1997-8669`, 1997. BOE-A-1997-8669.

[2] Real decreto 488/1997, de 14 de abril, 1997. Accessed: 2024-07-21.

[3] Aftabuzzaman, M., and Mazloumi, E. Achieving sustainable urban transport mobility in post peak oil era. *Transport Policy 18*, 5 (2011), 695–702.

[4] Agarwal, A. K. Biofuels (alcohols and biodiesel) applications as fuels for internal combustion engines. *Progress in Energy and Combustion Science 33*, 3 (2007), 233–271.

[5] Arrhenius, S. On the influence of carbonic acid in the air upon the temperature of the ground. *Philosophical Magazine and Journal of Science* (1896).

[6] BP. bp statistical review of world energy 2022 — 71st edition.

[7] Britannica, E. Steam engine, 2024. Accessed: 2024-07-17.

[8] Cardoso, J. S., Silva, V., Rocha, R. C., Hall, M. J., Costa, M., and Eusébio, D. Ammonia as an energy vector: Current and future prospects for low-carbon fuel applications in internal combustion engines. *Journal of Cleaner Production 296* (2021), 126562.

[9] Carnot, N. L. S. *Reflections on the Motive Power of Fire.* 1824.

[10] Chu, S., and Majumdar, A. Opportunities and challenges for a sustainable energy future. *Nature 488* (08 2012), 294–303.

[11] CMT Motores Térmicos, U. P. d. V. Cmt - motores térmicos, 2024. Accessed: 2024-07-17.

[12] Desantes, P. F. P. P. J. M. *Motores de combustion interna alternativos.* 2011.

[13] El-Adawy, M., Nemitallah, M. A., and Abdelhafez, A. Towards sustainable hydrogen and ammonia internal combustion engines: Challenges and opportunities. *Fuel 364* (2024), 131090.

[14] et al., I. R. Hydrogen as fuel of tomorrow. *INTERNATIONAL JOURNAL OF SCIENTIFIC RESEARCH IN ENGINEERING AND MANAGEMENT* (2024).

[15] Evans, B. Ammonia as a future fuel. In *29th Annual International Ammonia Energy Conference* (2012). Accessed: 2024-07-16.

[16] Heywood, J. B. *Internal Combustion Engine Fundamentals.* McGraw-Hill Education, New York, 1988.

[17] IEA. Iea (2023), world energy outlook 2023.

[18] IEA. Energy statistics data browser, 2024.

[19] International Energy Agency. Ammonia technology roadmap. Tech. rep., International Energy Agency, 2021. Accessed: 2024-07-10.

[20] Ioan James, U. O. O. *Remarkable Engineers.* 2010.

[21] Lee, H., and Romero, J. Ipcc, 2023: Climate change 2023: Synthesis report. contribution of working groups i, ii and iii to the sixth assessment report of the intergovernmental panel on climate change.

[22] Li, T., Duan, Y., Wang, Y., Zhou, M., and Duan, L. Research progress of ammonia combustion toward low carbon energy. *Fuel Processing Technology 248* (2023), 107821.

[23] Li, Y., Gong, J., Deng, Y., Yuan, W., Fu, J., and Zhang, B. Experimental comparative study on combustion, performance and emissions characteristics of methanol, ethanol and butanol in a spark ignition engine. *Applied Thermal Engineering 115* (2017), 53–63.

[24] Lin, L., Cunshan, Z., Vittayapadung, S., Xiangqian, S., and Mingdong, D. Opportunities and challenges for biodiesel fuel. *Applied Energy* (2011).

[25] López, J. M. *Estudio Computacional de la Influencia del Levantamiento de Aguja Sobre el Flujo Interno y el Fenómeno de la Cavitación en Toberas de Inyección Diesel.* Phd thesis, Universidad Politécnica de Valencia, Valencia, Spain, May 2013.

[26] Machaj, K., Kupecki, J., Malecha, Z., Morawski, A., Skrzypkiewicz, M., Stanclik, M., and Chorowski, M. Ammonia as a potential marine fuel: A review. *Energy Strategy Reviews 44* (2022), 100926.

[27] Mathews, J. Seven steps to curb global warming. *Energy Policy 35*, 8 (2007), 4247–4259.

[28] McGraw-Hill, S. R. T. *An introduction to combustion. Concepts and applications.* 1996.

[29] Mohammed El-Adawy, Medhat A. Nemitallah, A. A. Towards sustainable hydrogen and ammonia internal combustion engines: Challenges and opportunities. *Journal of Cleaner Production 364* (2024).

[30] Nations, U. Sustainable development goals, 2024. Accessed: 2024-07-17.

[31] Nguyen, D., and Turner, J. Towards carbon-free mobility: The feasibility of hydrogen and ammonia as zero carbon fuels in spark ignition light-duty vehicles. *International Journal of Engine Research* (2024).

[32] Office of Energy Efficiency and Renewable Energy. Hydrogen storage. `https://www.energy.gov/eere/fuelcells/hydrogen-storage`, 2023. Accessed: 2024-07-10.

[33] Payri, R., García-Oliver, J. M., Bracho, G., and Cao, J. Experimental characterization of direct injection liquid ammonia sprays under non-reacting diesel-like conditions. *Fuel 362* (2024), 130851.

[34] Payri, R., la Morena, J. D., Pagano, V., Hussain, A., Sammut, G., and Smith, L. One-dimensional modeling of the interaction between close-coupled injection events for a ballistic solenoid injector. *International Journal of Engine Research 20*, 4 (2019), 452–469.

[35] Payri, R., Salvador, F., Gimeno, J., and De la Morena, J. Influence of injector technology on injection and combustion development - part 1: Hydraulic characterization. *Applied Energy 88* (04 2011), 1068–1074.

[36] Payri, R., Tormos, B., Gimeno, J., and Bracho, G. The potential of large eddy simulation (les) code for the modeling of flow in diesel injectors. *Mathematical and Computer Modelling 52* (2010).

[37] Peterson, T. C., Connolley, W. M., and Fleck, J. The myth of the 1970s global cooling scientific consensus. *Bulletin of the American Meteorological Society* (2008).

[38] Piriou, B., Vaitilingom, G., Veyssière, B., Cuq, B., and Rouau, X. Potential direct use of solid biomass in internal combustion engines. *Progress in Energy and Combustion Science 39*, 1 (2013), 169–188.

[39] Press, O. U. *Oxford Dictionary of Physics*, 7th ed. Oxford University Press, 2015.

[40] Qi, Y., Liu, W., Liu, S., Wang, W., Peng, Y., and Wang, Z. A review on ammonia-hydrogen fueled internal combustion engines. *eTransportation 18* (2023), 100288.

[41] Rouchi, O. C. Development of an experimental test-rig to characterise the ammonia injection process based on momentum flux, 2023.

[42] Talens, M. C. *Thermal Effects Influence on the Diesel Injector Performance through a Combined 1D Modelling and Experimental Approach.* Doctoral thesis, Universitat Politècnica de València, 2016.

[43] Technologies, G. Gt-power. `https://www.gtisoft.com/gt-suite-applications/gt-power/`. Accessed: 2024-07-15.

[44] The Royal Society. Ammonia: zero-carbon fertiliser, fuel and energy store. Tech. rep., The Royal Society, 2020. Accessed: 2024-07-10.

[45] Valera-Medina, A., Xiao, H., Owen-Jones, M., David, W., and Bowen, P. Ammonia for power. *Progress in Energy and Combustion Science 69* (2018), 63–102.

[46] Verhelst, S., Turner, J. W., Sileghem, L., and Vancoillie, J. Methanol as a fuel for internal combustion engines. *Progress in Energy and Combustion Science 70* (2019), 43–88.

[47] White, F. M. *Fluid Mechanics*, 7th ed. McGraw-Hill Education, 2011.

Part II

Annex

Sensitivity analysis with diesel

Rail pressure

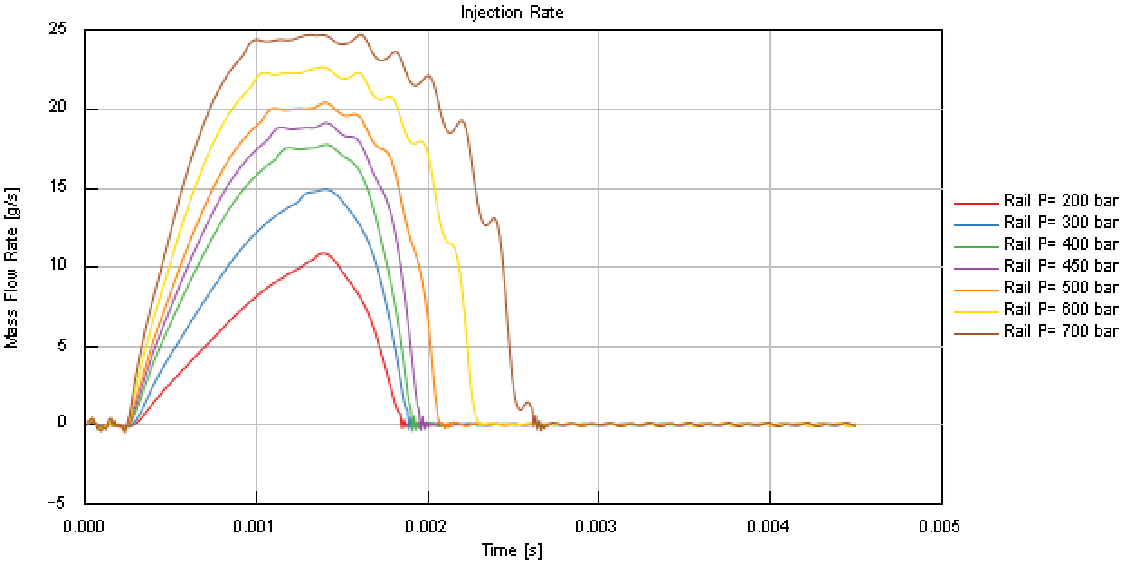


Figure 4.1: Injection rates for different rail pressures using diesel as a fuel and $EI = 1ms$

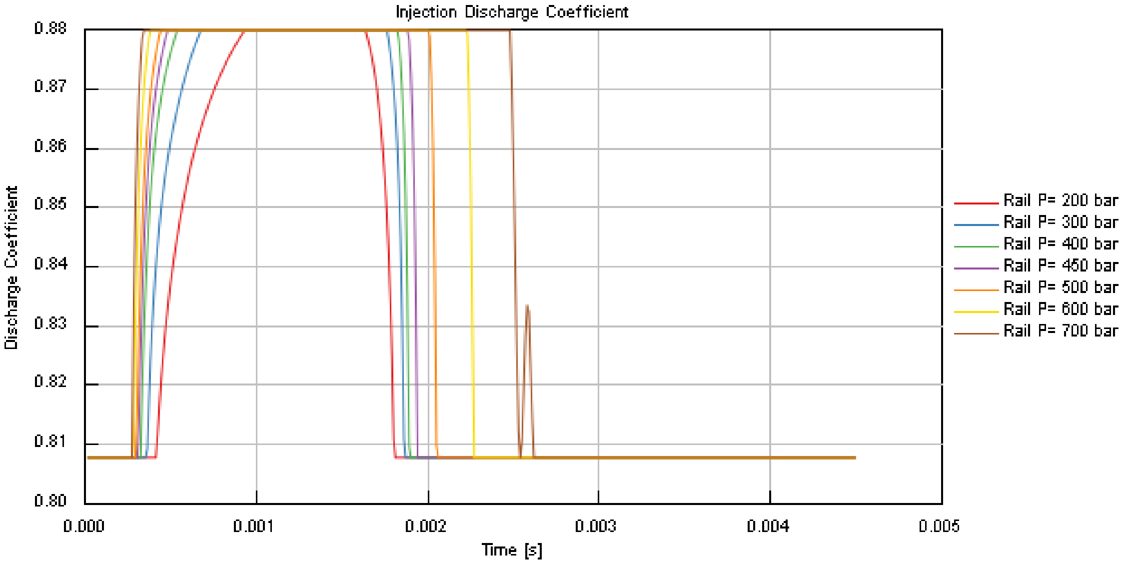


Figure 4.2: Discharge coefficients for different rail pressures using diesel as a fuel

Fuel Temperature

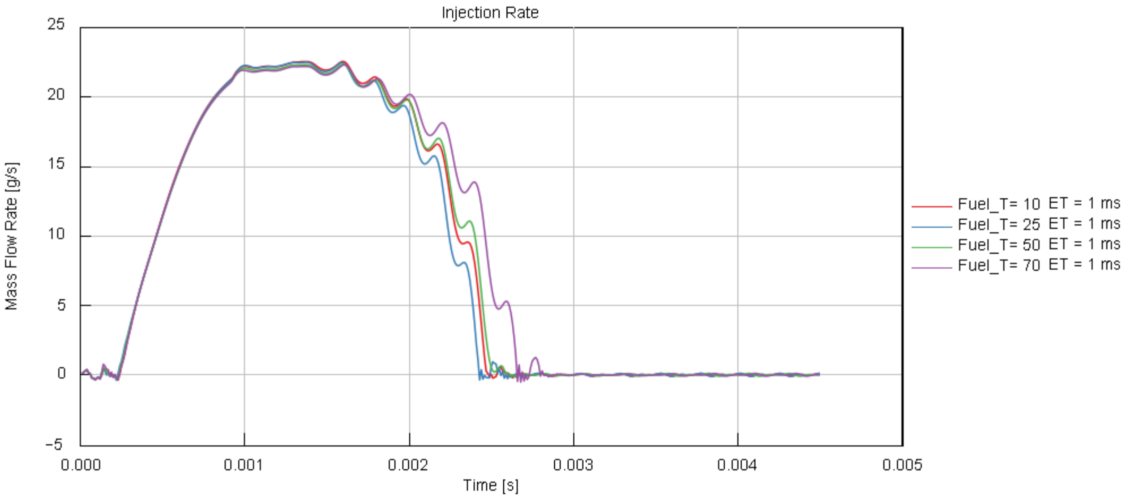


Figure 4.3: Injection rates for different fuel temperatures using diesel as a fuel and $EI = 1ms$

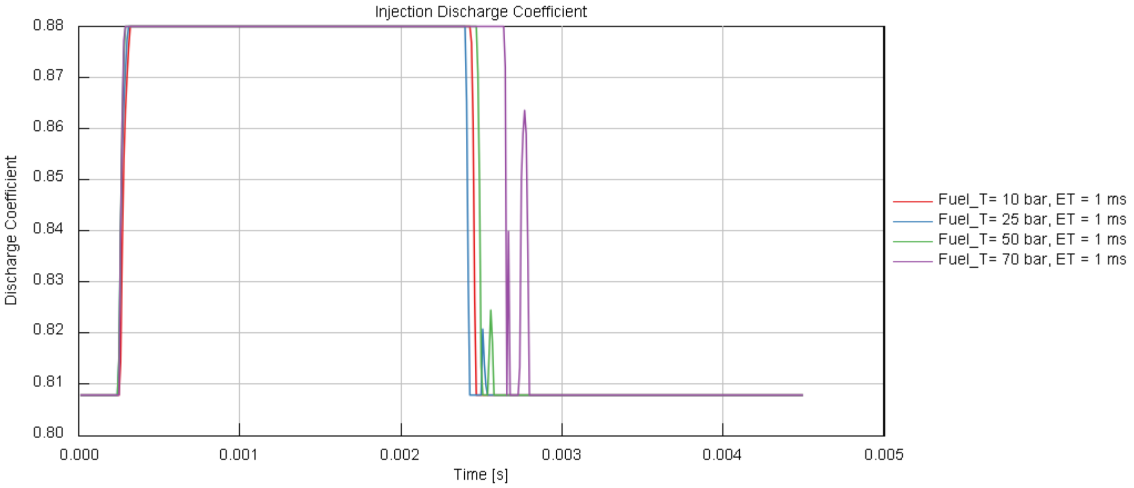


Figure 4.4: Discharge coefficient for different fuel temperatures using diesel as a fuel

Energizing time

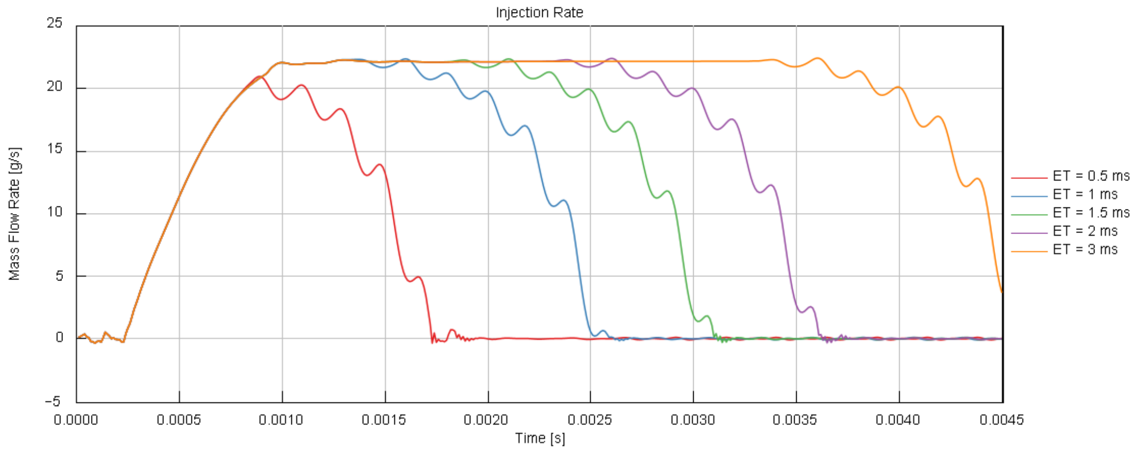


Figure 4.5: Injection rates for different energizing times using diesel as a fuel

