

Faculdade de Engenharia da Universidade do Porto

Application of Oxy-Combustion Technology for Drone Engine

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Abstract

In recent years, there has been a significant growth in the use of drones in areas such as defence, environmental monitoring and logistics. This growth drives for the demand for more efficient and compact propulsion systems with lower environmental impact. In this context, oxy-combustion technology emerges as a promising solution, as it involves burning fuel using oxygen-enriched air, typically with oxygen concentrations above 95 %. This approach allows for higher combustion temperatures, increases thermal efficiency, and reduces pollutants emissions.

To assess the potential of this technology, numerical simulation tools such as ANSYS Forte were used study combustion phenomena in engines, enabling a detailed analysis of the effects of oxygen enrichment on engine performance.

This work investigated the feasibility of applying oxy-combustion to drone engines, focusing on both two-stroke and four-stroke engines. The results obtained allow a comparison between conventional combustion operation and oxygen-enriched combustion, by evaluating parameters such as combustion efficiency, engine power, pressures, temperatures, and emissions, thereby contributing to the assessment of the potential of this technology for drone applications.

Simulation results showed oxy-combustion raises peak pressures and temperatures, reducing CO but increasing CO₂ and NO_x emissions. To prevent unburned O₂ and maximize engine performance, an optimal balance was found using 30 % O₂, alongside a 15 % fuel mass increase and recalibrating injection and ignition timings.

This work was developed in an industrial environment at TEKEVER, UAS, located in Caldas da Rainha, Portugal.

Key-words: drones; oxy-combustion; internal combustion engines; oxygen enrichment; numerical simulation; ANSYS Forte

Resumo

Nos últimos anos, tem-se registado um crescimento significativo na utilização de drones em áreas como a defesa, monitorização ambiental ou logística. Este crescimento impulsiona a procura por sistemas de propulsão mais eficientes, compactos e com impacto ambiental reduzido. Neste contexto, a tecnologia da oxi-combustão surge como uma solução promissora, uma vez que consiste na queima do combustível utilizando ar enriquecido com oxigénio, normalmente com concentrações acima de 95 %. Esta abordagem permite atingir temperaturas de combustão mais elevadas, aumentar a eficiência térmica e reduzir a emissão de poluentes.

Para avaliar o potencial desta tecnologia são aplicadas ferramentas de simulação numérica, como o software ANSYS Forte, com o objetivo de estudar os fenómenos de combustão em motores, permitindo uma análise detalhada dos efeitos do enriquecimento com oxigénio na performance do motor.

Este trabalho investigou a viabilidade da aplicação da oxi-combustão em motores de drones, em particular motores de dois e quatro tempos. Os resultados obtidos permitem comparar o desempenho do motor no regime de combustão convencional e de combustão enriquecida com oxigénio, através da avaliação de parâmetros como a eficiência da combustão, a potência do motor, pressões, temperaturas e emissões, contribuindo assim para a avaliação do potencial desta tecnologia em aplicações nos drones.

Os resultados das simulações mostraram que a oxi-combustão aumenta os picos de pressão e temperatura, reduz as emissões de CO, e aumenta as emissões de CO₂ e NO_x. Para evitar O₂ não queimado e maximizar o desempenho do motor, encontrou-se um equilíbrio ideal, utilizando 30 % de O₂, e aumentando a massa de combustível em 15 % e a recalibração dos tempos de ignição e injeção.

Este trabalho foi desenvolvido em ambiente empresarial, na empresa TEKEVER, UAS, localizada nas Caldas da Rainha, Portugal.

Palavras-chave: drones; oxi-combustão; motores de combustão interna; enriquecimento com oxigénio; simulação numérica; ANSYS Forte

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Abbreviations and Symbols

Abbreviations

AI – Artificial Intelligence

ASU – Air Separation Unit

BC – Bottom Centre Crank Position

BDC – Bottom Dead Centre

BLOS – Beyond Line-of-sight

CCS – Carbon Capture Systems

CCTs – Carbon Capture Technologies

CFD – Computational Fluid Dynamics

CI – Compression Ignition

CMCs – Ceramic Matrix Composites

EBCs- Environmental Barrier Coatings

ECU – Engine Control Unit

EGR – Exhaust Gas Recirculation

GCS – Ground Control System

HALE – High Altitude Long Endurance

HCs – Hydrocarbons

IC – Internal Combustion

IGCC – Integrated Gasification Combined Cycle

IMEP – Indicated Mean Pressure

ITM – Ion Transport Membranes

LOS – Line-of-sight

MALE – Medium Altitude Long Endurance

MHX – Main Heat Exchanger

MIEC – Mixed Ionic Electronic Conducting

MUAV – Mini Unmanned Aerial Vehicle

OEC – Oxygen-Enhanced Combustion

OTM – Oxygen Transport Membranes

PA – Polyamide

PANi – Polyaniline

PDMS – Polydimethylsiloxane

PI - Polyimide

PSA – Pressure Swing Adsorption

PSF – Polysulfone

PU – Polyurethane

R&D – Research and Development

RF – Radio Frequency

RPM – Rotation per minute

SAR – Synthetic Aperture Radars

SI – Spark Ignition

SPED – Density of Propulsive Energy

TBCs – Thermal Barrier Coatings

TC – Top Centre Crank Position

TDC – Top Dead Centre

Ti – Titanium

TUAV – Tactical Unmanned Aerial Vehicle

UAS – Unmanned Aerial System

UAVs – Unmanned Aerial Vehicles

UHCs – Unburnt Hydrocarbons

VOCs – Volatile Organic Compounds

VSA – Vacuum Swing Adsorption

VTOL – Vertical Takeoff and Landing

YSZ – Ytria-stabilized Zirconia

Symbols

b_e – Effective specific fuel consumption [g/kWh]

b_i – Indicated specific fuel consumption [g/kWh]

d_k – Piston diameter [mm]

$[CO_2]_{ambient}$ – Mass of carbon dioxide in environment [kg]

$[CO_2]_{exhaust}$ – Mass of carbon dioxide in exhaust gases [kg]

$[CO_2]_{intake}$ – Mass of carbon dioxide in intake manifold [kg]

EGR – EGR ratio $[-]$

E_K – Energy associated to fuel K [J]

H_u – Net Calorific value of fuel [J/kg]

L_{St} – Stoichiometric air requirement [kg_{air}/kg_{fuel}]

M – Third Collision Partner $[-]$

M_{O_2} – Molar weight of oxygen [kg/mol]

M_d – Torque [Nm]

m – Mass [kg]

m_K – Weight of fuel admitted [kg]

$\dot{m}_K$ – mass flow rate associate to fuel K [kg/s]

m_L – Actual mass of air [kg]

$m_{L,St}$ – Stoichiometric mass of air [kg]

$m_{O_2,St}$ – Mass of oxygen in standard conditions [kg]

N – Number of moles [mol]

n – Engine revolutions $[-]$

n_K – Number of moles of fuel [$kmol$]

$n_{O_2,St}$ – Number of moles of oxygen [$kmol$]

$\dot{W}$ – Power [W]

P – Pressure [Pa]

P_e – Effective power [W]

P_i – Indicated power [W]

R – Ideal Gas Constant [$J/mol \cdot K$]

R_u – Universal Gas Constant [$J/mol \cdot K$]

s – Piston stroke [mm]

s' – Residual stroke above the slots [mm]

T – Temperature [K]

t – Time [s]

V – Volume [m^3]

V_c – Compression or dead volume [cm^3]

V_H – Piston displacement [cm^3]

V_h – Total swept volume [cm^3]

V'_h – Dead volume above the slots [cm^3]

$\dot{V}_K$ – Volumetric flow rate [m^3/s]

V_{min} – Compression or dead volume [cm^3]

W_{KA} – Gas Work [J]

z – Number of cylinder [$-$]

Greek symbols

ε' – Effective compression ratio [$-$]

ε – Compression ratio [$-$]

η – Efficiency [$-$]

η_e – Effective efficiency [$-$]

η_i – Indicated efficiency [$-$]

λ – Air fuel ratio [$-$]

$\xi_{O_2,L}$ – Percentage by weight of oxygen in the air [%]

ρ_K – Density of fuel K [kg/m^3]

v – Specific Volume [m^3/kg]

ω – Angular speed [rad/s]

Chapter 1

Introduction

This dissertation is part of a Master's Degree in Mechanical Engineering at Faculdade de Engenharia da Universidade do Porto. The work was developed in cooperation with TEKEVER, UAS SA, located in Leiria, Portugal. The main objective of this dissertation is to analyse the effect of oxy-combustion in internal combustion engines, more specifically, in a two-stroke drone engine.

1.1 Project Context

From the Industrial Revolution through the first half of the 20th century, fossil fuels were the predominant source of energy generation worldwide.

However, the global warming issue has led the European Union to set some targets, among them to reduce carbon emissions by 55 % by 2030 and to become the first climate-neutral continent by 2050 (Raho et al. 2022).

One way to reduce carbon dioxide emissions is to utilize renewable energy sources, such as solar, wind, or geothermal energy. However, the cost of these technologies remains higher than the cost of oil, making them less competitive in today's market. At the same time, global energy demand is increasing, making the continued use of fossil fuels necessary (Nemitallah et al. 2017).

Consequently, if the use of fossil fuels continues to be a reality, it is necessary to develop strategies to reduce CO₂ emissions. Among these strategies are technological approaches for regulating emissions, such as carbon capture technologies (CCTs), with oxy-combustion being a prominent example (Raho et al. 2022).

In the last few years, the use of drones has grown significantly in areas such as logistics, environmental monitoring, and defence, so there is a need to develop more efficient, compact propulsion systems with lower environmental impact and an extended range.

A promising approach is oxy-combustion, which involves burning fuel using oxygen-enriched air, normally more than 95 % oxygen, instead of atmospheric air. In this way, it will be possible to obtain higher combustion temperatures, improve thermal efficiency, and reduce the emission of pollutants, especially nitrogen oxides (NO_x).