OA and OZ geometries

OZ diameter

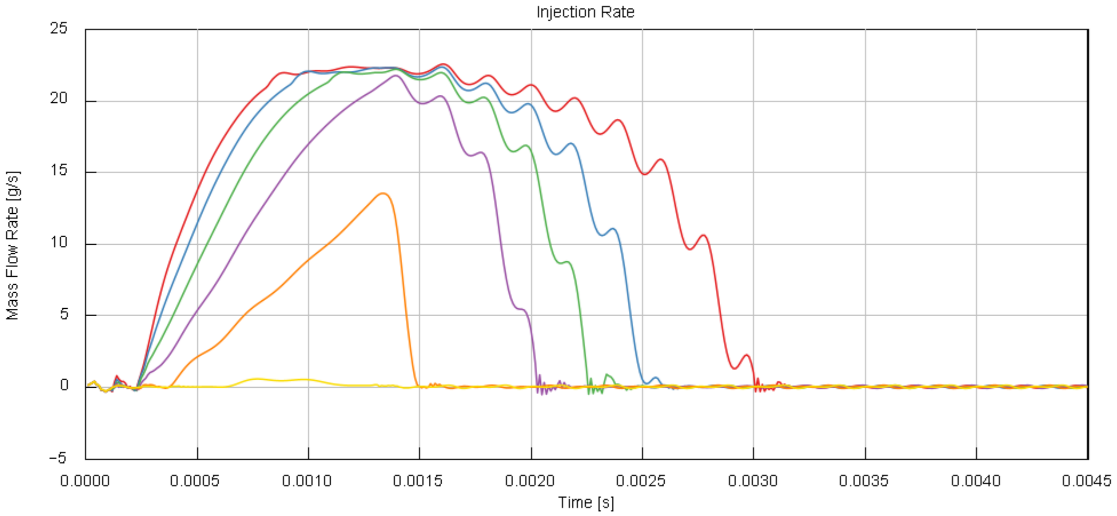


Figure 4.6: Injection Rate for OZ Diameters (ET=1 ms)

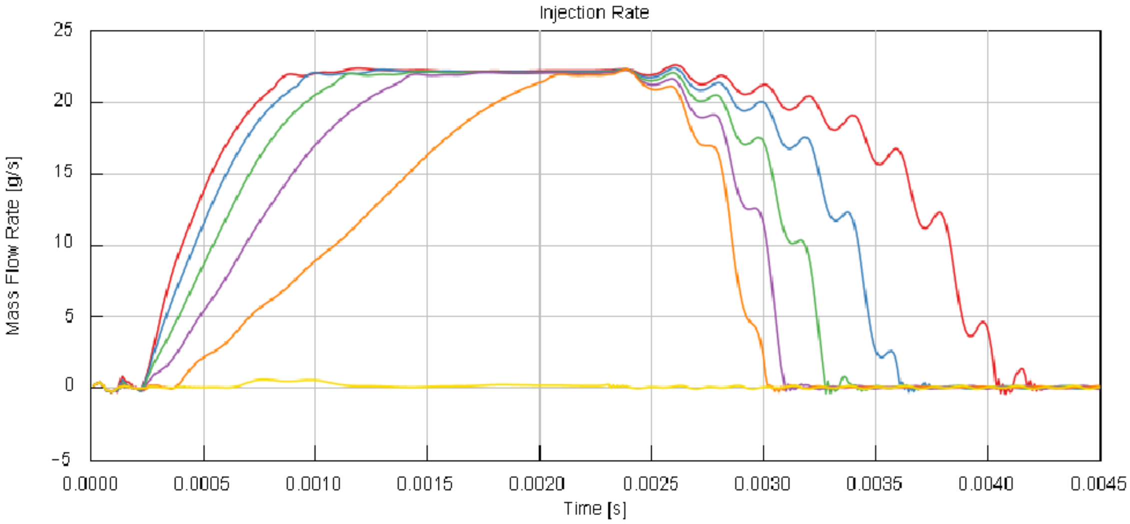


Figure 4.7: Injection Rate for OZ Diameters (ET=2 ms)

Effects in OZ

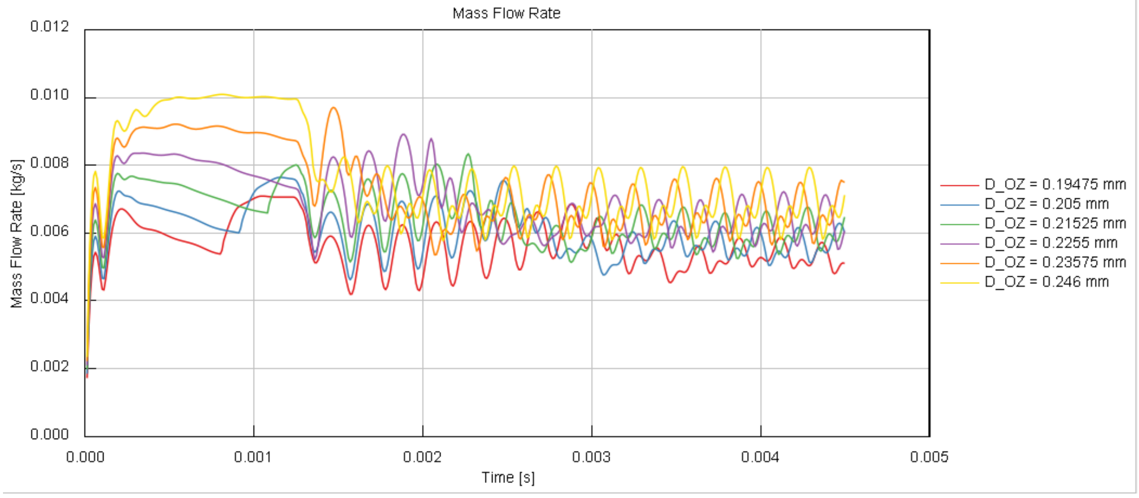


Figure 4.8: Mass flow rate through OZ for different OZ diameters

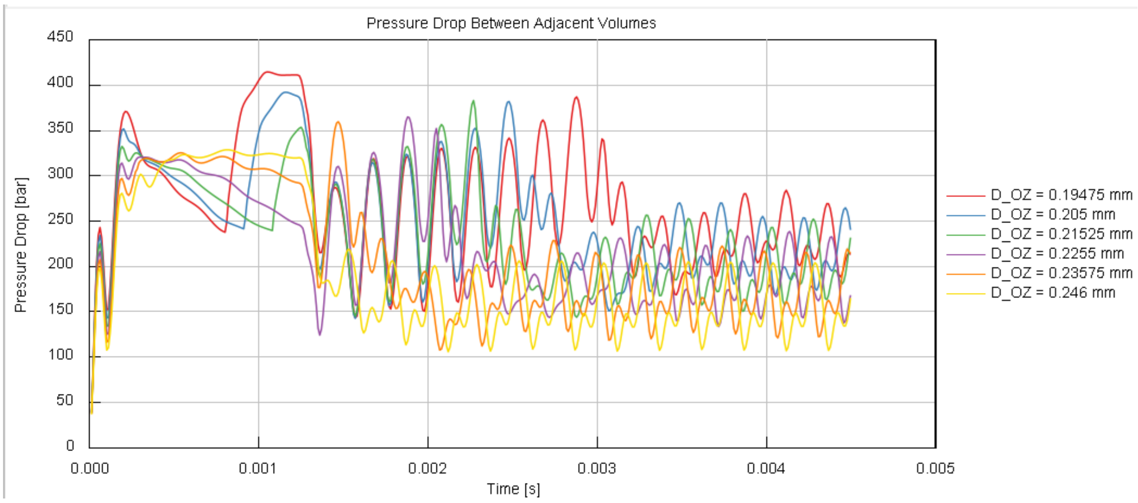


Figure 4.9: Pressure drop through OZ for different OZ diameters

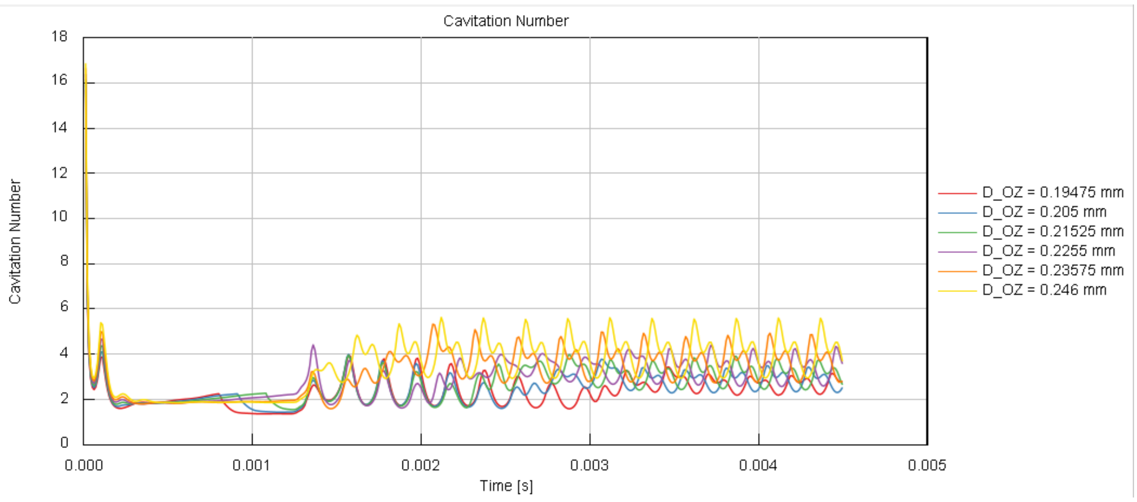


Figure 4.10: Cavitation number in OZ for different OZ diameters

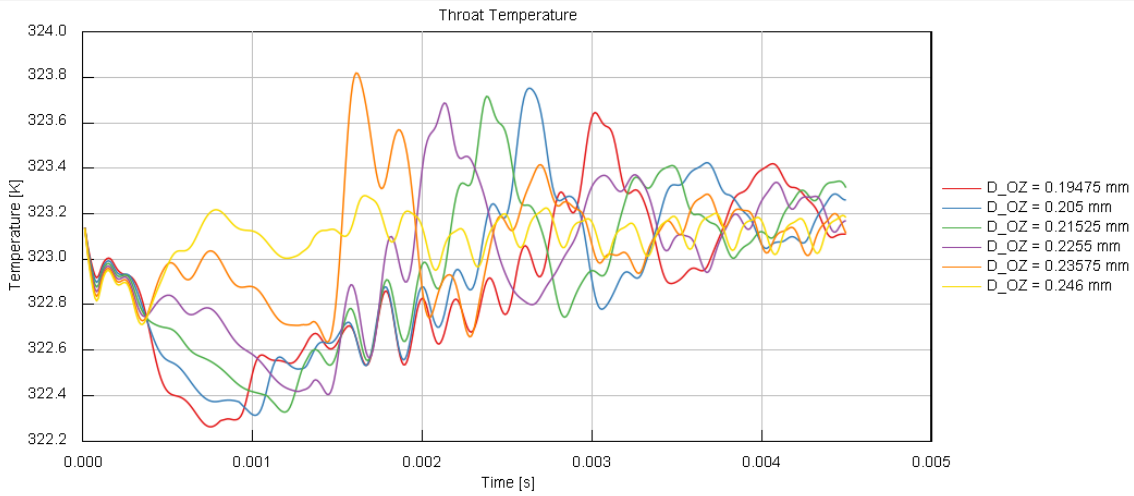


Figure 4.11: Throat temperature in OZ for different OZ diameters

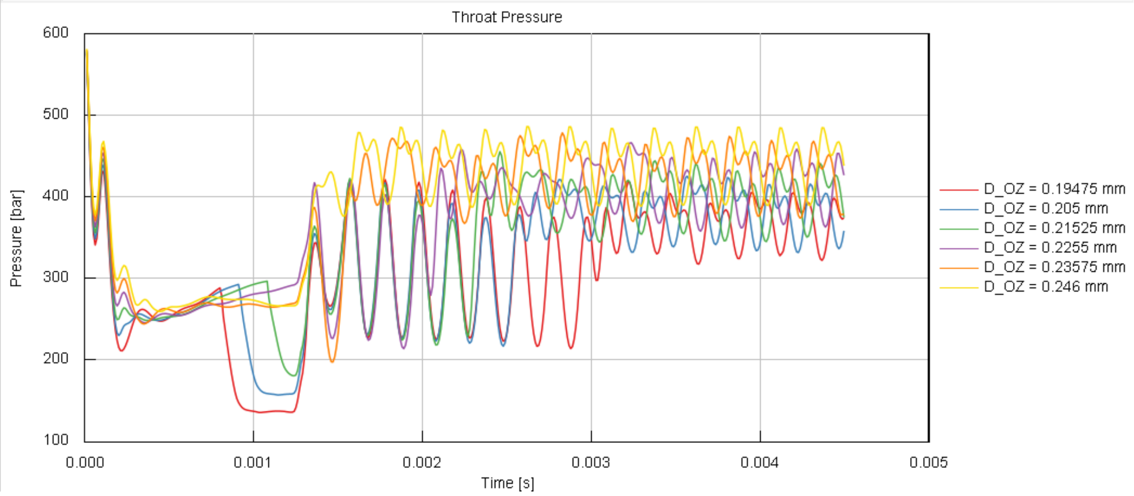


Figure 4.12: Throat pressure in OZ for different OZ diameters

Effects in OA

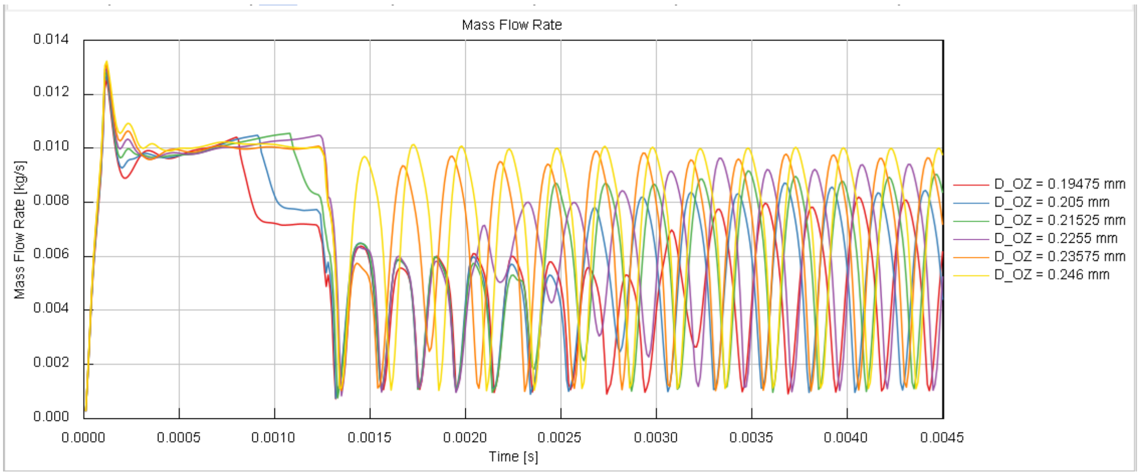


Figure 4.13: Mass flow rate through OA for different OZ diameters

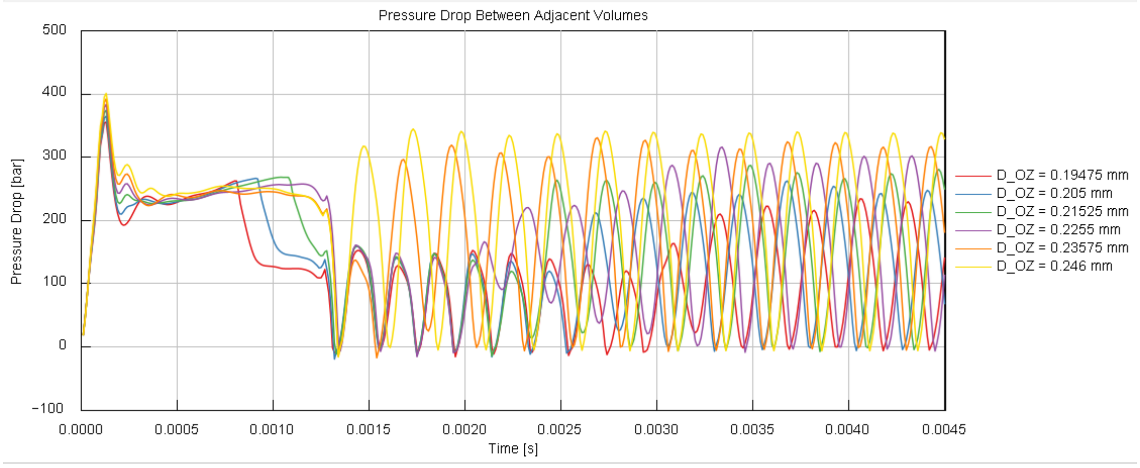


Figure 4.14: Pressure drop through OA for different OZ diameters

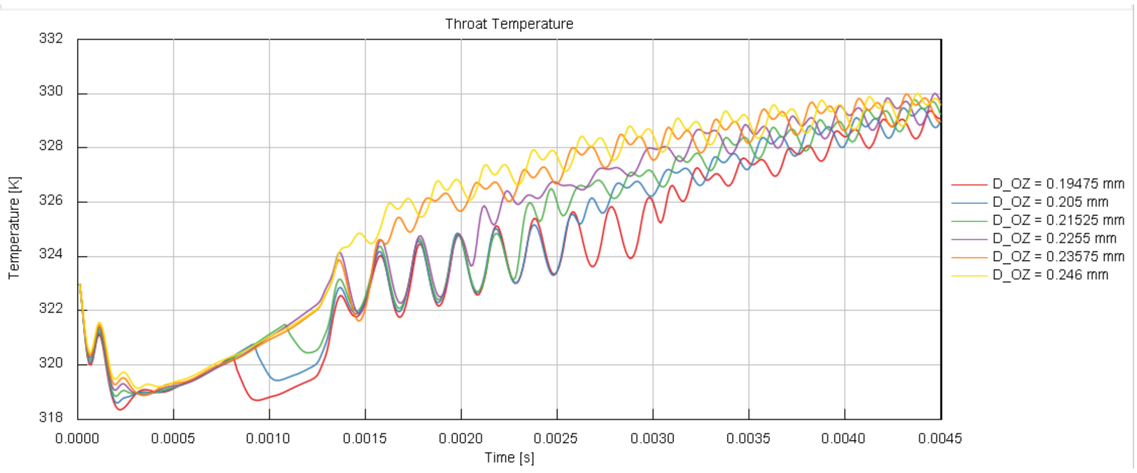


Figure 4.15: Throat temperature in OA for different OZ diameters

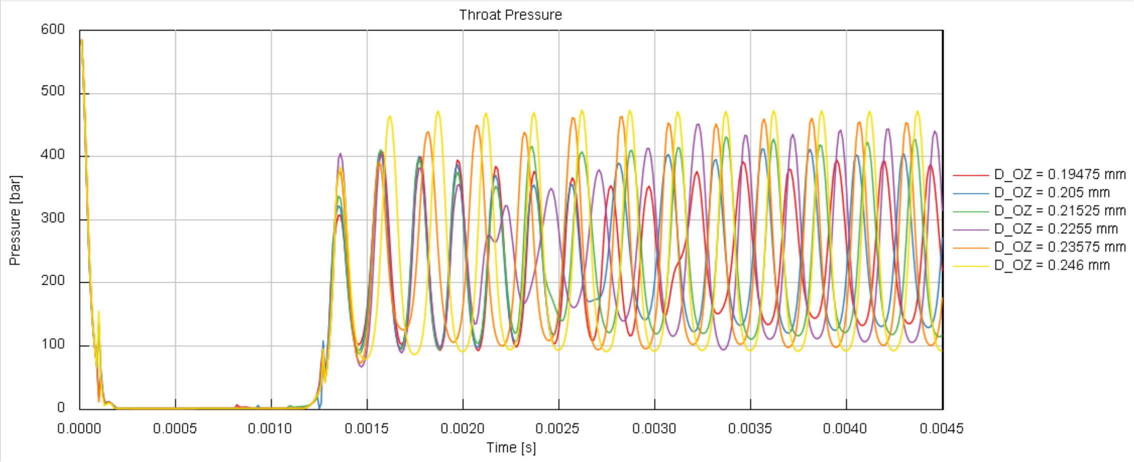


Figure 4.16: Throat pressure in OA for different OZ diameters

OA diameters

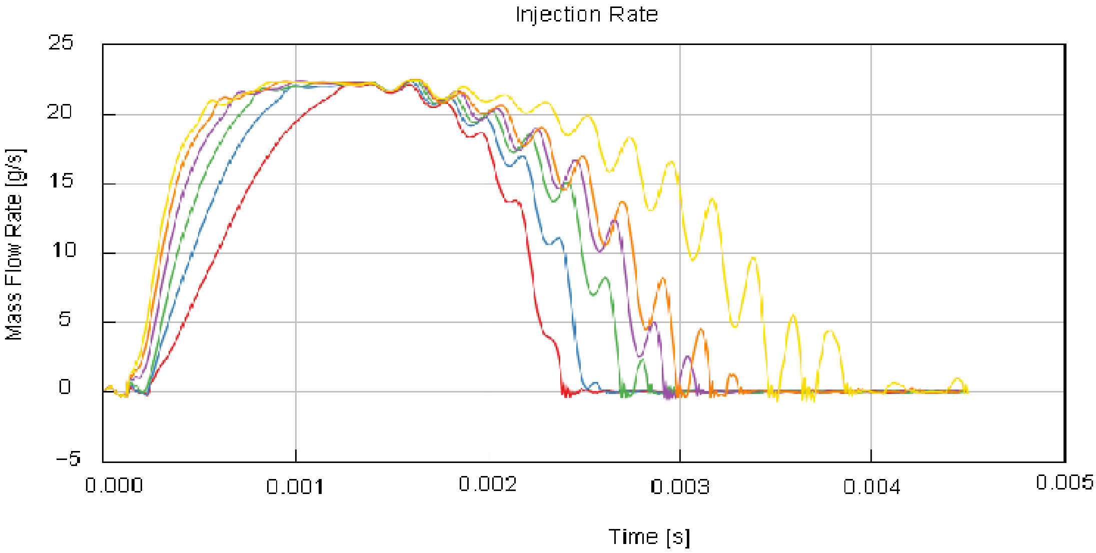


Figure 4.17: Injection Rate for OA Diameters (ET=1 ms)

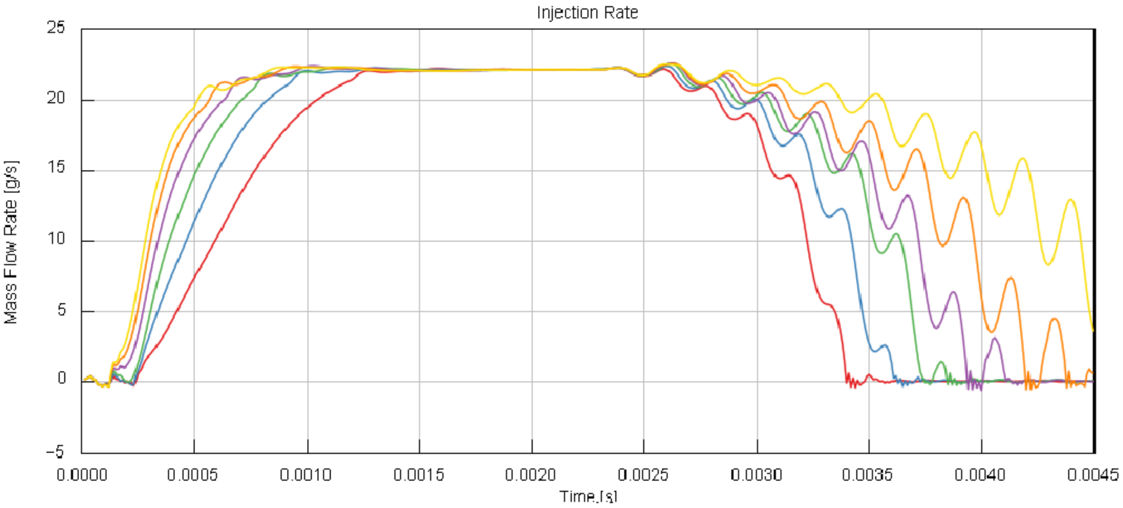


Figure 4.18: Injection Rate for OA Diameters (ET=2 ms)