The effects of oxy-combustion in internal combustion engines have been widely studied through ANSYS simulations, which allow for a detailed analysis of the intake flow and combustion behaviour. This makes it a valuable tool for evaluating oxy-combustion in lightweight applications, such as drone engines. Thus, this work aims to investigate the application of oxy-combustion in a two-stroke drone engine, based on simulating the behaviour of oxygen-enriched air in the engine intake, using ANSYS Software, and assessing the feasibility of using an oxygen separation system.

1.2 Background and Motivation

In recent decades, advancements have led to the development of vehicles that do not require human presence to operate. Those vehicles, which are Unmanned Aerial Vehicles (UAVs), have witnessed huge improvements. Recently, UAVs have been used to accomplish tasks in urban, suburban, and rural areas. Among all the possible applications, it is possible to highlight surveillance, delivery of medical supplies to remote places, coastguard and sea-lane monitoring, fire-detection and response services (Ariante and Del Core 2025).

Depending on the type of mission, fuel engines can be used, in particular, piston engines. Piston engines are internal combustion engines that use fuel as an energy source to convert chemical energy into mechanical energy. One of the advantages of using this type of technology is that it is a mature technology, the structure is simple, and it is a low-cost

system. Although it has some disadvantages: low power-to-weight ratio when compared with turbine engines and has speed limitations (Zhang et al. 2022).

Nowadays, there is a huge concern about global warming and greenhouse gas emissions. To overcome those concerns, adaptations or changes to existing systems and technologies must be adopted. On one hand, it is possible to change fuel engines for hybrid fuel-electric engines or pure electric engines. On the other hand, adaptations to existing fuel engines can be adopted. To reduce greenhouse gas emissions, it is possible to adopt an oxy-combustion system.

Oxy-combustion is a combustion with oxygen-enriched air, normally more than 95% of oxygen, instead of atmospheric air. The only products of this type of combustion are water vapor and carbon dioxide. As oxy-combustion doesn't use atmospheric air, there are no nitrogen oxides in flue gases, only carbon dioxide, which can be reused to cool the engine or can be captured by one of the carbon capture technologies.

The focus of this dissertation work is to apply oxy-combustion technology to internal combustion engines, and more specifically to two and four-stroke drone engines, in order to increase engine efficiency and power, and reduce pollutant emissions. To understand the feasibility of the use of oxy-combustion, an internal combustion engine was simulated using the Ansys Forte software.

One of the limitations of this work is the fact that there is no research about oxy-combustion in drone engines, although in the literature, it is possible to find studies of oxy-combustion applied to internal combustion engines, such as Diesel engines or spark ignition engines. This helps to understand if oxygen-enriched combustion could be a future technology applied to drone engines.

1.3 Objectives

The main objective of this work is to evaluate the feasibility and potential advantages of applying oxy-combustion technology in drone propulsion systems.

To achieve this overarching goal, three specific objectives are established:

- Develop and implement a compact, integrated oxygen separation system for UAVs.
- Simulate oxygen-enriched air in an internal combustion engine using *ANSYS® Forte*, developed by *ANSYS, Inc.*
- Compare engine performance (e.g., efficiency, power output, emissions) between conventional air-fuelled combustion and oxygen-enriched combustion.

Thus, it is expected that these objectives will provide a comprehensive assessment of the technical and environmental feasibility of oxy-combustion as an innovative approach for UAV propulsion.

1.4 Sustainable Development Goals (SDGs)

This research is closely aligned with the United Nations Sustainable Development Goals (SDGs) (Figure 1), specifically addressing the global demand for more efficient and sustainable technological solutions in the aerospace sector.

Primarily, this work contributes to SDG 9 (Industry, Innovation and Infrastructure) by fostering technological advancement in unmanned aerial systems (UAS). The exploration of oxy-combustion in two-stroke and four-stroke engines represents a significant innovation in propulsion systems, directly upgrading the technological capabilities required for modern drone applications in logistics, defence, and environmental monitoring.

Furthermore, the optimization of the engine operational parameters supports SDG 12 (Responsible Consumption and Production). By identifying an optimal balance between oxygen-enrichment alongside with changes in fuel mass and engine calibration adjustments, this study maximizes thermal and combustion efficiency. This approach promotes a more rational and efficient use of energy resources, ensuring that enhanced efficiency engine performance is achieved through optimized fuel consumption.

Finally, the broader implication of this technology intersects with SDG 13 (Climate Action). Although the localized in-cylinder thermodynamics of oxy-combustion lead to

higher NO_x and CO₂ formations due to high peak temperatures, the technology itself is critical. Oxy-combustion facilitates a more complete burn (evidenced by reduced CO emissions) and produces an exhaust stream with a higher CO₂ concentration, which is a fundamental requirement for the future integration of carbon capture technologies. Moreover, providing highly efficient propulsion systems ensures that drones, can be more effectively deployed in vital environmental and climate monitoring missions.



Figure 1 – SDGs applied to this work.

1.5 Methodology

In an initial stage, the approach consisted of developing the literature review and researching internal combustion engines, UAS technology, oxy-combustion, oxygen separation methods, Computational Fluid Dynamics (CFD), and Ansys Forte modelling and materials that can be used in high temperature engines. Simultaneously, an engine model was developed to be used in previous simulations. For that, measurements were made, and a 3D model of a two-stroke engine was created using SolidWorks software.

Subsequently, using Ansys Forte and a four-stroke engine, previously modelled and validated, some simulations were made. First, to run the simulations, the intake air composition was changed from 21 % to 99 % O₂. Second, with the same range of oxygen composition, the intake temperature and pressure were changed. The results of the different simulations were analysed in order to understand which O₂ concentration is most suitable for a four-stroke engine.

With the chosen composition, new simulations were conducted. This time, the engine's angular speed was changed from 1500 to 5000 rpm. After that, the power curves were represented for each composition, with the main purpose of selecting a fuel mass capable of equalling the engine's reference power, in this case, close to engine power for an oxygen concentration of 21 %.

1.6 Hosting Company

TEKEVER is a leading provider of advanced unmanned aerial systems for maritime surveillance. The company specializes in developing drones powered by an AI-centric platform that integrates Edge AI, satellite communications, and cloud computing to deliver real-time data and advanced analytics. These solutions are accessible via intuitive web and mobile interfaces. TEKEVER is also a recognized expert in satellite communication, particularly in Inter-Satellite Links and satellite RF payloads for Earth observation and space exploration.

With a strong focus on research, development, and engineering, TEKEVER's talent excels in cutting-edge technology implementation. The company has R&D, engineering, and production facilities in Portugal, France, and the UK. TEKEVER collaborates with a global partner network, ensuring local support to customers worldwide.

1.7 Dissertation Structure

The document is organized in six chapters and is complemented with additional information in the appendices at the end of the document. This first chapter presents an introduction and an overview of the work developed during this Master's Dissertation.

The second chapter provides an overview of the current state of the environment, as well as the levels of pollutant gas emissions, highlighting the need to find alternatives to reduce these emissions. Accordingly, a possible solution—oxy-combustion—is presented, along with its applicability within the scope of the present work. Alongside

that, the chapter contains the theoretical background of the study, addressing topics such as unmanned aerial vehicles (UAVs), internal combustion engines, combustion fundamentals, oxy-combustion, and possible methods for oxygen separation.

The third chapter covers the modelling process and the use of the ANSYS Forte combustion simulation software, in which all the parameters employed are explained in detail.

In the fourth chapter, the results are presented, and comparisons are made between the simulations performed after varying some of the combustion parameters.

Finally, the fifth chapter presents the conclusions of the work and proposes directions for future research that may be developed as a continuation of this study.

Chapter 2

Literature Review

2.1 UAVs Technology

In recent years, UAVs (Unmanned Aerial Vehicles) have seen significant improvements in their structure, working methodology, flying features, and navigation control. UAVs are a very versatile technology, with a wide range of applications and for that reason, are a promising technology (Ahmed et al. 2022).

The use of these systems has increased in the last few years, and they are crucial for surveillance, monitoring, and conservation. Therefore, it is important to understand their working principles, systems, and classifications to develop new approaches and optimize performance.

2.1.1 UAS Concept

A UAS (Unmanned Aerial System) is described as the complete system, which includes the aircraft, control stations, and data links (Figure 2). Considering there is no pilot in a UAV, the aircraft is remotely piloted by an operator and, for that, uses command, control, and communication systems. These operations can be accomplished in a Ground Control System (GCS) or can be pre-programmed, allowing the aircraft to fly autonomously.



Figure 2 - UAS components (Ariante and Del Core 2025).

Historical evolution

The first UAV was manufactured in 1916 by the two American citizens Lawrence and Sperry. The system used was the beginning of “attitude control”, which started being used for automatic piloting of an aircraft. The device was called “aviation torpedo” and Lawrence and Sperry flew a distance of approximately 48 km.

But the major development of UAVs started in the 1950s, taking advantage of the Vietnam War and the Cold War. After the Vietnam War, the U.S. and Israel began to develop smaller and cheaper UAVs. These were small aircraft that used small motorcycles or snowmobiles engines. They carried video cameras and transmitted images to the operator's location. During the Gulf War in 1991, the U.S. put UAVs into practical use, and UAVs for military applications developed rapidly from there (Gupta, Ghonge, and Jawandhiya 2013).

2.1.2 UAV Classification

Unmanned Aerial Vehicle classification methods are based on the use of UAV features. UAVs can be classified according to the following characteristics (Tachinina, Lysenko, and Kutiepov 2022):

Type of aircraft

According to the type of aircraft, the main types of UAVs are aircraft-type, helicopter-type, and multi-rotor.