Effects in OZ

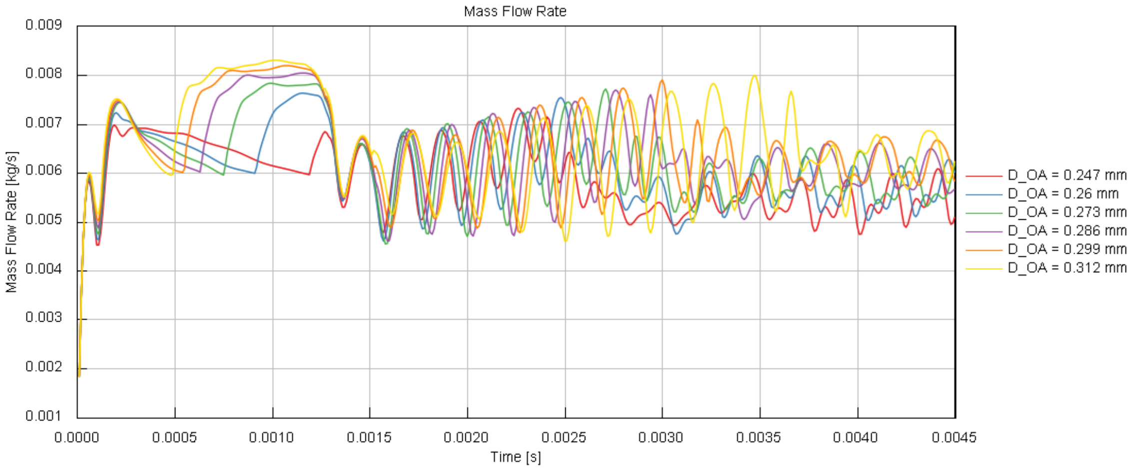


Figure 4.19: Mass flow rate through OZ for different OA diameters

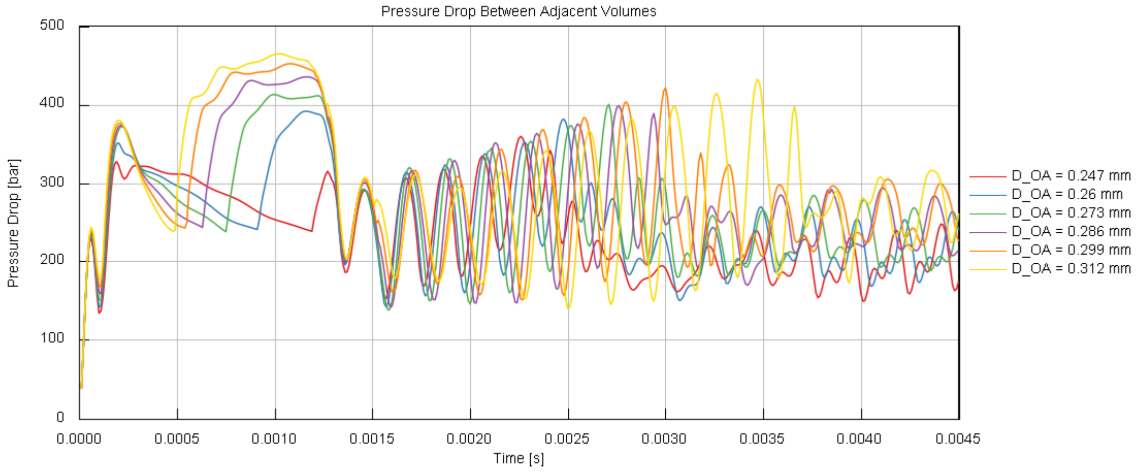


Figure 4.20: Pressure drop through OZ for different OA diameters

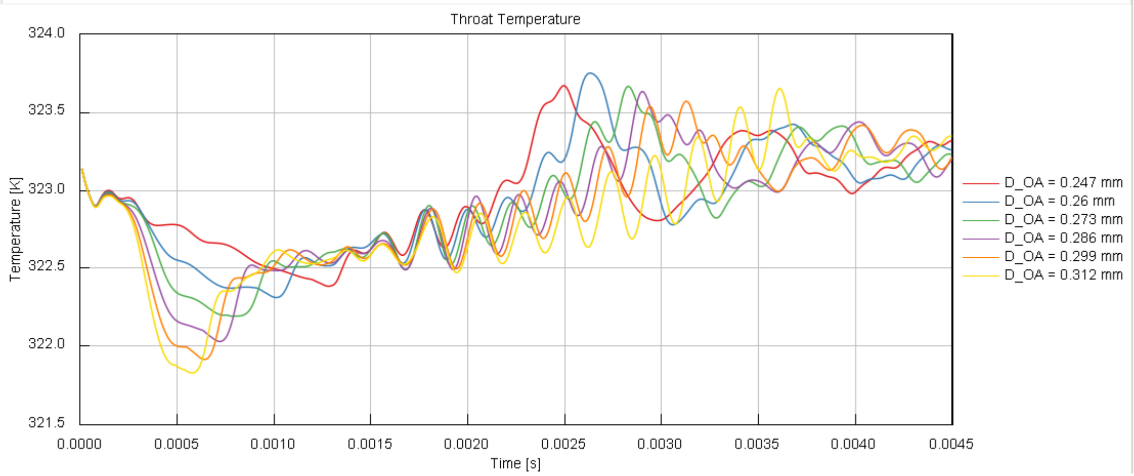


Figure 4.21: Throat temperature in OZ for different OA diameters

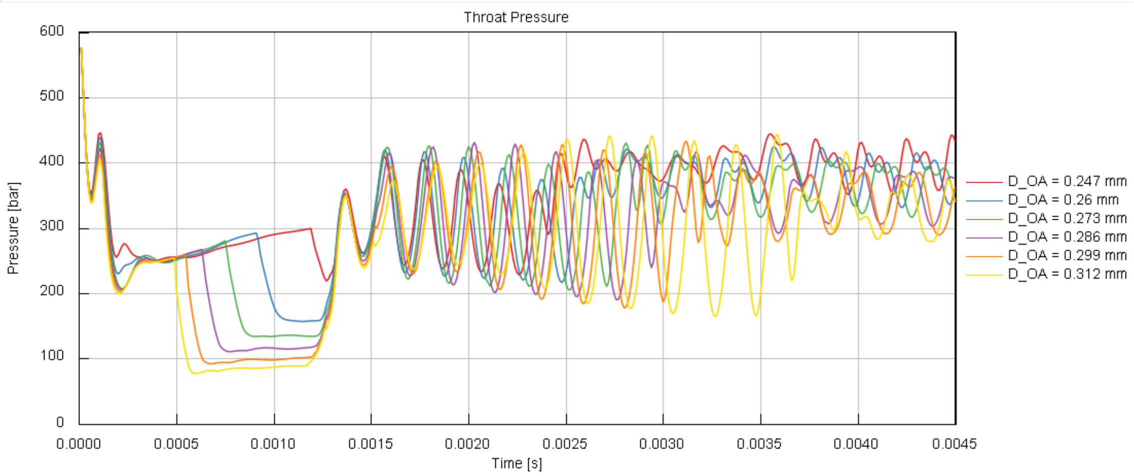


Figure 4.22: Throat pressure in OZ for different Oa diameters

Effects in OA

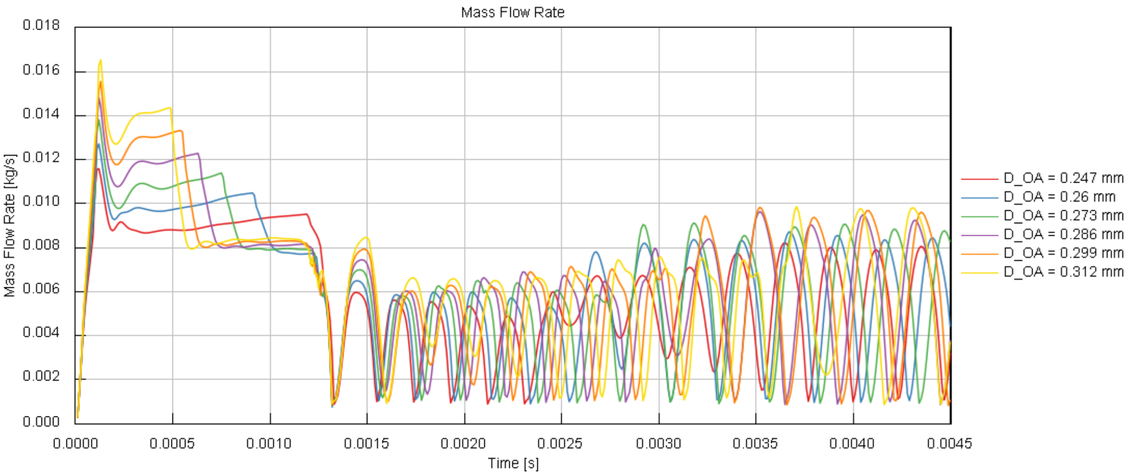


Figure 4.23: Mass flow rate through OA for different OA diameters

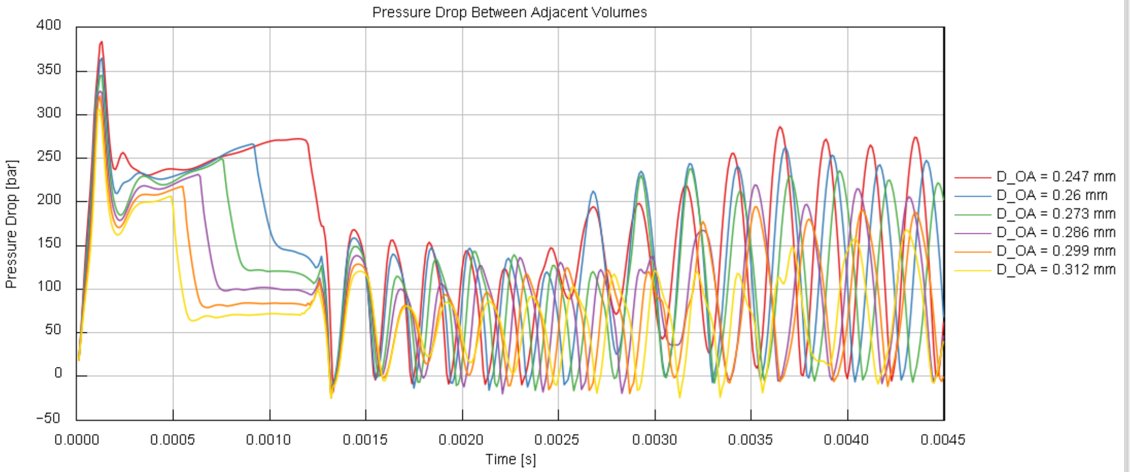


Figure 4.24: Pressure drop through OA for different OA diameters

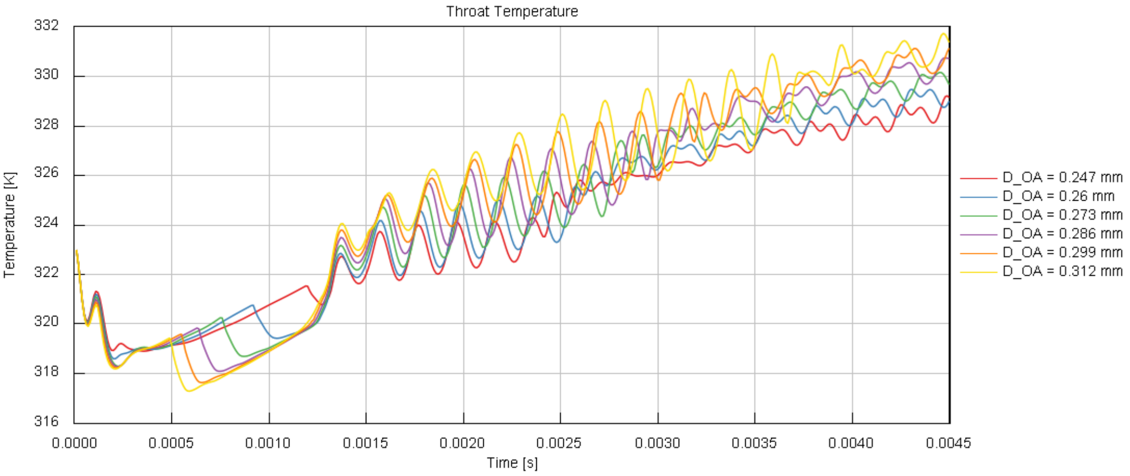


Figure 4.25: Throat temperature in OA for different OA diameters

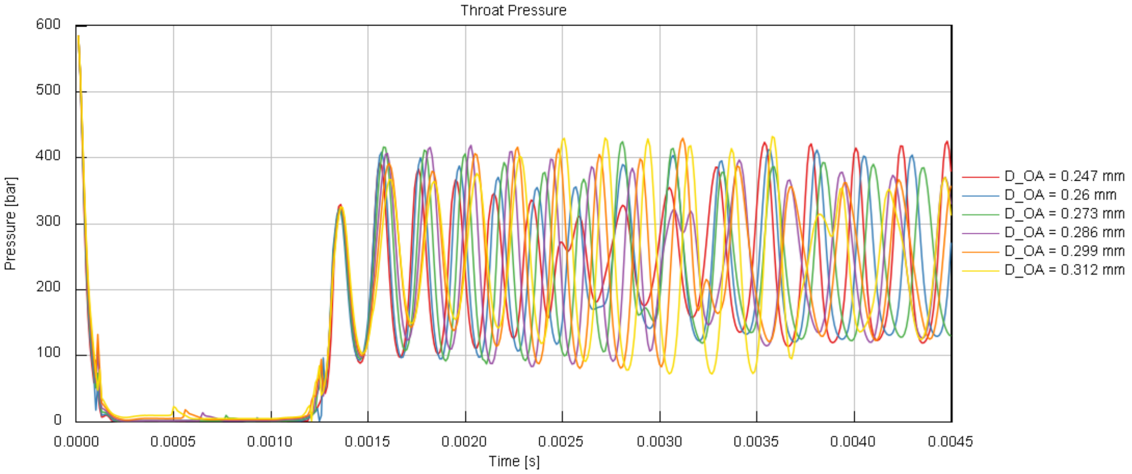


Figure 4.26: Throat pressure in OA for different OA diameters

Other parameters

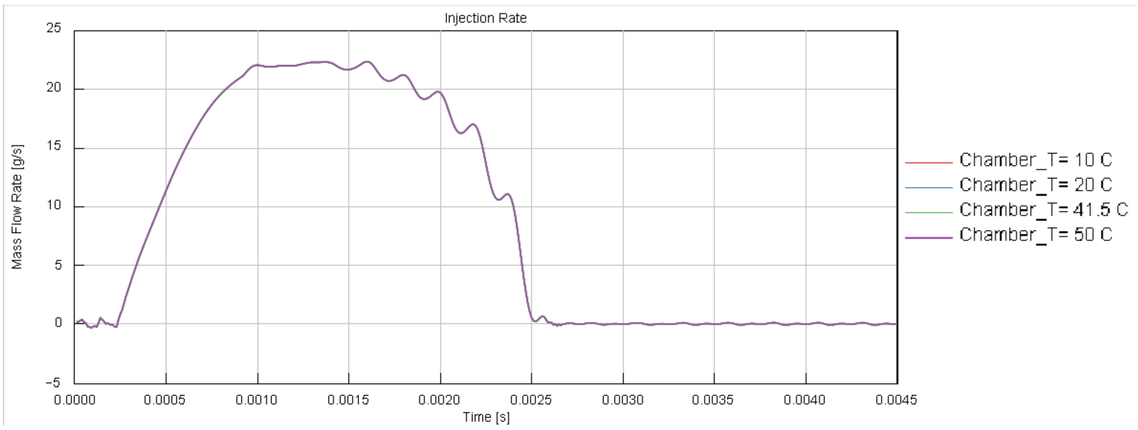


Figure 4.27: Injection Rate for different chamber temperatures (ET=1 ms)

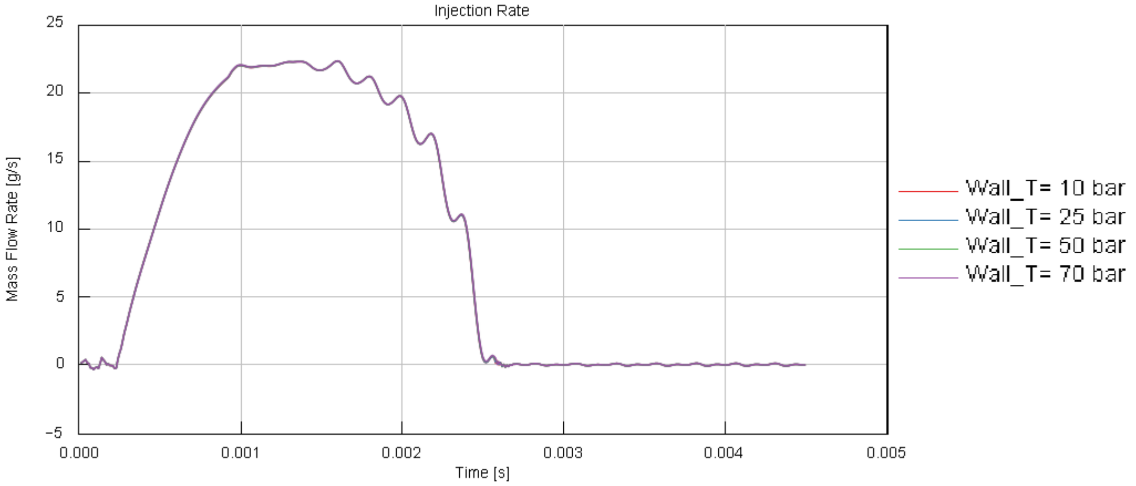


Figure 4.28: Injection Rate for different wall temperatures (ET=1 ms)

Sensitivity analysis with ammonia

Rail pressure

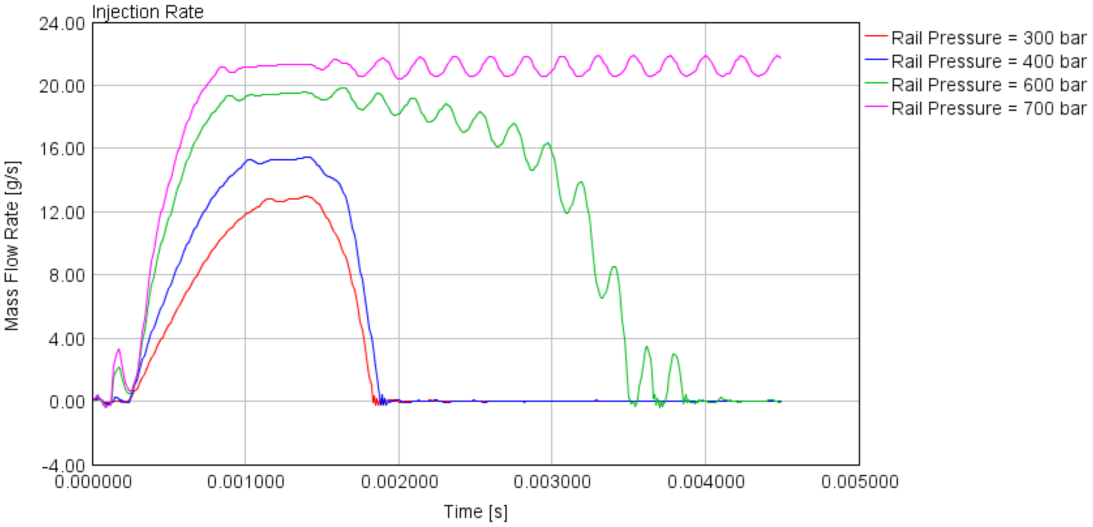


Figure 5.1: Injection rates for different rail pressures using ammonia as a fuel and $EI = 1ms$

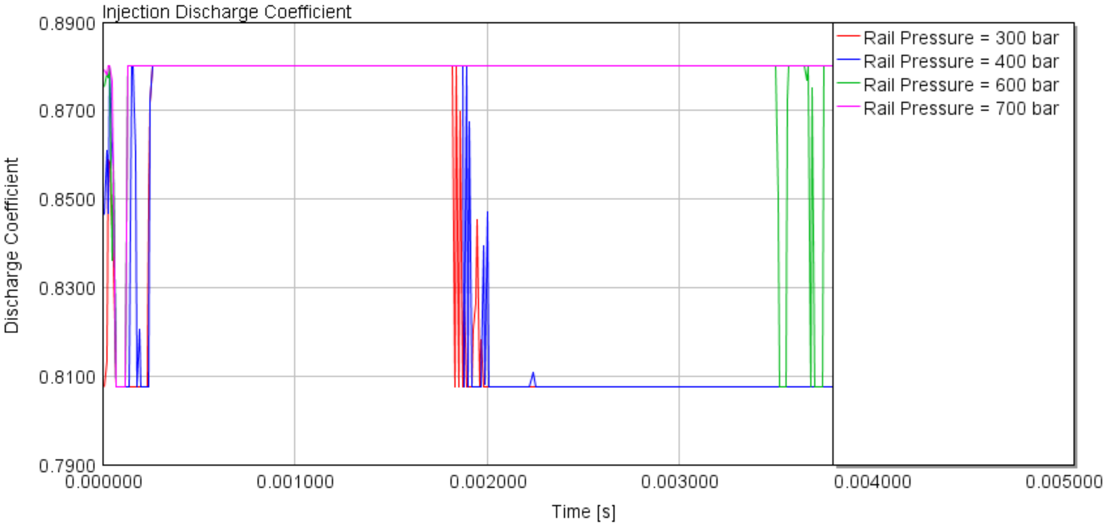


Figure 5.2: Discharge coefficients for different rail pressures using ammonia as a fuel

Fuel Temperature

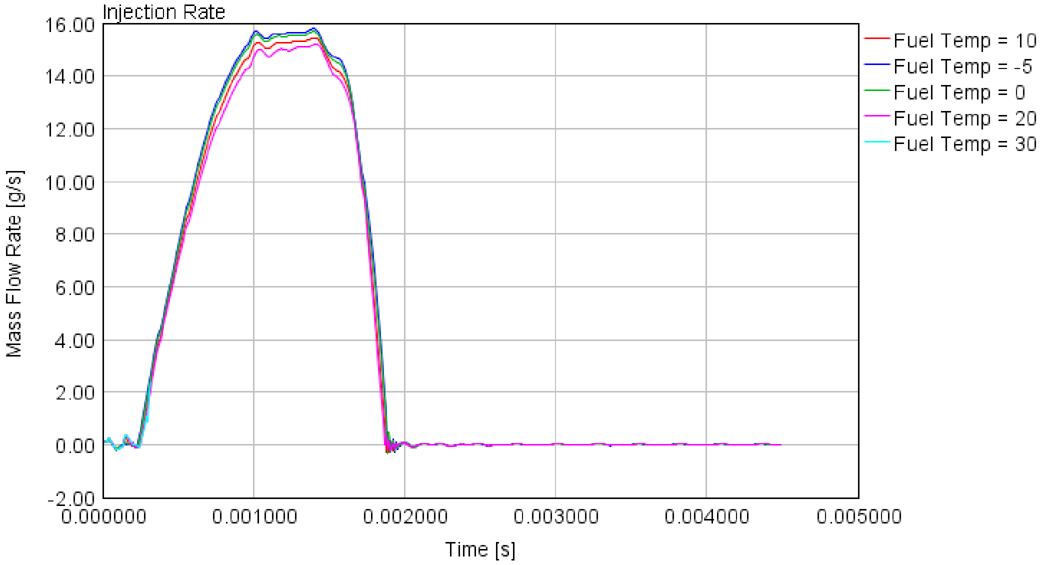


Figure 5.3: Injection rates for different fuel temperatures using ammonia as a fuel and $EI = 1ms$

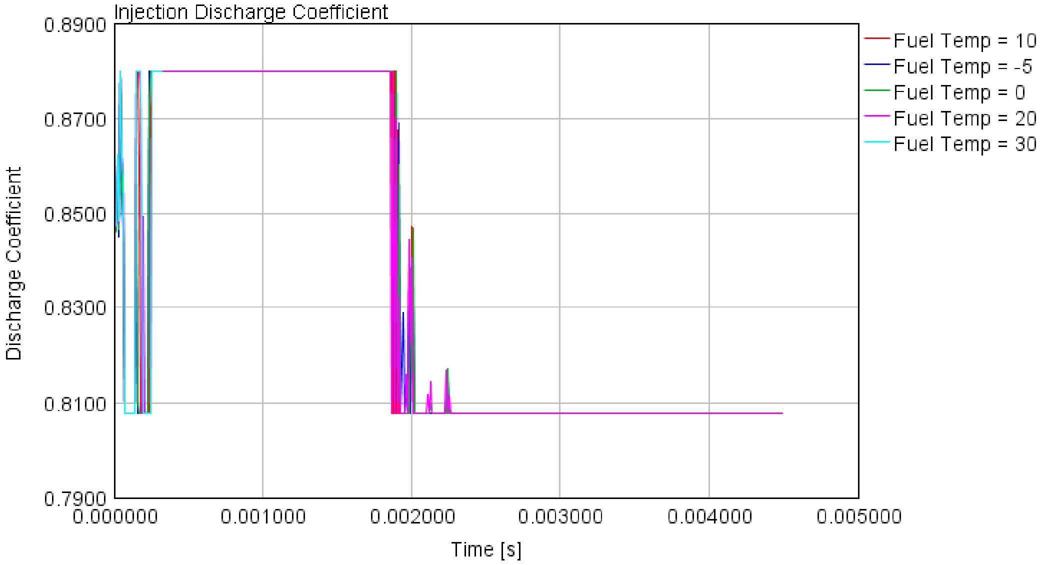


Figure 5.4: Discharge coefficient for different fuel temperatures using ammonia as a fuel