Aircraft-type UAVs are also known as fixed-wing UAVs. In this type of aircraft, lift is generated through an aerodynamic method, using the pressure of the air flowing on the fixed wing. The design of this type of UAVs has the same configuration as the ones used in manned aviation. This type of UAV is characterized by long flight duration, high maximum flight altitude, and high speed.

Helicopter-type UAVs are also known as rotary-wing, with the lift generated aerodynamically by the rotating propeller blades rather than by wings as in fixed-wing UAVs. In these types of UAVs, wings are completely absent or play a secondary role. The ability to hover at a point and high manoeuvrability are some of the advantages of rotary-wing UAVs.

Multi-rotor UAVs have more than one rotor, and the most commonly used designs are tricopters, quadcopters, hexacopters, and octocopters.

Finally, there are hybrid fixed-wing VTOL (Vertical Takeoff and Landing), which have the stability of a fixed-wing UAV as well as the ability to hover, take off, and land vertically (Tachinina, Lysenko, and Kutiepov 2022).

Dimension

UAVs can also be classified according to size, using the following subclasses: Very small UAVs, Small or Mini UAVs, Medium UAVs, and Large UAVs.

The very small UAV class (Figure 3) refers to UAVs whose size ranges from 30 to 50 cm. They are extremely small and very lightweight. Depending on the desired manoeuvrability, they may have rotary or flapping wings, and the last design allows them to land on very small surfaces.

Small UAVs or Mini UAVs refer to UAVs with at least 50 cm and at most 2m. Many designs in this type of UAV are based on fixed-wing models, most of which are launched manually, being thrown into the air.

Medium UAVs (Figure 3) are UAVs that are too heavy to be carried by a single person, but smaller than light aircraft. Usually, they have a wingspan of about 5 to 10 m and can carry a payload of 100 to 200 kg.

Finally, the large UAV class (Figure 3) refers to UAVs used for military purposes, typically with more than 10 m (Model 2025).

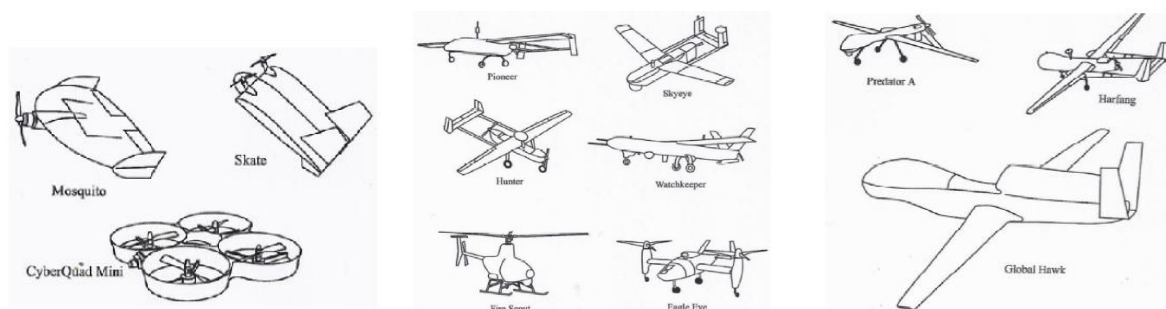


Figure 3 - Examples of: Very Small UAVs; Medium UAVs; Large UAVs (from left to right) (Tachinina, Lysenko, and Kutiepov 2022).

Range, endurance and altitude

High-Altitude Long Endurance (HALE) vehicles fly at altitudes above 15000 m and has more than 24 hours of endurance. They carry out extremely long-range reconnaissance and surveillance, and some are armed. This technology is usually operated by Air Forces from fixed bases.

Medium Altitude Long Endurance (MALE) vehicles fly between 5000 and 15000 m altitude and have 24 hours of endurance. They play a similar role to HALE, but generally operate over shorter ranges, around 500 km, and from fixed bases.

Medium Range or Tactical UAV (TUAV) vehicles have a range between 100 and 300 km, and the systems are smaller and simpler than HALE or MALE systems. Inside this UAVS group, are also Close-Range UAVs, which can be used for military or civilian purposes and operate in ranges up to 100 km.

Mini UAV (MUAV) is a UAV under 20 kg, but not as small as Micro UAV, capable of being launched by hand and with a range of up to 30 km. MUAVs are also used for military and civilian purposes (Gupta, Ghonge, and Jawandhiya 2013).

Engine type

The characteristics, advantages, and disadvantages of the different engine types are summarized in Table 1.

Table 1 - Advantages and disadvantages of UAVs engines (Tachinina, Lysenko, and Kutieпов 2022).

Piston Engine - Two-stroke engine	
Advantages	Disadvantages
• Low mass • High power-to-weight ratio (P/W) • Better SPED (density of propulsion energy) values	• High noise level compared to a four-stroke or Wankel engine.
Four-stroke engine	
• Better fuel economy than the Wankel engine	• Rather noisy • Not commonly used due to its heavy weight • Very low power-to-weight ratios compared with two-stroke engines
Wankel engine	
• High power-to-weight ratio • Simple construction • Endurance and reliability of operation • Valveless system • Possibility of using lower-octane fuel • Easy start at low temperatures	• Rather noisy • High carbon dioxide emissions • High cost of production • High fuel consumption • Relatively low torque
Jet propulsion	
• Very high power-to-weight ratio • Very low weight	• Very high fuel consumption
Turbojet engine	
• Very high power-to-weight • Relatively light	• Very high fuel consumption
Turboprop engine	
• Consume cheaper fuel (aviation kerosene) • Efficient at low cruising speeds • Lightweight • Ongoing maintenance is less complicated than in other engines.	• No disadvantages to point
Electric Motor	
• More efficient • Low weight • Good power-to-weight ratio	• Low SPED • Not suitable for long distances, due the batteries capacity.

Degree of autonomy

UAVs can also be classified by their degree of autonomy. There are seven levels from level 0 to level 5.

Level 0 – No automation: The pilot has full control of the aircraft, and it is totally manually controlled.

Level 1 – Pilot assistance: The pilot continues to control the operation and safety of the UAV; however, a drone can take over at least one vital function for a limited period of time.

Level 2 – Partial automation: The pilot remains responsible for safety and must be ready to take control of the drone if something happens. Most manufacturers currently build drones at this level, where the platform can assist with navigation functions and allow the pilot to delegate some tasks.

Level 3 – Conditional automation: Very similar to level 2, but the UAV notifies the human pilot if intervention is necessary.

Level 3+ - Automated drone deployment: No human supervision is required during the flight.

Level 4 – High automation: The UAV can be controlled by a human, but it is not always necessary. The drone is expected to use backup systems if a system fails and remains operational.

Level 5 – Full automation: The UAV controls itself under any conditions without human intervention. At the moment, there are no UAVs of this type (Tachinina, Lysenko, and Kutieпов 2022).

2.1.3 Structure and main systems

UAS is composed of aircraft, communication systems, command and control elements, and payload (Figure 4).

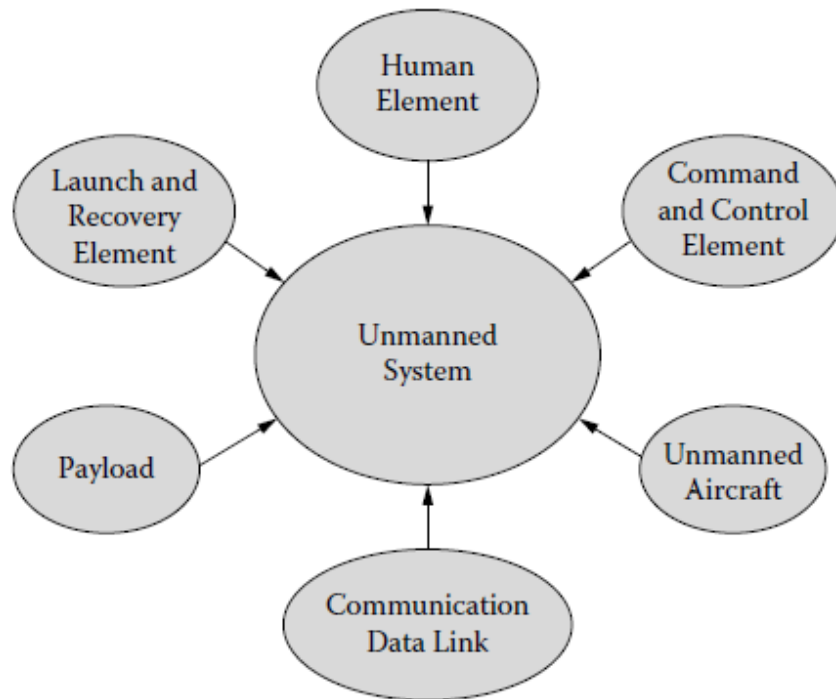


Figure 4 - Elements of an Unmanned System (Barnhart, Marshall, and Shappee 2021).

In chapter 2.1.2, the types and classifications of aircraft available on the market were presented.

Regarding the command-and-control elements, the aircraft can be autopiloted, which means that the aircraft is fully autonomous from takeoff to landing. Another command system is Ground Control Station (GCS), which is a land- or sea-based control centre that provides facilities for human control of UAVs. GCS vary in size, can be as small as a handheld transmitter or as large as a self-contained facility with multiple workstations. A GCS consists of at least a pilot station: the pilot-in-command operates the aircraft and its systems, and a sensor station: the operator manages the sensor payload and radio communications. Complex UAS may require more workstations.

Data link is the term used to describe how the UAS command and control information is sent and received, both to and from the GCS and autopilot. UAS operations can be divided into two categories: radio frequency line-of-sight (LOS) and beyond line-of-sight (BLOS).

Line-of-sight (LOS) operations refer to operating a UAV via direct radio waves. Most of the frequencies used in these systems are unlicensed and are regulated by governmental directives.

Beyond line-of-sight (BLOS) refers to operating UAVs via satellite communications or using a relay vehicle, usually another aircraft.

Most of the time, UAVs are used to accomplish a mission, and the mission usually requires a payload. The payload can be related to surveillance, weapons delivery, communications, or cargo. For surveillance, for example, sensor payloads are used. Examples of sensors are electro-optical cameras, infrared cameras, synthetic aperture radars (SAR), or laser range finders/designators. These systems can be installed on the UAV by permanent mounting, giving the operator a fixed view, or the UAV can employ a system called a gimbal or turret. This system gives the sensor a predetermined range of motion, usually in two axes (vertical or horizontal).

Electro-optical cameras use electronics to pivot, zoom, and focus the image, and these cameras operate in the visible light spectrum. Infrared cameras operate in the infrared range of the electromagnetic spectrum. Laser range finders are used to determine the distance to an object, while laser range designator is used to designate a target. The use of lasers has some inconveniences, such as it may not be accurate when the atmospheric conditions are unfavourable, the laser can be absorbed by special paints, or reflect incorrectly (Barnhart, Marshall, and Shappee 2021).

2.1.4 Challenges and future

It is expected that research on autonomous aerial vehicles will continue in the next years.

Future work may include developments in hybrid aerial robotics, air-ground drones, long flight drones with smart technology batteries, and VTOL with high accuracy.

However, several challenges must be properly addressed in the research and development of UAVs. These include UAVs communications, dynamic path planning, privacy and security, efficient energy for UAVs, union of UAVs and AI (Artificial

Intelligence), and integration of different segments, for network communication between air, ground, and space UAVs; (Ahmed et al. 2022).

2.2 Internal Combustion Engines

Internal combustion engines are piston engines, in which the working fluid – air – is simultaneously the source of the oxygen necessary for combustion. Fuel combustion produces exhaust gases. Combustion is a cyclical process, and the differentiation lies in the working principle and the type of fuel used, such as gasoline, diesel, or hybrid engines.

One way to classify internal combustion engines is according to their working cycles, which can be four-stroke or two-stroke cycles (Figure 5). For the case studied, it is necessary to understand two-stroke cycles (Basshuysen and Schaefer 2016).

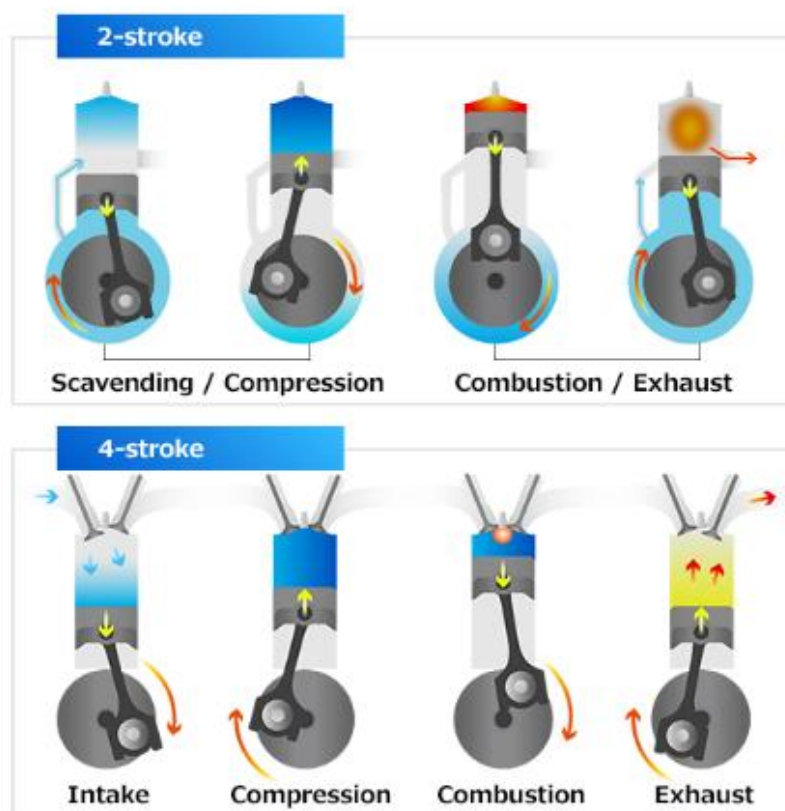


Figure 5 - Scheme of Two and Four-Stroke engines working principles (Motorcycle 2026).

2.2.1 Two-stroke Engines

At the end of the 19th century, the two-stroke engine was invented by Sir Dugald Clerk. Motorcycles were among the first applications of this type of engine.

Since its invention, the two-stroke engine has been employed by numerous car manufacturers and adapted for use in light aircraft, including those designed for meteorological data collection or for military purposes. (Blair 1996)

Working principle

The cycle of a two-stroke engine comprises four processes – intake, compression, expansion, and exhaust – completed in just two strokes of the piston, as shown in Figure 5.

1st stroke – Scavenging and Compression

The piston, moving from BDC, moves upward, closing the inlet port and subsequently the exhaust port. As the stroke continues, the piston compresses the air–gasoline mixture in the cylinder. Simultaneously, the piston uncovers the inlet port, and the pre-mixture is admitted into the crank case. The second stroke ends when the piston reaches the Top Dead Centre (TDC) (Martins 2013).

2nd stroke – Combustion and Exhaust

The piston moves upward, compressing the mixture in the combustion chamber, and the spark plug ignites it, causing combustion and resulting in an increase in pressure and temperature. Then, the piston moves downward from the Top Dead Centre (TDC), transferring energy to the crankshaft.

Before the end of the stroke, the piston uncovers the exhaust port, through which the exhaust gases are expelled under a pressure higher than atmospheric pressure. During the downward movement, the mixture in the crankcase is compressed, and the piston

uncovers the inlet port, allowing the fresh pre-compressed gases in the crankcase to flow into the cylinder.

Finally, the piston reaches the Bottom Dead Centre (BDC) (Martins 2013).

2.2.2 Four-Stroke Engines

In 1876, one of the most significant steps in the development of internal combustion engines was made when Nicolaus Otto patented and produced the first four-stroke engine. This engine was more silent than the free-piston engines, one of the first engines invented.

Working principle

The cycle of a four-stroke engine comprises four processes – intake, compression, expansion, and exhaust – completed in just four piston strokes, as shown in Figure 4.

Intake stroke

This stroke starts with the piston at the top-centre crank position (TC) and ends with the piston in the bottom-centre crank position (BC), which intakes fresh mixture into the cylinder. To increase the inducted mass, the inlet valve opens shortly before the stroke starts and closes after it ends.

Compression stroke

This stage occurs when both valves are closed, and the mixture inside the cylinder is compressed to a small fraction of its initial volume. Near the end of the compression stroke, combustion is initiated, and the cylinder pressure rises more rapidly.

Combustion stroke

Starts with the piston at TC and ends at BC, as the high-temperature and high-pressure gases push the piston down, forcing the crank's rotation. About five times more work is done on the piston during the power stroke than the piston performs during compression. When the piston approaches the BC, the exhaust valve opens to initiate the exhaust process and reduce the cylinder pressure to close the exhaust pressure.

Exhaust stroke

The remaining burned gases leave the cylinder: first, because the pressure in the cylinder is higher than the exhaust pressure; second, they are swept out by the piston as it moves toward TC. When the piston approaches TC, the inlet valve opens. Immediately after the TC, the exhaust valve closes, and the cycle starts again (Heywood 1998).

2.2.3 Engine Characteristics

Engine characteristics are important to design fundamental dimensions and evaluate and compare different engines.

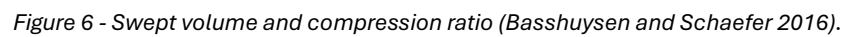
Piston Displacement

Piston displacement or swept volume V_h for an engine cylinder is the distance travelled by the piston during one stroke, between BDC and TDC, and is calculated using Equation 1 (Basshuysen and Schaefer 2016).

$$V_H = V_h \cdot z = \frac{\pi \cdot d_k^2}{4} \cdot s \cdot z \quad (1)$$

Where s is the piston stroke, d_k is the piston diameter or piston bore, V_H is the piston displacement for one cylinder, V_h is the total swept volume of the engine, and z the number of cylinders.

The compression ratio is the quotient between the maximum and the minimum cylinder volumes: the maximum volume is reached when the cylinder is at BDC, and the minimum when the cylinder is at TDC position, as shown in Figure 6.


$$\varepsilon = \frac{V_{max}}{V_{min}} = \frac{V_h + V_C}{V_C} \quad (2)$$

Where $V_c = V_{min}$ = Compression or dead volume.

In two-stroke engines with slot control, a distinction is made between geometric compression ratio, ε , and the effective compression ratio, ε' . The effective compression only starts when the intake and exhaust slots are closed. The effective compression ratio is given by Equation 3 and 4.

$$\varepsilon' = \frac{V_h' + V_c}{V_c} \quad (3)$$

$$V_h' = \frac{\pi \cdot d_k^2}{4} \cdot s' \quad (4)$$

Where, V_h' is the dead volume above the slots and s' is the residual stroke above the slots.

For two-stroke engines, the compression ratio ranges between 7.5 and 10. For a four-stroke engine, particularly a direct injection engine, the compression ratio is between 9 and 12.

Torque and Power

The power is defined by Equation 5 from the torque and engine revolutions.

$$P_e = M_d \cdot \omega = M_d \cdot 2 \cdot \pi \cdot n \quad (5)$$

According to Equation 5, an increase in power can be achieved by increasing the rotational speed or the torque.

Fuel Consumption

The energy admitted by the fuel per unit of time is defined by Equation 6.

$$E_K = m_K \cdot H_u \quad (6)$$

where m_K is the weight of fuel admitted and H_u is the net calorific value of fuel

Fuel consumption is measured as a volumetric flow or as mass flow, being defined by Equation 7.

$$\dot{m}_K = \frac{m_K}{t} = \rho_K \cdot \dot{V}_k \quad (7)$$

Where, ρ_K is the fuel density.