Energizing time

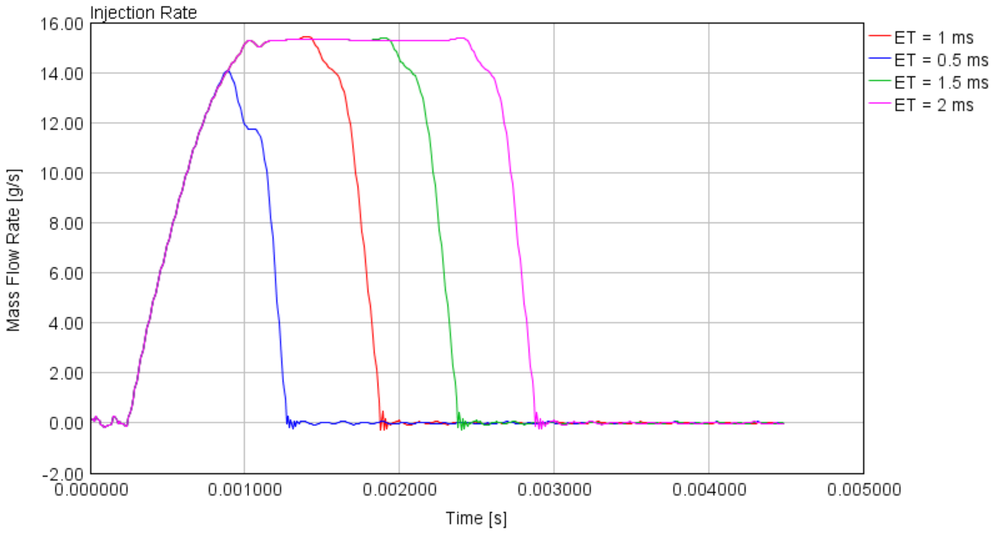


Figure 5.5: Injection rates for different energizing times using ammonia as a fuel

OA and OZ geometries

OZ diameter

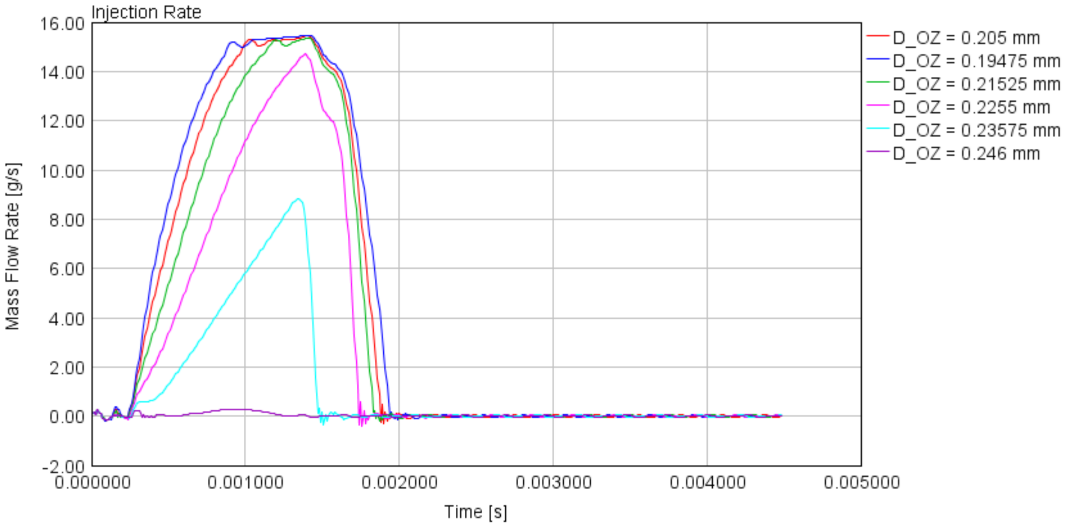


Figure 5.6: Injection Rate for OZ Diameters (ET=1 ms)

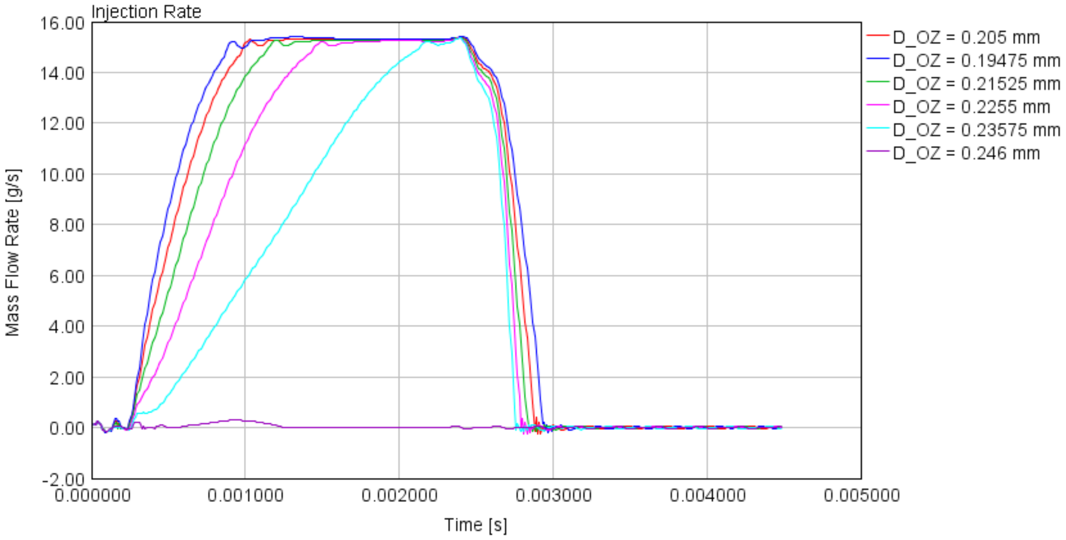


Figure 5.7: Injection Rate for OZ Diameters (ET=2 ms)