For better comparability, fuel consumption can also be referred to the indicated power or effective power. The indicated specific fuel consumption is defined by Equation 8.

$$b_i = \frac{\dot{m}_K}{P_i} = \frac{1}{\eta_i \cdot H_u} \quad (8)$$

Where, η_i is the indicated efficiency or internal effectiveness.

Effective specific fuel consumption is

$$b_e = \frac{\dot{m}_K}{P_e} = \frac{1}{\eta_e \cdot H_u} \quad (9)$$

Where, η_e is the effective efficiency.

Efficiency

In internal combustion engines, a distinction is made among the indicated, effective, and mechanical efficiencies.

The indicated and the effective efficiencies are essentially determined from the energy stored in the fuel.

The energy per unit of time admitted with the fuel is given by Equation 10.

$$\frac{E_K}{t} = \dot{m}_K \cdot H_u \quad (10)$$

where $\dot{m}_K$ is the admitted mass of fuel per unit of time, H_u is the net calorific value of the fuel.

If P is the engine power, and it is the output of the engine process, and the admitted fuel energy per unit of time is the input, then the efficiency η can be calculated using Equation 11.

$$\eta = \frac{\text{Power}}{\text{Fuel}} = \frac{P}{\frac{E_K}{t}} = \frac{P}{\dot{m}_K \cdot H_u} \quad (11)$$

Indicated Mean Pressure

The indicated mean pressure (p_{mi}) represents the equivalent specific work acting on the piston. For better understanding, the indicated mean pressure will be designated as IMEP.

IMEP is determined from the cylinder pressure curve and the swept volume, which means that it is possible to use the $p - V$ diagram and use the area below the $p - V$ to calculate the IMEP.

After some equation manipulation, it is possible to calculate the IMEP using Equations 12 and 13.

$$W_{KA} = \oint p \, dV_\alpha \quad (12)$$

$$IMEP = \frac{W_{KA}}{V_h} \quad (13)$$

where dV_α = change in volume = $f(\text{crank angle } \alpha)$, V_h is the piston displacement for one cylinder, and W_{KA} is the gas work at piston per working cycle.

Air-fuel ratio

During combustion in the engine, the ratio of the air mass actually present in the cylinder to the stoichiometric air mass is referred to as the air/fuel factor λ .

The stoichiometric air requirement L_{St} is defined as the quotient between the air mass and the fuel mass under stoichiometric conditions, that is

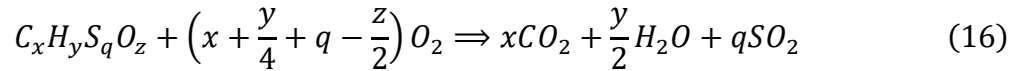
$$L_{St} = \frac{m_{L,St}}{m_K} \quad (14)$$

$$\lambda = \frac{m_L}{m_{L,St}} = \frac{m_L}{m_K \cdot L_{St}} \quad (15)$$

where, $m_{L,St}$ is the air mass under stoichiometric conditions and m_K is the fuel mass.

The stoichiometric air requirement can be calculated from the weight percentage of the chemical elements contained in the fuel, also taking into account the combustion products (exhaust gases) resulting from the combustion.

The most important products in complete combustion are carbon dioxide (CO_2), water (H_2O), and sulphur dioxide (SO_2), as well as nitrogen (N_2). Considering a fuel with the composition $C_xH_yS_qO_z$, the chemical equation is obtained:



With the stoichiometric components

$$x = \frac{M_K}{M_C} \cdot c ; y = \frac{M_K}{M_H} \cdot h ; q = \frac{M_K}{M_S} \cdot s ; z = \frac{M_K}{M_O} \cdot o$$

Where, c, h, s, o are the weight percentages of the elements carbon (c), hydrogen (h), sulphur (s) and oxygen (o) contained in the fuel, M_C, M_H, M_S, M_O are the molar weights of the elements in the fuel, and M_K is the molar weight of the fuel.

Considering the weight percentage of oxygen in the air, $\xi_{O_2,L}$, the stoichiometric air requirement is obtained as:

$$L_{St} = \frac{1}{\xi_{O_2,L}} \cdot \frac{m_{O_2,St}}{m_K} = \frac{1}{\xi_{O_2,L}} \cdot \frac{M_{O_2}}{M_K} \cdot \frac{n_{O_2,St}}{n_K} \quad (17)$$

Where M_{O_2} is the molar weight of oxygen and $n_{O_2}; n_K$ are the volumes of oxygen and fuel.

Based on the chemical reaction equations, the relation $n_{O_2,St} = x + \frac{y}{4} + q - \frac{z}{2}$ and $n_K = 1$, the following expressions are obtained:

$$L_{St} = \left(\frac{1}{\xi_{O_2,L}} \cdot \frac{M_{O_2}}{M_K} \cdot c + \frac{1}{4} \cdot \frac{M_{O_2}}{M_H} \cdot h + \frac{M_{O_2}}{M_S} \cdot s - o \right) \quad (18)$$

$$L_{St} = \frac{1}{0.232} \cdot (2.664 \cdot c + 7.937 \cdot h + 0.988 \cdot s - o) \quad (19)$$

A “lean mixture” ($\lambda > 1$) is a mixture with excess of air, while a rich mixture ($\lambda < 1$) is a mixture with air deficiency, and it is stoichiometric mixture when $\lambda = 1$. In the case of two-stroke engine, they operate with an air deficiency and four-stroke engine under stoichiometric conditions (Basshuysen and Schaefer 2016).

2.3 Combustion

2.3.1 Combustion Fundamentals

Combustion can be defined as rapid oxidation that generates heat or both light and heat. It is an important process that transforms energy stored in chemical bounds to heat, which can be used in several processes or systems (Turns 2000).

Combustion Modes and Flame Types

There are two types of combustion modes: flame or nonflame mode (Figure 7), and flames can be categorized as premixed flames or non-premixed (diffusion) flames.

Flame mode typically occurs in spark-ignition engines, where the fuel is mixed with air in the engine’s intake system. After compression of this fuel-air mixture, an electric

discharge initiates the combustion process, then a flame develops from the “kernal” created by the spark discharge and spreads throughout the cylinder to the combustion chamber walls. The nonflame mode occurs in diesel engines, where the fuel is injected into the cylinder in air that is already at high pressure and temperature, near the end of the compression stroke. Then an undesirable phenomenon, named “autoignition”, occurs, and portions of the developing mixture of already injected and vaporized fuel with this hot air start the combustion process, which spreads rapidly (Heywood 1998).

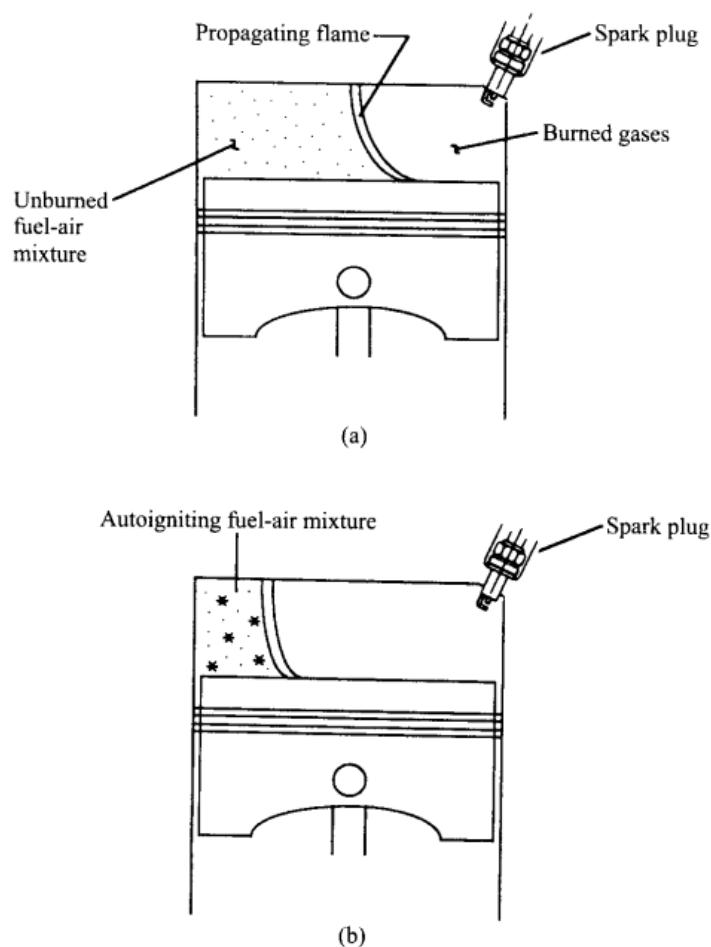


Figure 7 - (a) Flame and (b) nonflame modes (Turns 2000).

The types of flame are related to the mixing state of the reactants. In a premixed flame, the fuel and oxidizer are uniformly mixed in the same region where the reaction occurs. A non-premixed or diffusion flame occurs when the reactants are not premixed and must

mix in the same region where the reaction occurs, with the mixing taking place through a diffusion process.

The flame can also be classified according to the character of the gas flow through the reaction zone: whether it is laminar or turbulent. Laminar flow occurs at low Reynolds numbers, and turbulent flow, a chaotic and random state of motion, occurs at high Reynolds numbers. The Reynolds number is the ratio between inertial and viscous forces ($\text{density} \times \text{velocity} \times \text{length scale} / \text{viscosity}$) (Heywood 1998).

Simple laminar flows can be solved analytically using the continuity equation and Navier-Stokes equation, whereas more complex problems require the use of CFD modelling to be solved.

In engineering, most of the flows studied are turbulent, and fluid engineers have access to viable tools capable of representing the effects of turbulence through turbulence physics and CFD modelling (Versteeg 2007).