Effects in OZ

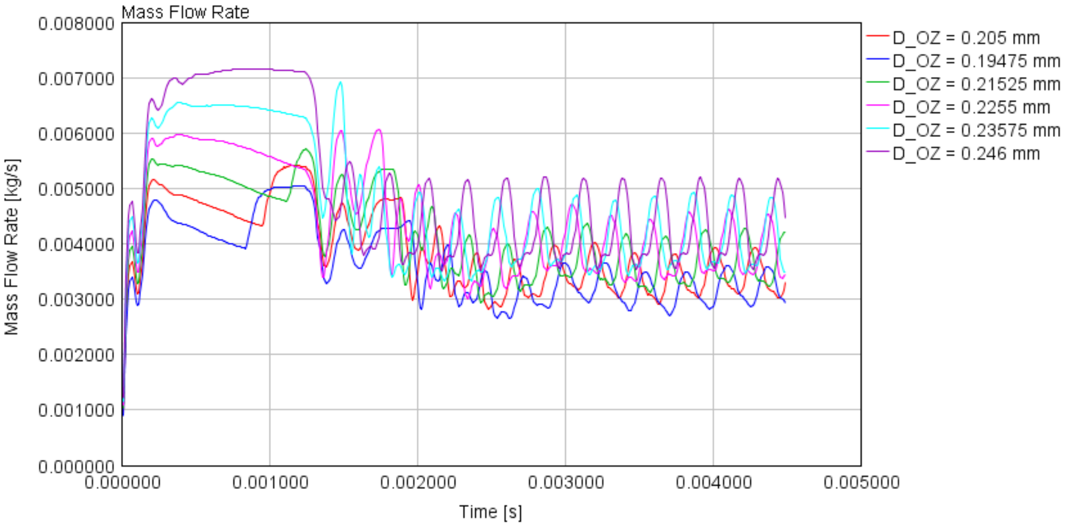


Figure 5.8: Mass flow rate through OZ for different OZ diameters

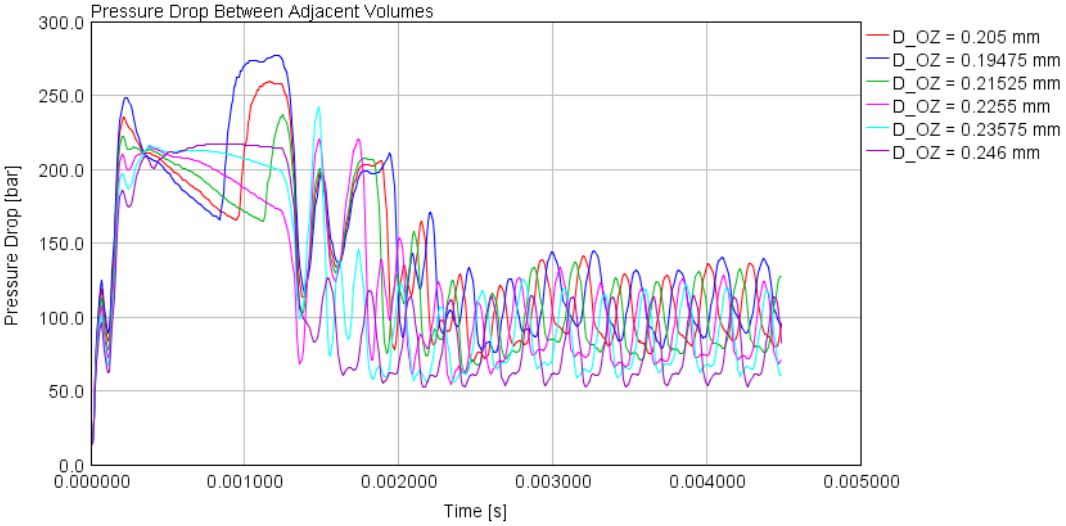


Figure 5.9: Pressure drop through OZ for different OZ diameters

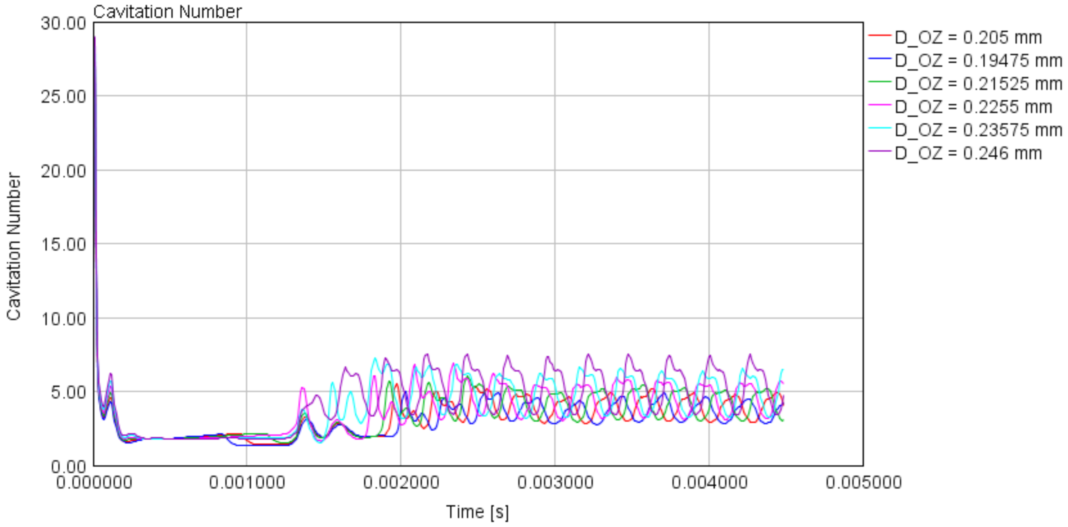


Figure 5.10: Cavitation number in OZ for different OZ diameters

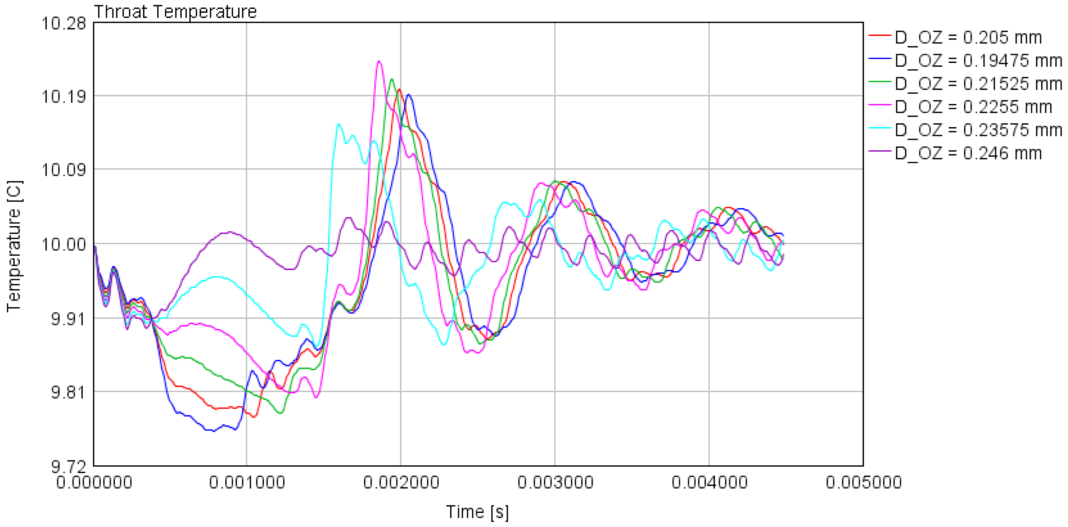


Figure 5.11: Throat temperature in OZ for different OZ diameters

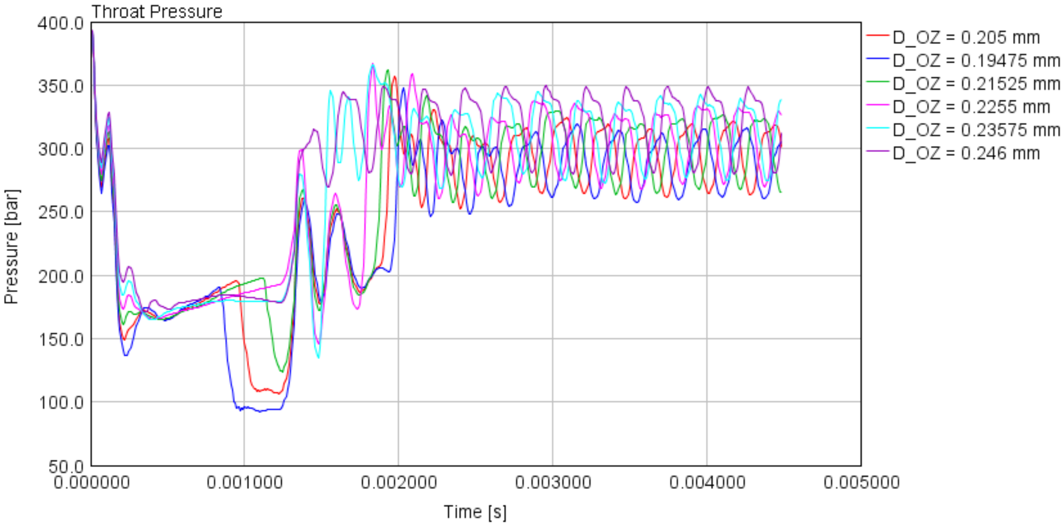


Figure 5.12: Throat pressure in OZ for different OZ diameters

Effects in OA

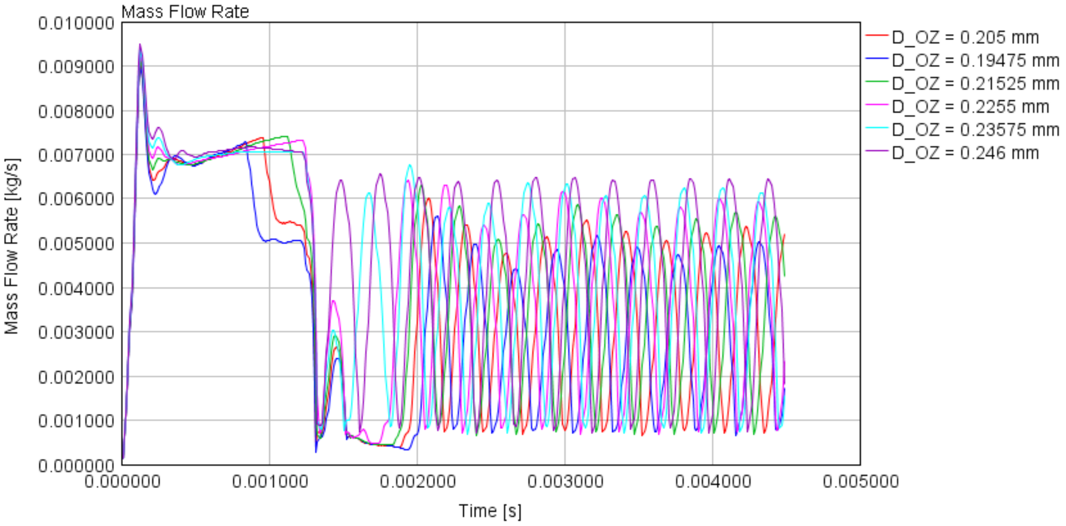


Figure 5.13: Mass flow rate through OA for different OZ diameters

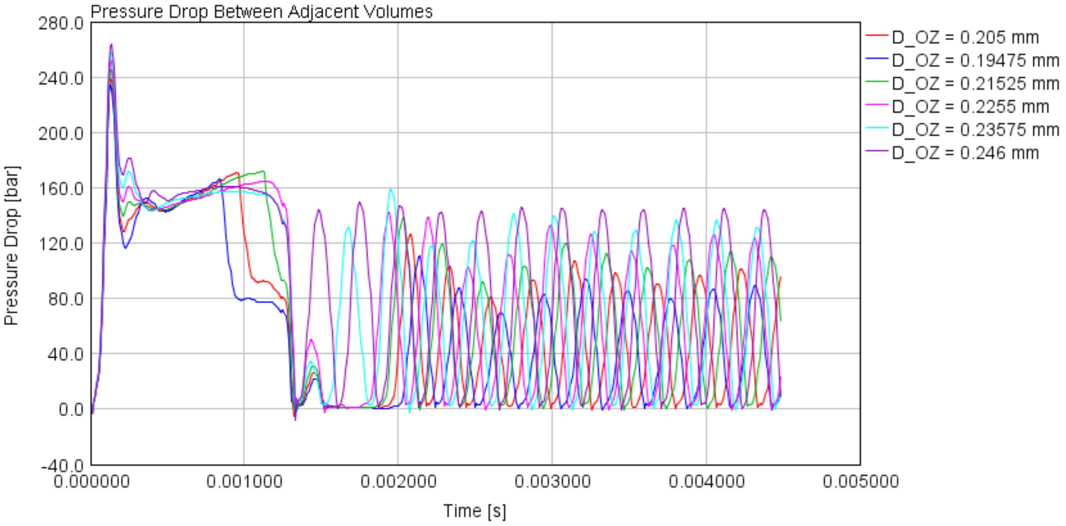


Figure 5.14: Pressure drop through OA for different OZ diameters

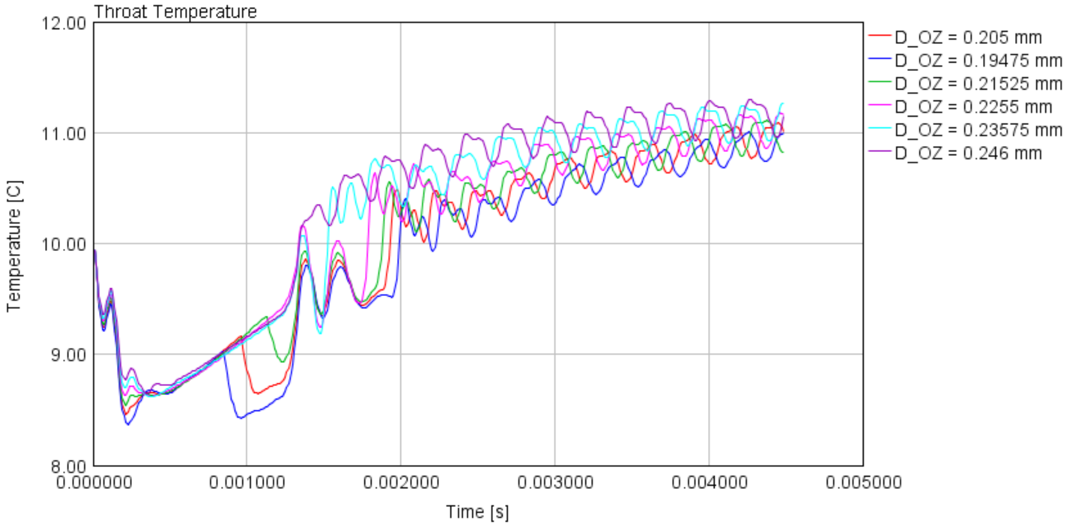


Figure 5.15: Throat temperature in OA for different OZ diameters

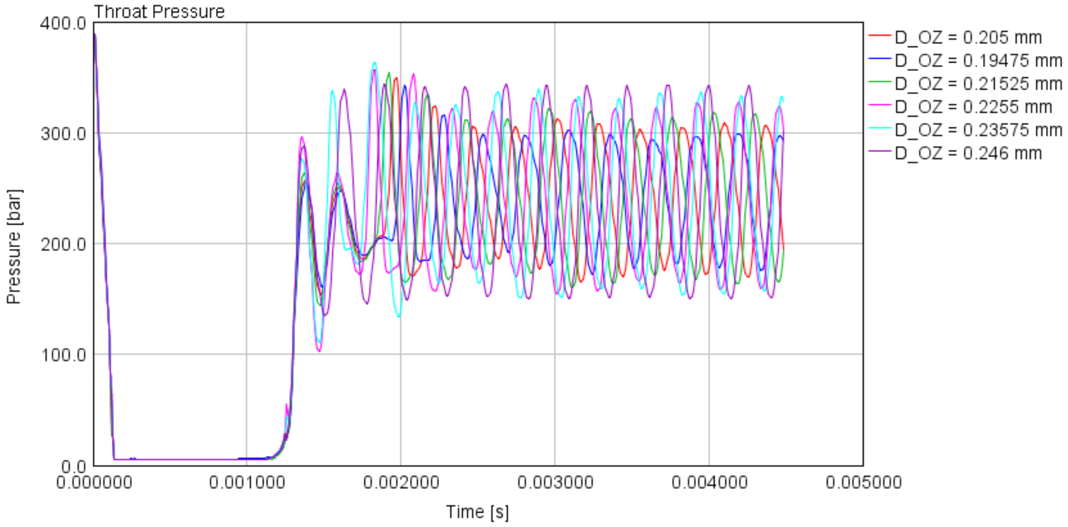


Figure 5.16: Throat pressure in OA for different OZ diameters

OA diameters

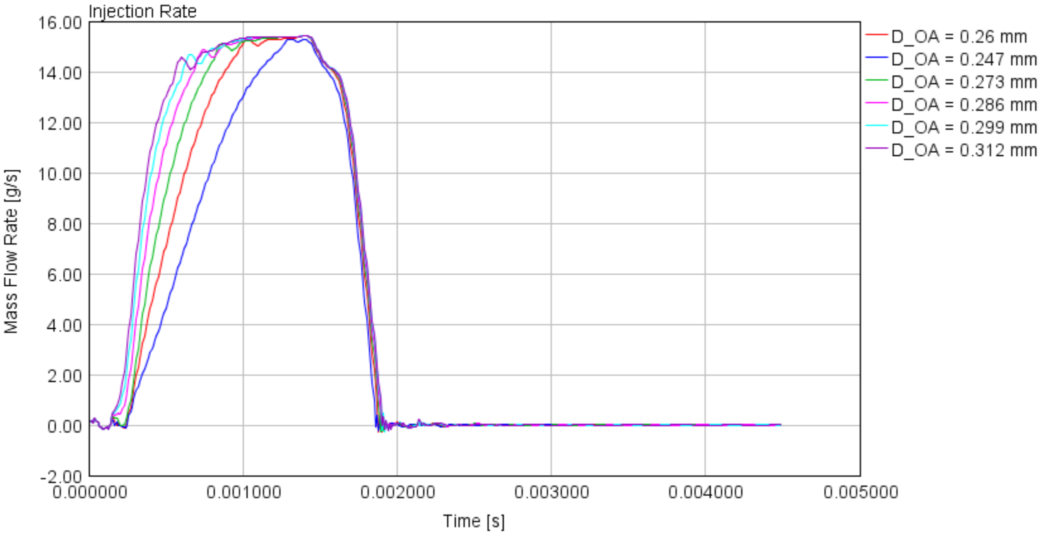


Figure 5.17: Injection Rate for OA Diameters (ET=1 ms)

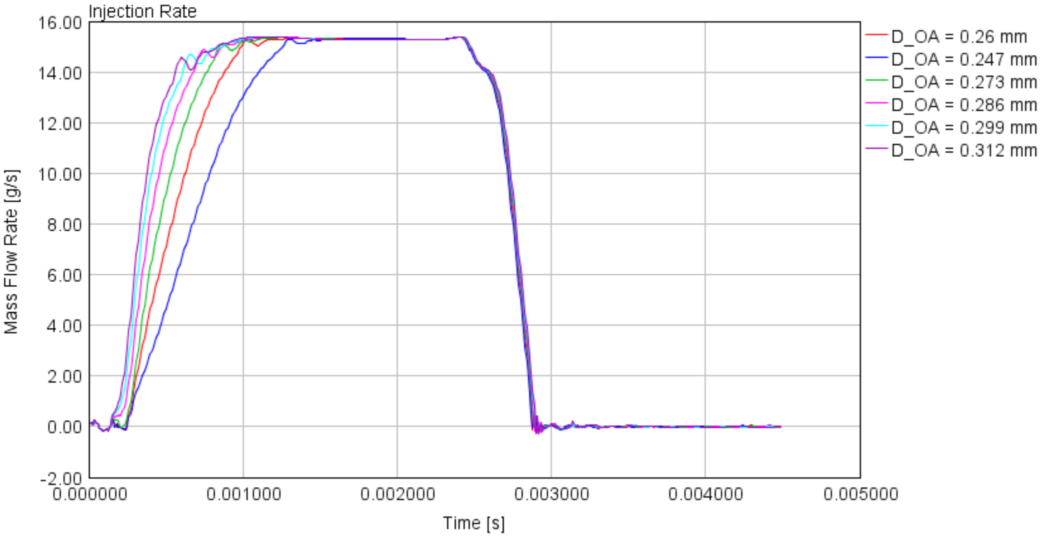


Figure 5.18: Injection Rate for OA Diameters (ET=2 ms)