2.3.2 Combustion and Thermochemistry

Equation of state

The equation of state provides a relationship between the pressure (P), temperature (T) and volume (V) (or specific volume v). For an ideal-gas, a gas can be modelled neglecting intermolecular forces, and the equation of state can have the following equivalent forms:

$$PV = NR_u T \quad (20a)$$

$$PV = mRT \quad (20b)$$

$$Pv = RT \quad (20c)$$

Or

$$P = \rho RT \quad (20d)$$

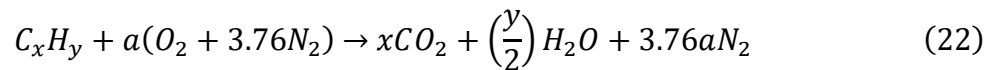
Where the specific gas constant R is related to the universal gas constant R_u (=8315 J/kmol·K) and the gas molecular weight MW by

$$R = \frac{R_u}{MW} \quad (21)$$

The density ρ , in Equation d is related with the specific volume by $\rho = \frac{1}{v} = \frac{m}{V}$ (Turns 2000).

Stoichiometry

The stoichiometric quantity of oxidizer is the amount needed to completely burn a certain quantity of fuel. If more than the stoichiometric quantity of oxidizer is supplied, the mixture is said to be a poor mixture, while supplying less than the stoichiometric quantity results in a rich mixture. The stoichiometric oxidizer or fuel ratio is determined by writing atom balances, assuming that the fuel reacts to form an ideal set of products. For a hydrocarbon fuel (C_xH_y), the stoichiometric relation is written as



Where

$$a = x + \frac{y}{4} \quad (23)$$

For simplicity, it is assumed that the composition of air is 21 % O_2 and 79 % N_2 (by volume), that means that for one mole of O_2 , there are 3.76 moles of N_2 .

The stoichiometric fuel ratio is then,

$$\left(\frac{A}{F}\right)_{stoic} = \left(\frac{m_{air}}{m_{fuel}}\right)_{stoic} = \frac{4.76a}{1} \frac{MW_{air}}{MW_{fuel}} \quad (24)$$

And the equivalence ratio, Φ , used to indicated if the mixture is lean, rich or stoichiometric is,

$$\Phi = \frac{\left(\frac{A}{F}\right)_{stoic}}{\left(\frac{A}{F}\right)} = \frac{\left(\frac{F}{A}\right)}{\left(\frac{F}{A}\right)_{stoic}} \quad (25)$$

From this definition, if $\Phi > 1$, the mixture is fuel-rich, if $\Phi < 1$ the mixture is fuel-lean and if $\Phi = 1$ the mixture is stoichiometric (Turns 2000).

Adiabatic Flame Temperature

There are two definitions for the adiabatic flame temperature: one for constant-pressure combustion and another for constant-volume.

If a fuel-mixture burns adiabatically at constant pressure, the absolute enthalpy of the reactants in the initial state ($T = 298 \text{ K}$, $P = 1 \text{ atm}$) is equal to the absolute enthalpy of the products in the final state ($T = T_{ad}$, $P = 1 \text{ atm}$), resulting in the following equations:

$$H_{reac}(T_i, P) = H_{prod}(T_{ad}, P) \quad (26a)$$

Or, equivalently, if equation 26a is divided by mass,

$$h_{reac}(T_i, P) = h_{prod}(T_{ad}, P) \quad (26b)$$

The statement of the first-law of thermodynamics (Equation 26) defines the adiabatic flame temperature at constant-pressure. The concept of adiabatic flame temperature is simple and is illustrated in Figure 8.

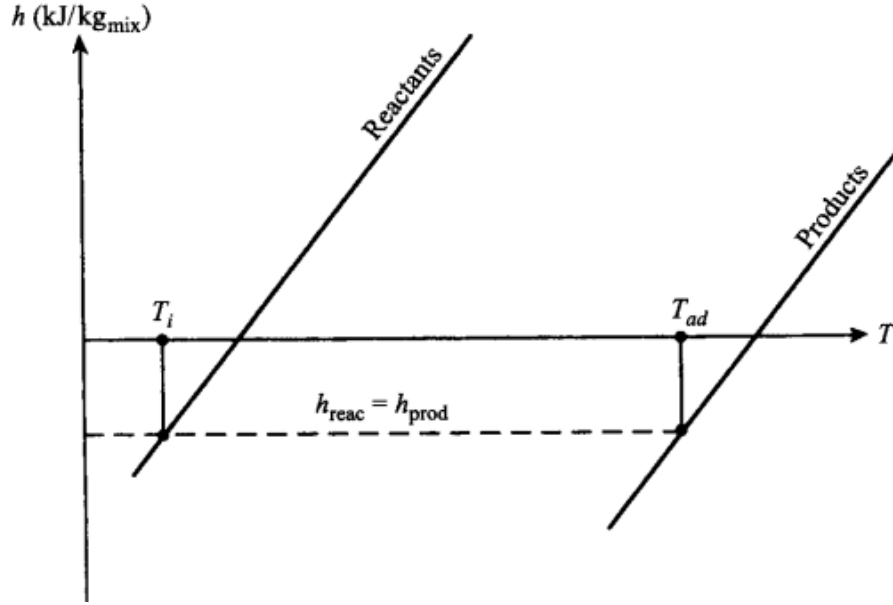


Figure 8 - Constant-pressure adiabatic flame temperature. (Turns 2000)

When analysing the temperature of the adiabatic flame at constant-volume, an ideal analysis of the Otto-cycle, for example, is necessary. The first law of thermodynamics requires:

$$U_{reac}(T_{int}, P_{int}) = U_{prod}(T_{ad}, P_f) \quad (27)$$

Where U is the absolute internal energy of the mixture. Graphically, Equation 27 resembles the sketch (Figure 7), used to illustrate the adiabatic flame at constant-pressure, except that internal energy replaces enthalpy. Since most thermodynamic property calculations provide values for H instead of U , it is possible to rearrange equation 27 to the following form:

$$H_{reac} - H_{prod} - V(P_{init} - P_f) = 0 \quad (28)$$

And the ideal gas law can be applied to eliminate PV terms:

$$P_{init} = \sum_{reac}^N R_{uT_{init}} = N_{reac} R_u T_{init}$$

$$P_f = \sum_{prod}^N R_{uT_{ad}} = N_{prod} R_u T_{ad}$$

Therefore,

$$H_{reac} - H_{prod} - R_u(N_{reac}T_{init} - N_{prod}T_{ad}) = 0 \quad (29)$$

An alternative form of Equation 29, based on the per-mass-of-mixture basis, can be obtained by dividing Equation 29 by the mass of mixture, m_{mix} , and recognizing that:

$$\frac{m_{mix}}{N_{reac}} \equiv MW_{reac} \quad (30)$$

Or

$$\frac{m_{mix}}{N_{prod}} \equiv MW_{prod} \quad (31)$$

And obtain:

$$h_{reac} - h_{prod} - R_u \left(\frac{T_{init}}{MW_{reac}} - \frac{T_{ad}}{MW_{prod}} \right) = 0 \quad (32)$$

Since the composition of the product mixture depends on both temperature and pressure, using Equation 29 or 32 with the ideal-gas law and appropriate equation of state, i.e., (only, ideal gas), to find it is straightforward, but not trivial (Turns 2000).

2.3.3 Chemical Equilibrium

In high-temperature combustion, the products of combustion are not resumed in a simple mixture of ideal products, as suggested in atom-balance used to determine stoichiometry. The major species dissociate, producing minor species. For example, in a hydrocarbon combustion with air, the ideal combustion products are CO_2 , H_2O , O_2 , and N_2 , although the dissociation of those products yields the following species: H_2 , OH , CO , H , O , N , NO , and others.

As it is possible to observe in Figure 9, for CO_2 dissociation, there is an increasing of CO mole fraction with temperature and pressure.

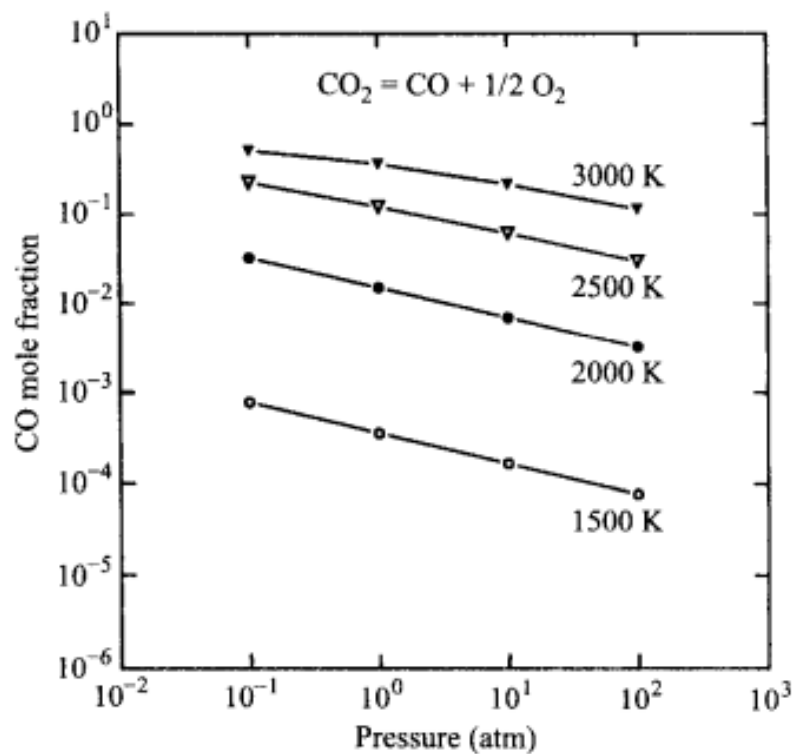


Figure 9 - CO mole fraction resulting from CO_2 dissociation at various pressures and temperatures.

Pressure has a significant effect on dissociation. Figure 9 also shows that the CO mole fraction decreases with increasing pressure (Turns 2000).

2.3.4 Chemical Kinetics

Chemical kinetics is the study of elementary reactions and their rates during combustion. In combustion processes, the rate of chemical reactions controls the combustion rate, and chemical rates are important for determining the formation and destruction of pollutants.

Understanding chemical kinetics and detailed chemical mechanisms is important for determining pollutant emission levels, and for this, there are computational models that allow predicting pollutant values after combustion (Turns 2000).

Global reactions express chemistry in a specific problem, but it does not provide a basis for understanding what is actually happening in a system. There are many intermediate processes, involving intermediate species. For example, considering the global reaction:



Equation 33 represents the conversion of hydrogen and oxygen into water, but the following elementary equations are important:



Where M is the third-body collision partner.

These overall reactions that involve multiple steps are called a reaction mechanism (Turns 2000).

2.3.5 Important Chemical Mechanisms

Carbon Monoxide Oxidation

Carbon Monoxide (CO) plays an important role in hydrocarbon oxidation. Hydrocarbon combustion can be characterized as a two-step process: the first step is the transformation of the fuel into CO, and the second step is the final oxidation of the CO into CO₂.

CO is slow to oxidize, unless there are some hydrogen-containing species present (small quantities of H₂O or H₂), which can improve the oxidation rate. These species promote faster oxidation of CO.

Nitrogen Oxides Formation

Nitrogen oxides and their formation mechanism play a significant role in combustion and, consequently, in air pollution.

In the combustion of fuels that do not contain nitrogen, nitrogen oxides can be formed by three chemical mechanisms: thermal or Zeldovich mechanism, the Fenimore or prompt mechanisms, and the N_2O - intermediate mechanism.

The thermal mechanism dominates in high temperature combustion, while the Fenimore mechanism is particularly important in rich combustion. The N_2O -intermediate mechanism is important in lean combustion and low-temperature processes.

The thermal or Zeldovich mechanism consists of two chain reactions:



Which can be extended by adding the following reaction,



The Fenimore mechanism (Figure 10) is related to the hydrocarbon combustion. Fenimore discovered that NO was rapidly produced near the flame zone of laminar premixed flames than the NO formed by the thermal mechanism, which is the reason why Fenimore mechanism is also called prompt NO. The hydrocarbon radicals react with molecular nitrogen, forming amines or cyano compounds, and then the amines and cyano compounds are converted into intermediate compounds that ultimately form NO. The process is described in the following equations:



When the equivalence ratio is above 1.2, the conversion of hydrogen cyanide, HCN, to form NO follows the following chain reactions:



In the atmosphere, nitric oxide oxidizes, forming nitrogen dioxide, which consequently produces acid rain and photochemical smog. In many combustion processes, significant fractions of oxides of nitrogen are emitted as NO_2 ($\text{NO}_x = \text{NO} + \text{NO}_2$), and the elementary reaction for forming NO_2 prior to exhausting of combustion products into the atmosphere is the following:

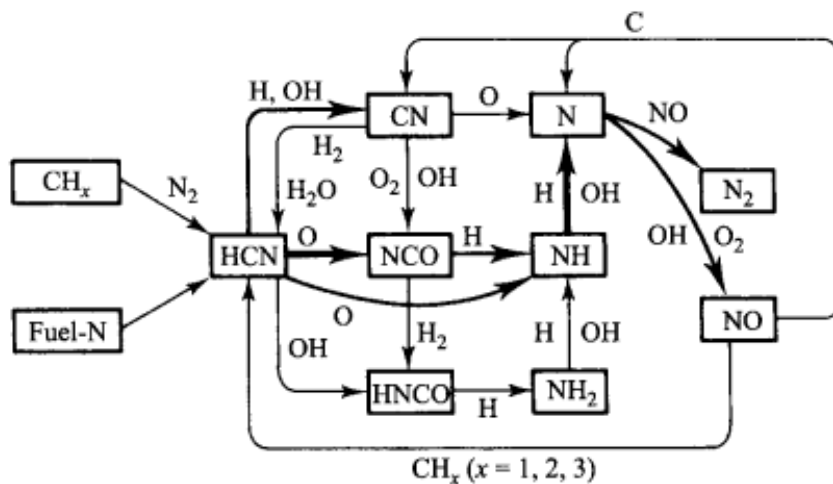


Figure 10 - NO production associated with the Fenimore prompt mechanism.

2.4 Oxy-combustion Technology

The use of fossil fuels continues to be a reality, so it is necessary to create strategies to reduce CO_2 and other pollutant emissions. Among these strategies are technological

approaches for regulating emissions, such as carbon capture technologies (CCTs), with oxy-combustion being a prominent example (Raho et al. 2022).

In oxy-combustion, atmospheric air is replaced by oxygen-enriched air, leading to a reduction in NO_x emissions. However, this substitution results in higher combustion temperatures. To overcome this problem, it is necessary to create and develop strategies to minimize the impact.

2.4.1 Carbon Capture Technologies

The carbon capture technologies (CCTs) (Nemitallah et al. 2017), also known in the literature as carbon capture sequestration (Raho et al. 2022) or carbon capture and storage systems (Li et al. 2021) (CCS), are systems that currently allow achieving net-zero CO_2 emissions, even when it is necessary to continue using fossil fuels (Li et al. 2021).

Among the available CCTs, three of the most common and efficient can be highlighted (Figure 11):

- Pre-combustion carbon capture.
- Post-combustion carbon capture.
- Oxy-combustion.

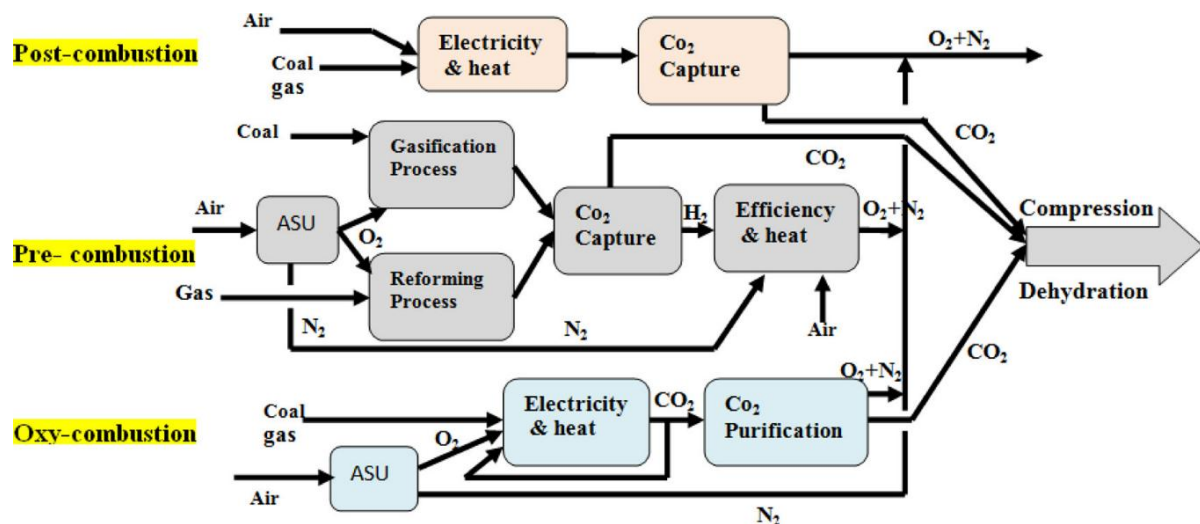


Figure 11 - Scheme of the three carbon capture technologies available. (Nemitallah et al. 2017)

Pre-combustion carbon capture

In pre-combustion capture technology, the carbon is, as the name says, removed before the combustion occurs. Firstly, the fuel is gasified to form a synthetic gas or syngas.

Integrated gasification combined cycle (IGCC) is a typical application of the pre-combustion capture method. This method is also used to produce fertilizers, chemical gaseous fuels and power (Zheng and Liu 2017).

Post-combustion Carbon Capture

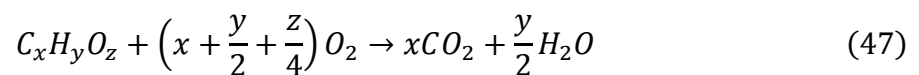
This method is applied to most of the power plants, and it consists in CO₂ capture after the fuel burning.

The CO₂ is scrubbed from the flue gas by chemical solvents, solid minerals, among others (Zheng and Liu 2017).

The most common and important methods of CO₂ separation are absorption, adsorption, cryogenic processes, and membrane separation (Rubin et al. 2012)

2.4.2 Oxy-combustion

Oxyfuel combustion technology is the concept of using pure oxygen instead of air to burn the fuel. The products of this combustion reaction are mainly water vapor and carbon dioxide (Nemitallah et al. 2017), as can be seen in Equation 47 (Li et al. 2021):



As can be observed, there is no presence of nitrogen (N₂), and this is the main difference between oxy-combustion and air-fuel combustion (Li et al. 2021). The absence of nitrogen oxides (NO_x) emissions in the initial mixture is completely eliminated, unless there are leaks from outside air or impurities in the fuel, and it also leads to smaller

volumes in the combustion chamber and different combustion characteristics when compared to combustion using atmospheric air (Nemitallah et al. 2017).

2.5 Oxygen enrichment methods

For oxygen separation, there are several processes available, with the purpose of using it in oxy-combustion. Among all the available processes, the most notable are Pressure Swing Adsorption (PSA), Vacuum Swing Adsorption (VSA), and Membrane Separation Technologies, which are used for small-scale oxygen production (<200 t/d). For large-scale production, cryogenic oxygen production is used, which currently corresponds to a production of 4000 t/d (Luo and Liu 2018).