Effects in OZ

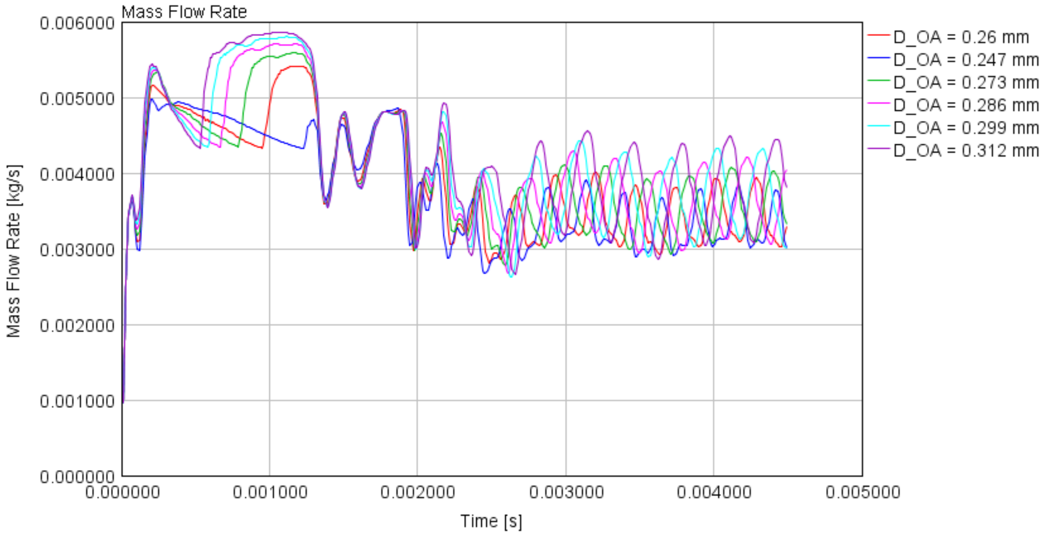


Figure 5.19: Mass flow rate through OZ for different OA diameters

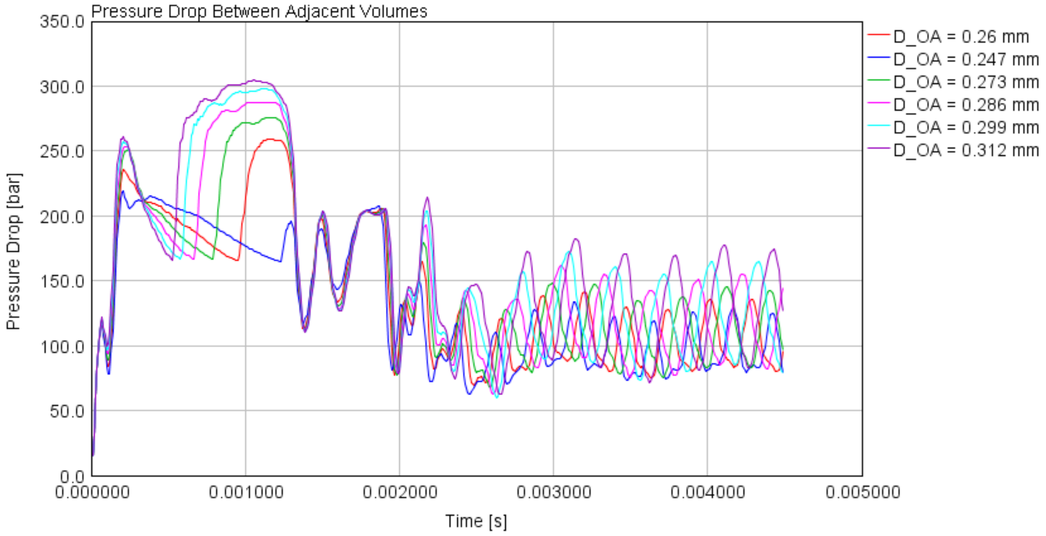


Figure 5.20: Pressure drop through OZ for different OA diameters

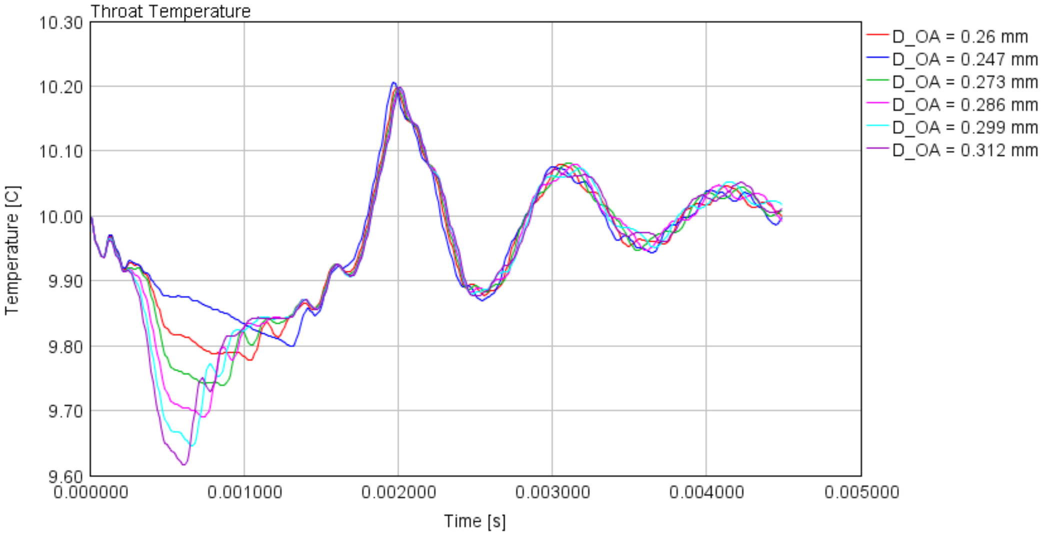


Figure 5.21: Throat temperature in OZ for different OA diameters

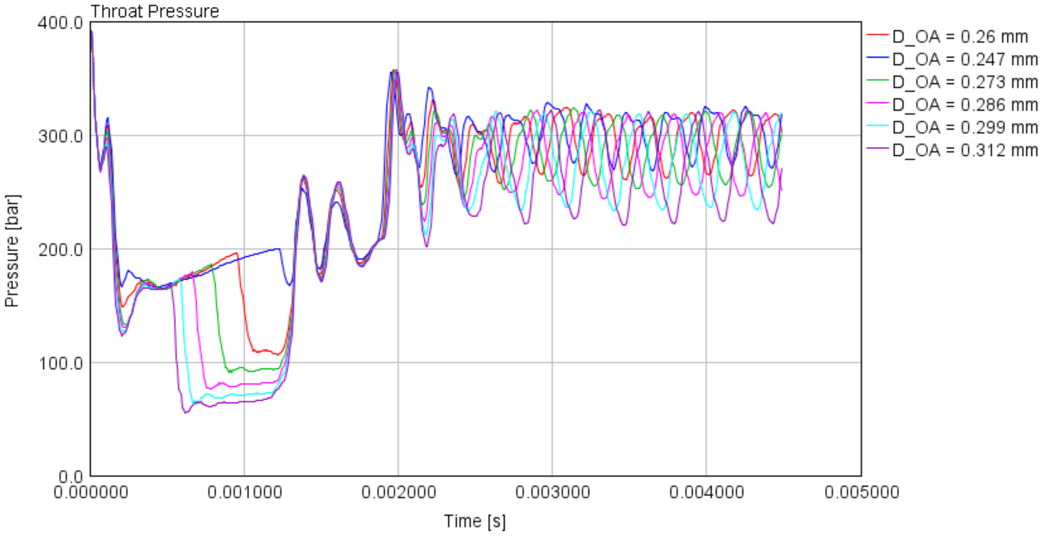


Figure 5.22: Throat pressure in OZ for different Oa diameters

Effects in OA

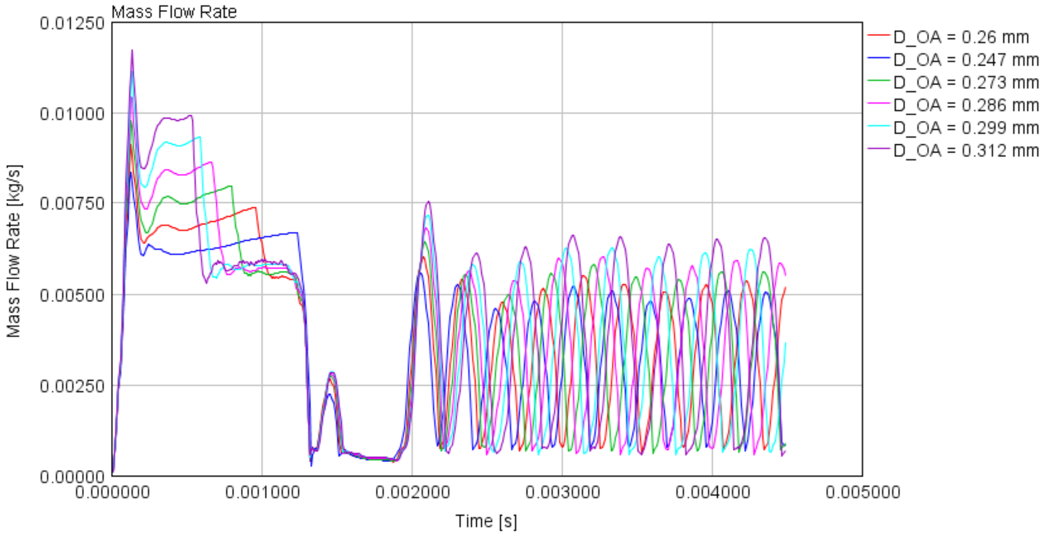


Figure 5.23: Mass flow rate through OA for different OA diameters

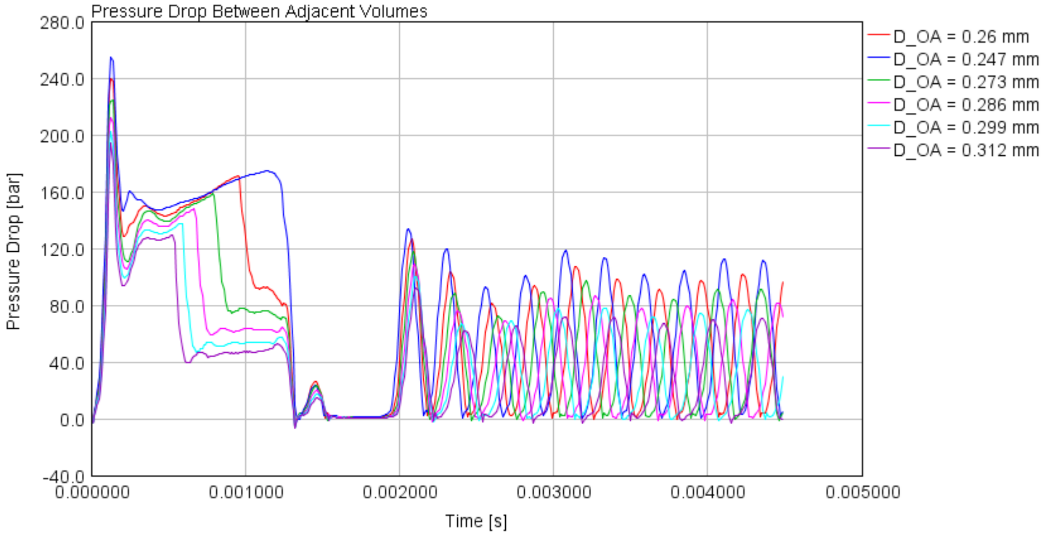


Figure 5.24: Pressure drop through OA for different OA diameters

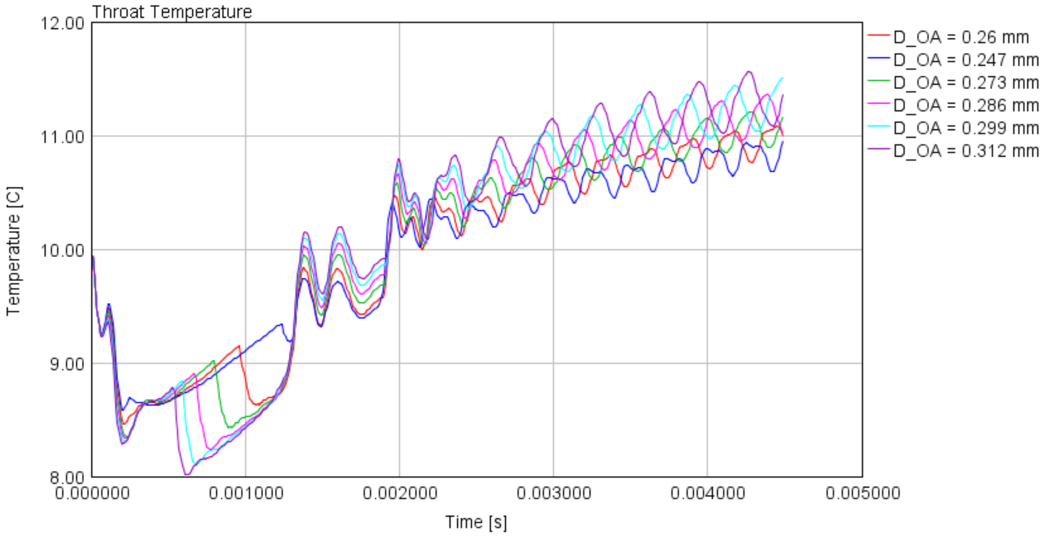


Figure 5.25: Throat temperature in OA for different OA diameters

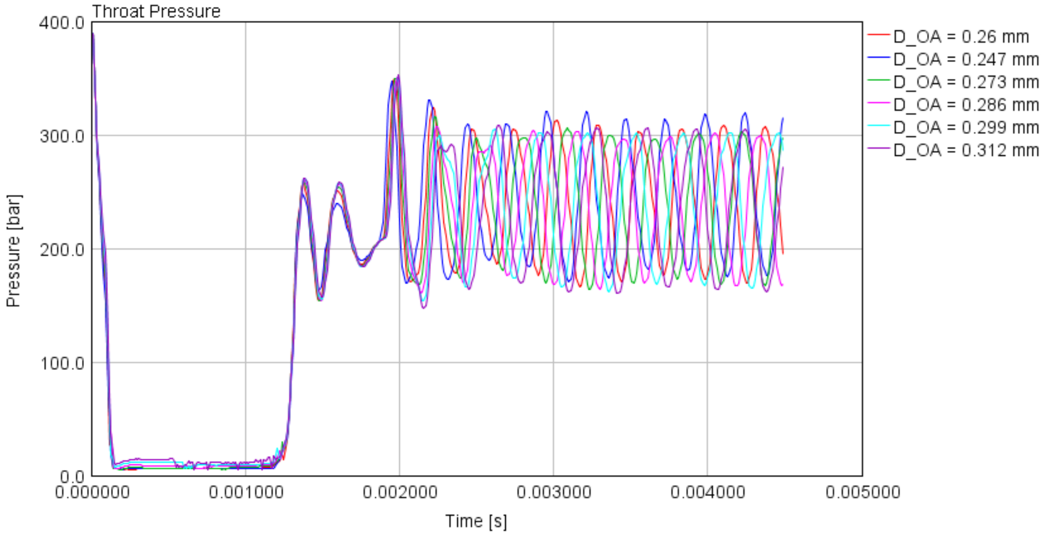


Figure 5.26: Throat pressure in OA for different OA diameters

Comparison with methanol

Injection rate at 400 bar

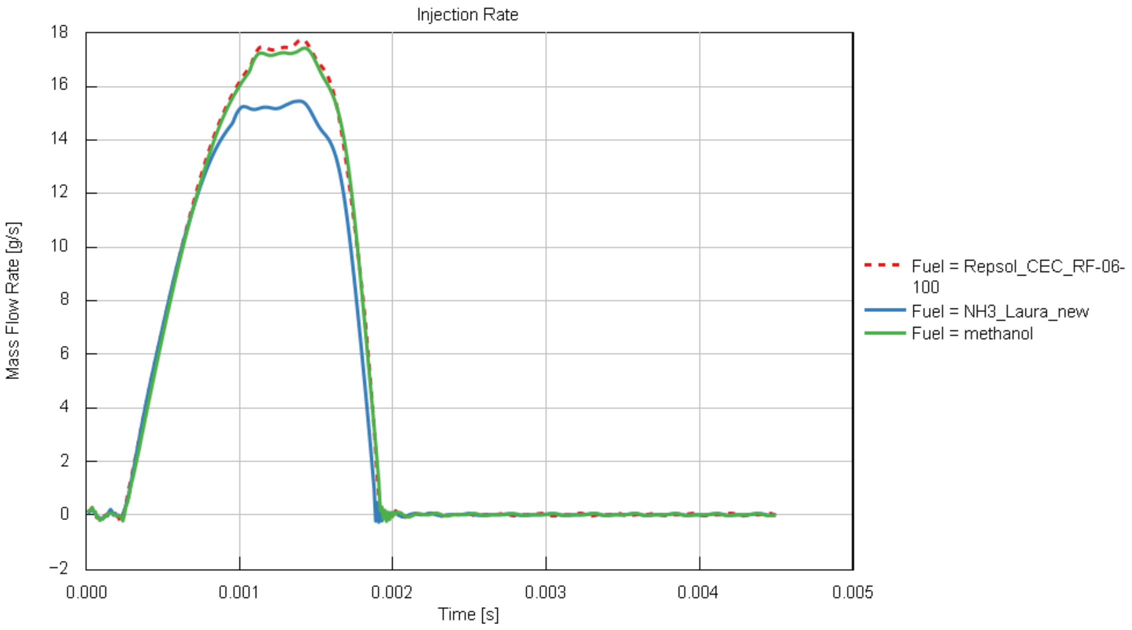


Figure 5.10: Injection rate comparison of different fuels

Injected mass at 400 bar

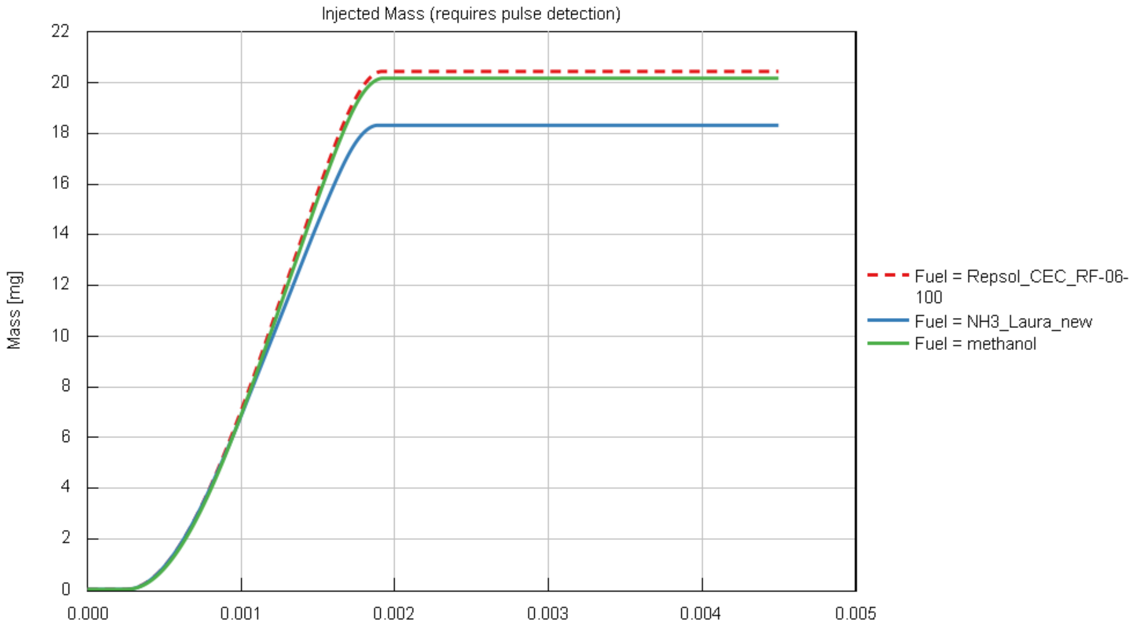


Figure 5.11: Injected mass comparison of different fuels

Injected volume at 400 bar

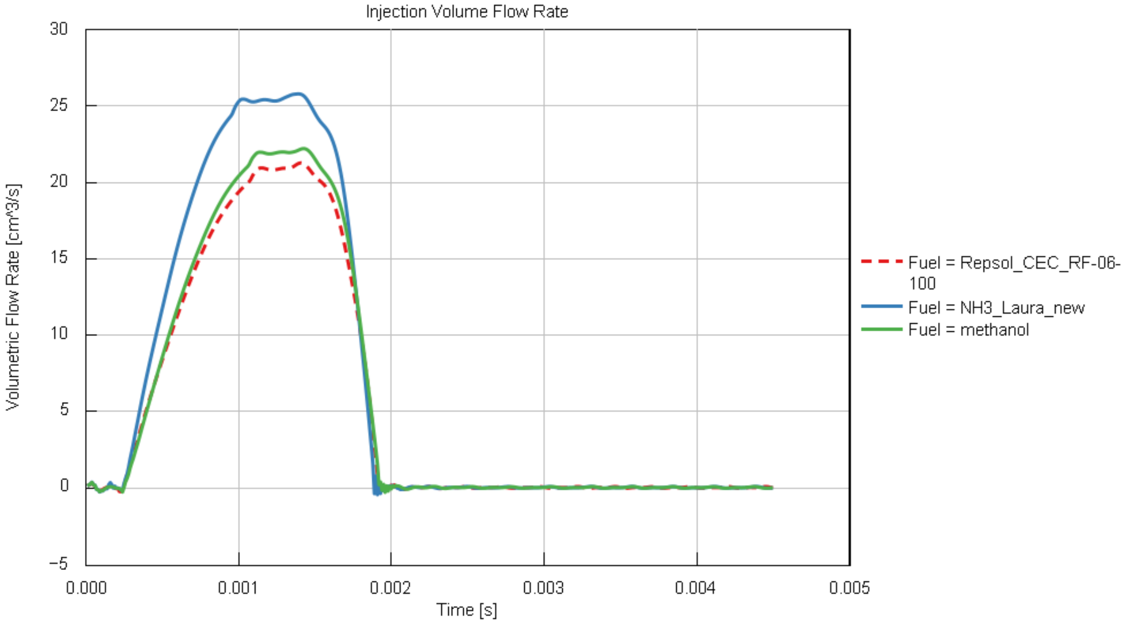


Figure 5.12: Injected volume comparison of different fuels

Mass flow in OZ at 400 bar

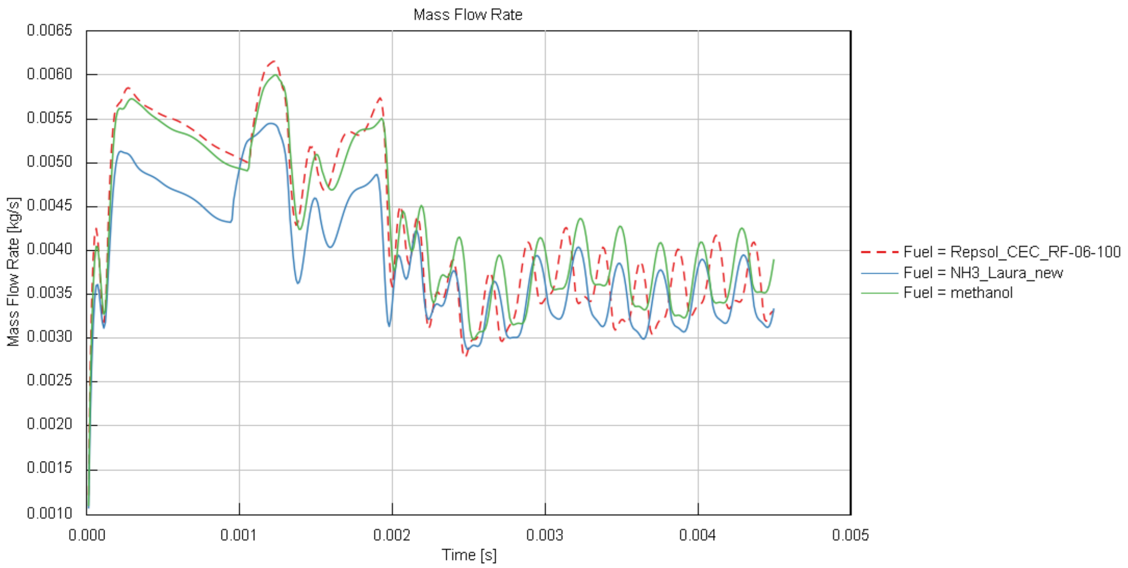


Figure 5.13: Mass flow in OZ at 400 bar

Throat temperature in OZ at 400 bar

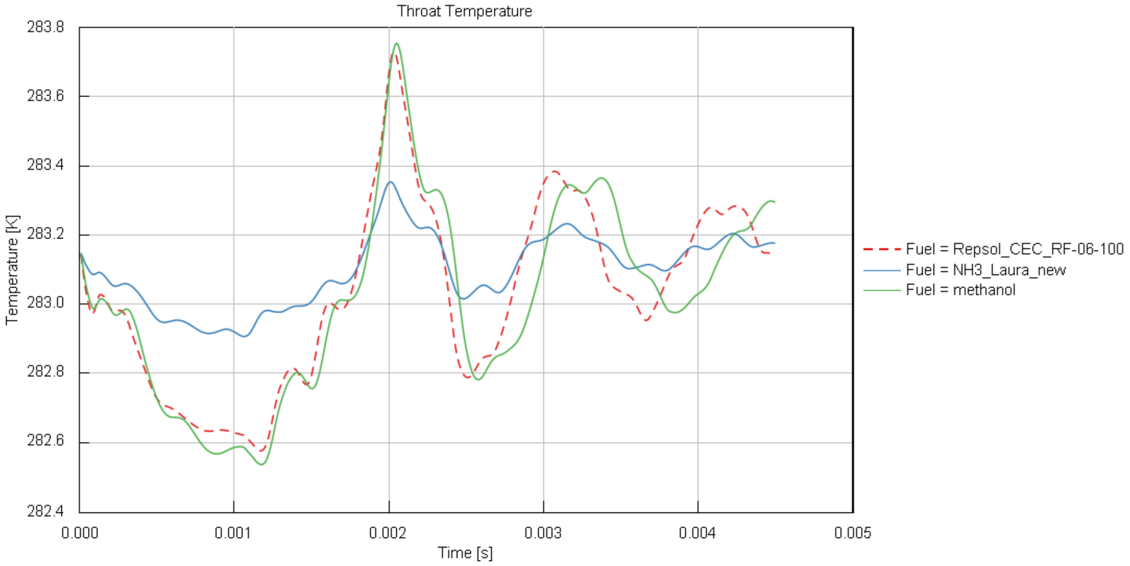


Figure 5.14: Throat temperature in OZ at 400 bar

Throat temperature in OA at 400 bar

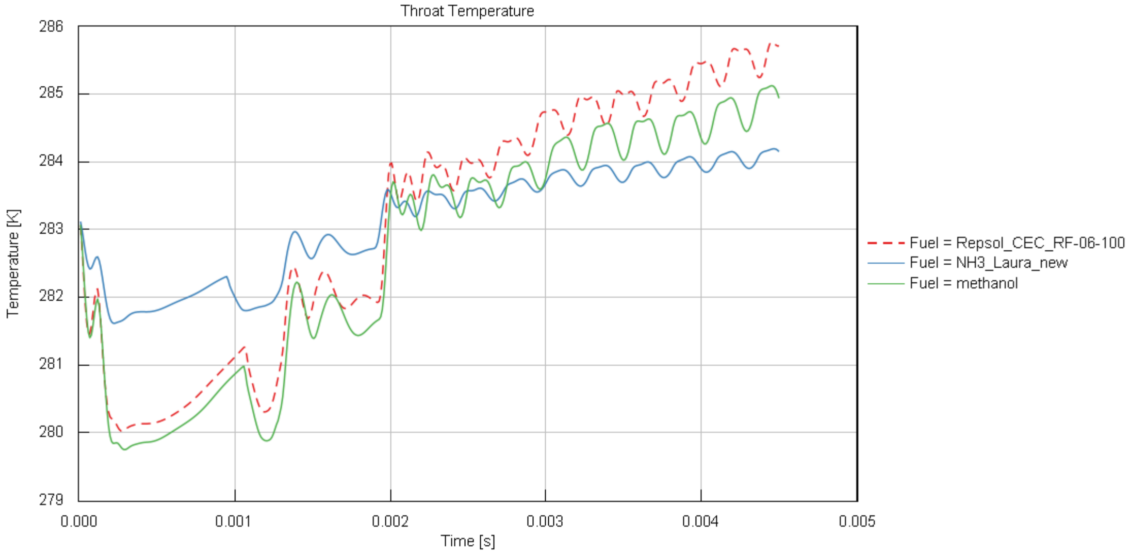


Figure 5.15: Throat temperature in OA at 400 bar

Throat pressure in OA at 400 bar

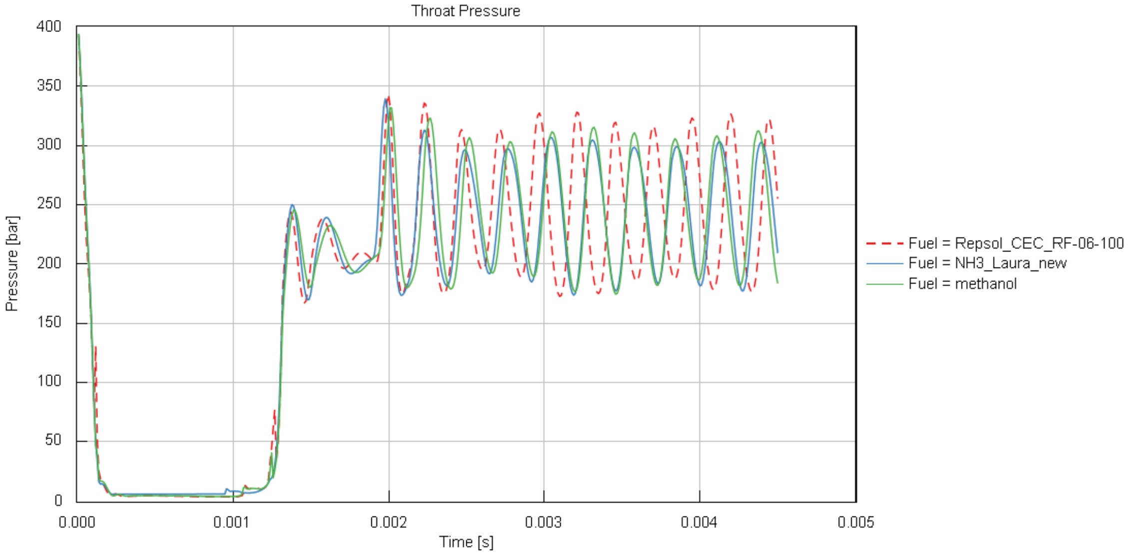


Figure 5.16: Throat pressure in OA at 400 bar

Part III

Specifications Document

Specifications Document

Introduction

The specifications document of a project generally consists of outlining each of the technical and legal requirements that must be covered. The formality of the specifications document refers to the conditions that this document must meet for the preparation of this project. To better explain this section, the document is divided into general conditions and specific conditions. The general conditions describe the hygiene and safety formalities of the project, and the specific conditions list the characteristics that the work equipment must have.

More generically, a specifications document must have necessary characteristics such as precision and reliability. Precision might be the most important of all since the results depend on the tolerances selected by the author and the project director. Reliability ensures that the project's objective can be achieved, relying on the tools available at the Clean Mobility and Thermofluids department. The control of the data obtained in the model produced by GT-SUITE allows for a decisive comparison with the experimental data being collected in the department for ongoing research.

GENERAL CONDITIONS OF THE DOCUMENT

During this section, each of the general conditions related to the development of this project will be stipulated. The author's work environment must meet all the requirements reflected in Royal Decree 488/1997 of April 14 [2], which specifically addresses clarifications related to the environment and its characteristics, whether concerning the quality of the infrastructure or the determination of the tools and equipment used in the process. The chosen facilities must meet all the needs of the study participants, ensuring their safety and physical integrity.

Since no specific installation or test room was required, the general conditions document is broken down as follows: mandatory conditions, which establish the required knowledge level for this study, and workplace conditions, summarizing the minimum needs for the author to develop their work capabilities.

MANDATORY CONDITIONS

The mandatory conditions describe each of the components involved in the work's progress. In addition to naming the capabilities of each part, it also refers to the rights and obligations that the members must fulfill to enhance this research's aptitude.

The promoter is a person or entity that professionally promotes the work of another. In this case, it is a research team from the Department of Clean Mobility and Thermofluids at the Polytechnic University of Valencia. The project director's role is to coordinate and supervise each process carried out during the research. They can resolve issues that arise during the investigation and propose modifications based on the results obtained.

Before starting the project, both the engineer and the director must establish a roadmap that first defines the project's purpose, followed by breaking down the plan into different parts with respective timelines. It also includes an estimate of the equipment and materials that will be required for each part.

The engineer must possess technical and practical skills related to the research topic to introduce variations in the simulation parameters and interpret the results obtained from these simulations. Additionally, the responsibility level is high since a large amount of data has been provided by the Department of Clean Mobility and Thermofluids due to a previous study, requiring careful handling of this data under confidentiality terms.

Finally, the engineer, knowing the project's purpose, must demonstrate a critical capacity concerning the results obtained in each part of the project, drawing the appropriate conclusions, always supervised and corroborated by the project director.

ENGINEER'S DUTIES AND RIGHTS

In addition to all the requirements that the engineer must meet, this section will list the rights and obligations that this member is exposed to. The engineer must show initiative in preparing each process in the research. Together with the project director, a series of guidelines and working methods must be established, providing any tool that allows the progress of the research at all times.

Regarding rights, the engineer needs support from other project members and financial backing for its production. Therefore, the availability of the project director is crucial to address all progress and issues that arise in the study in a consensual manner, always verifying the validity of the obtained results.

To conclude this section, the engineer must be provided with the necessary materials, tools, and equipment for the project's completion. This responsibility falls on the Department of Clean Mobility and Thermofluids as the promoter.

WORKPLACE CONDITIONS

The conditions related to the workplace are reflected in Royal Decree 486/1997 of April 14 [1], which specifically addresses each condition to be described. Almost the entire project has been developed in a computational environment; no testing was required for its development, and consequently, no access to a specially designated room or defined workspace was requested.

SPECIFIC CONDITIONS OF THE DOCUMENT

A series of characteristics related to the conditions of both the software and the computer equipment will be listed below. It is worth noting that calculation tools, text generation tools, and graph creation tools will be used for this project. Regarding the requirements for computer equipment, having a powerful computer is not necessary to handle this volume of data.

This project is primarily developed using two programs, which must be legally obtained. This is achieved through the licenses of each program. Once the product license is requested, users must comply with the requirements imposed by the creators of these tools.

The document grants the user legal use, stipulating each term that authorizes the use of the copy. Besides all conditions outlined in the document, the current Intellectual Property Law must be followed. The Department of Clean Mobility and Thermofluids, or alternatively, the Polytechnic University of Valencia, has covered the cost of these licenses, which will be specified in the budget document.

The work was carried out using a personal computer without any specific requirements. This equipment modeled the injector, performing each proposed simulation during the research. Finally, it graphically presented a correct display of these results.

Part IV

Budget

Budget

Overview of Project Costs

In this document, we will outline the budget required for the project, separating the types of costs to obtain partial budgets. We can distinguish between labor and computational equipment, and the sum of each of these parts yields the total budget.

All the equipment used in this study are located at the facilities of the Department of Clean Mobility and Thermofluids. The costs for equipment and licenses have been itemized, including the purchase of a computer, the necessary GT-SUITE software and licenses, and a Microsoft Office license. These components are essential for the project's technical and administrative tasks.

In this case, the types of costs will be divided according to their nature and summed to obtain the total budget, as there is no experimental part included in this project, only labor and computational equipment.

Thus, the total budget will be the sum of the partial budgets for labor and specified equipment. Subsequently, a 13% increase is estimated due to general expenses. Finally, a 21% Value Added Tax (VAT) is applied to this value. The monetary unit is the euro (€).

Labour

This section describes the hours worked by each of the project participants. In this case, the student's hours have been accounted for, corresponding to the credits of the Final Degree Project (TFG) (in the table 5.1). Additionally, the assistant professor's hours have been estimated approximately. The time dedicated by each participant is shown in the table 5.2.

Table 5.1: Time Allocation

Concept	**Quantity**	**Units**
TFG Credits	12	Credits
Time per credit	30	hours/credit
Total time	360	hours
Additional writing and formatting time	80	hours

Table 5.2: Total Hours Calculation

Concept	**Quantity**	**Units**
Student-Junior Engineer	360	Hours
Professor	40	Hours

To estimate the hourly cost of the project participants, their gross salaries must be considered. In this case, only the base salary will be valued, so no supplements will be considered.

The data has been obtained from the agreement referred to the Teaching and Research Staff of the Polytechnic University of Valencia during the 2023-2024 academic year. This information can be observed in the table 5.3.

Table 5.3: Hourly Rates

Concept	**Quantity**	**Units**
Student- Junior Engineer	18.88	€/hour
Professor	47.50	€/hour

Once the hourly costs of each project member are justified in previous sections, table 5.4 estimates a partial budget corresponding to labor, excluding equipment and materials.

Table 5.4: Labor Cost

Concept	**Quantity**	**Units**
Student- Junior Engineer	6796.80	€
Professor	1900.00	€
Total	8696.80	€

Therefore, the total cost of labor in this project is **EIGHT THOUSAND SIX HUNDRED NINETY-SIX EUROS AND EIGHTY CENTS**.

Computational Cost

In the computational part, each of the elements that make up the work equipment will be specified. The costs for equipment and licenses have been itemized, including the purchase of a **computer**, the necessary **GT-SUITE software** and **licenses**, and a **Microsoft Office license**. These components are essential for the project's technical and administrative tasks. Their final costs are depicted in table 5.5.

For this project, the availability of a personal computer was necessary. The depreciation cost of this PC will be calculated based on its purchase value (649 euros), its depreciation period (4 years), and its residual value concerning the purchase value (85%).

Formula for calculating the annual cost (C.A.) of an asset:

$$C.A. = \frac{(1 - \text{Residual Value Factor}) \times \text{Purchase Cost}}{\text{Depreciation Period}} \tag{5.1}$$

Where:

- Residual Value Factor is the percentage of the purchase cost that remains at the end of the depreciation period, expressed as a decimal.
- Purchase Cost is the initial cost of the asset (649 euros).
- Depreciation Period is the number of years over which the asset is depreciated (in this case 4).

For this specific project, the applied values are:

$$C.A. = \frac{(1 - 0.15) \times 649}{3} = 183.88\,/\text{year} \tag{5.2}$$

In this section, the calculation of **consumable materials** used in the project has been omitted as it mainly involves the cost of electricity. This will be considered in *general expenses* as it is difficult to quantify.

Table 5.5: Computational Costs

Concept	**Quantity**	**Cost (€)**
Computer	1	183.88
GT-SUITE software and license (for 1 year)	1	5000
Microsoft Office License (for 1 year)	1	69.00
Subtotal of Equipment and Licenses		**5252.88**

Therefore, the total cost of the computational part in this project is **FIVE THOUSAND TWO HUNDRED FIFTY-TWO EUROS AND EIGHTY-EIGHT CENTS**.

Budget Summary

Table 5.6: Total Project Cost

Description	**Total Cost (€)**
Subtotal of Equipment and Licenses	5252.88
Total Cost of Human Labor	8696.8
General expenses (13%)	1813.46
VAT [IVA] (21%)	3310.26
Total Cost of the Project	**19073.40**

Thus, the total budget required for the completion of this project is estimated to be **NINETEEN THOUSAND SEVENTY-THREE EUROS AND FORTY CENTS**.