2.5.1 Cryogenic Oxygen Production

Cryogenic Oxygen Production is a distillation process, and it is a very complex process. Although with cryogenic oxygen production, it is possible to achieve high-purity oxygen, between 90 % and 99.9 % (Baukal Jr 2013).

For this technology, an Air Separation Unit (ASU) (Figure 12) is used, and the following operations are performed:

- Pretreatment to remove CO₂, water and some hydrocarbons.
- Cooling the air to cryogenic temperatures to allow the separation of components.
- Separation of air into its components.
- Refrigeration to maintain the energy balance of the ASU.
- Compression of gaseous products and storage of the liquid.

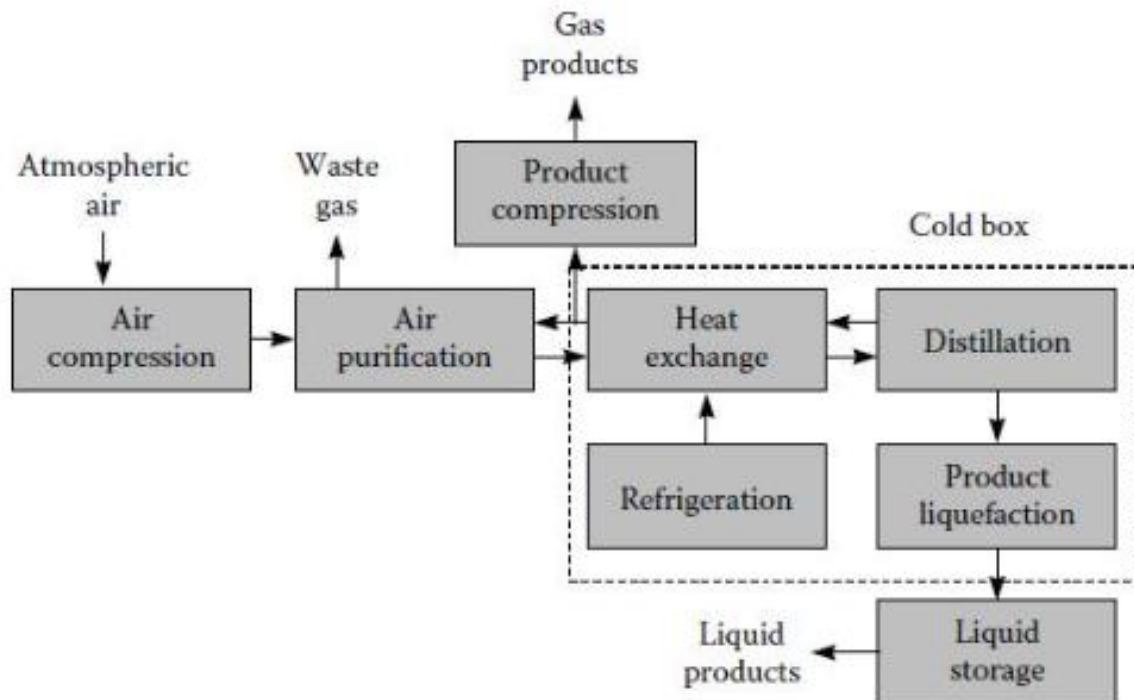


Figure 12 - Air Separation Unit block diagram (Baukal Jr 2013).

In the cryogenic ASU, the air is compressed and then treated to remove all contaminants, such as water, carbon dioxide, and hydrocarbons. The purified air is then cooled to cryogenic conditions in the main heat exchanger (MHX), after which it proceeds to a distillation unit. There, the air is separated into an oxygen and nitrogen stream, and sometimes an argon stream is produced. The products pass again through the MHX and are then compressed and pumped according to the project specifications.

There is a wide variety of designs for cryogenic air separation, and the main differences are related to the method of providing refrigeration, the method used to pressurize the products, the operating pressures, and the column configuration in the distillation section.

When argon production is not required, the most common configuration of the distillation section contains two columns (Figure 13). However, in some cases, due to the demand for oxy-fuel combustion, the distillation section may contain three columns (Luo and Liu 2018).

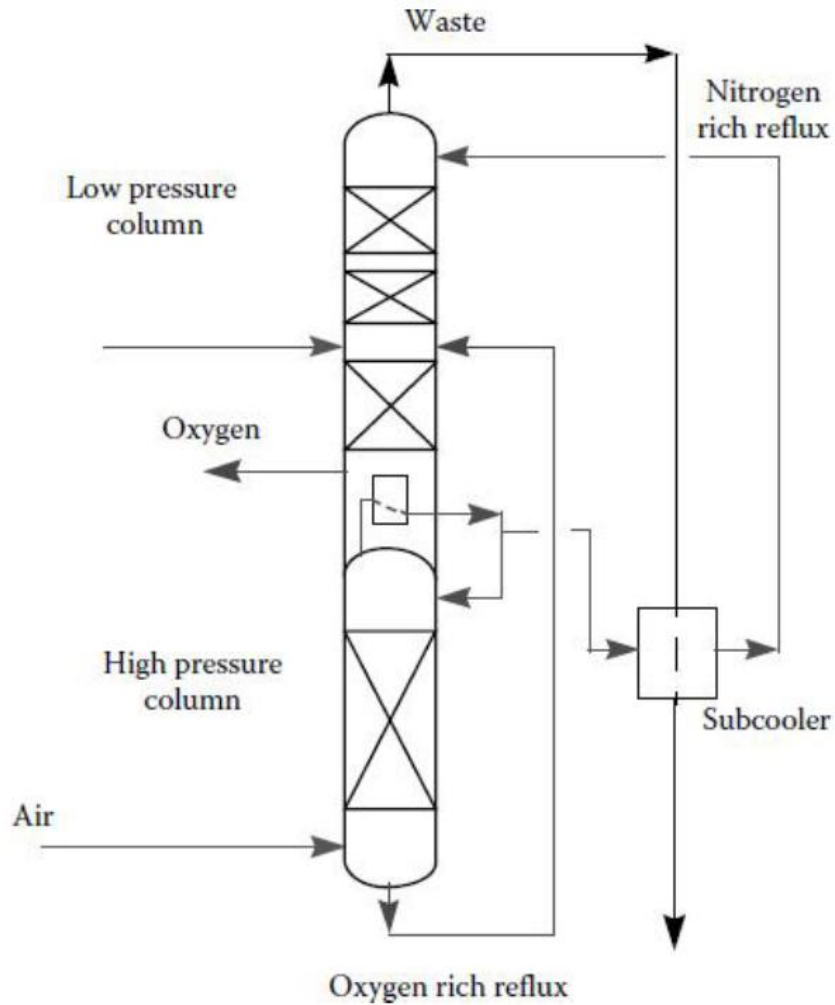


Figure 13 - - Double column design (Baukal Jr 2013).

2.5.2 Adsorption Processes

The main purpose of the adsorption process is to absorb nitrogen using natural or synthetic materials. To achieve this, zeolites can be used. They have non-uniform electrical fields in their pores, which promote the adsorption of molecules. During air separation, nitrogen molecules are more strongly adsorbed than oxygen or argon molecules. The air goes through a zeolite bed, and nitrogen is retained, while a stream of oxygen-enriched air exits the bed.

On the other hand, carbon molecular sieves can also be used, which have a similar pore size when compared to air molecules. Since air molecules are slightly smaller than nitrogen molecules, they diffuse more quickly into the adsorbent cavities.

Pressure Swing Adsorption (PSA) is a very versatile technology. This concept is simple and involves the separation of some components from an air mixture. The components are selectively adsorbed on a porous adsorbent at high pressure, usually above atmospheric pressure, by contact with the solid adsorbent inside a column, and the exiting air is enriched with the component that is not adsorbed. Inside the column, the adsorbed components are desorbed in the solid by a reduction in partial pressures (swing), and the adsorbent remains clean and can be reused (Sircar 2002).

For oxygen separation, Vacuum Swing Adsorption (VSA) can also be used. This process is based on the selective adsorption of nitrogen by an efficient zeolite at high temperatures, usually between 110-180 kPa, followed by nitrogen desorption under vacuum, usually at a pressure of 20-50 kPa (Budner et al. 1999).

If one of these technologies is used, it is possible to achieve an oxygen purity of 90-94 % (Budner et al. 1999).

2.5.3 Membrane Separation Technologies

Membrane technology is an emerging technique for oxygen separation, more economical, energy efficient, and environmentally friendly for O₂/N₂ separation (Singh, Prasad, and Ahn 2024).

In this method, air is drawn from the environment into the membrane module, and the gases of interest, O₂ and N₂, are separated based on their solubility and diffusivity. Inside the membrane module, the oxygen is separated from the air and collected due to its high diffusivity (Chong et al. 2016).

The purity of oxygen with this technology ranges from 25 to 40 % when a polymeric membrane is used (Chong et al. 2016), and can reach 99 % with ceramic membranes (Belousov and Fedorov 2020).

For O₂/N₂ separation membranes, several polymeric materials can be used, including polysulfone (PSF), polyamide (PA), polyurethane (PU), polydimethylsiloxane (PDMS), polyimide (PI), and polyaniline (PANi). There are many options, but the most promising

polymer for this application is PSF or PI. Studies have demonstrated that both polymers are advantageous for gas separation (Singh, Prasad, and Ahn 2024).

Recently, studies have been conducted to develop ceramic membranes for the separation of air components. This system is particularly efficient at high temperatures, between 800 and 900°C. To refer to high-temperature ceramic membranes, there are multiple acronyms that can be used: MIEC (Mixed Ionic Electronic Conducting); ITM (Ion Transport Membranes); and OTM (Oxygen Transport Membranes) (Hashim, Mohamed, and Bhatia 2010).

In this type of membrane, ionic and electric fluxes are involved. The driving force for the ionic transport in this case is the difference in partial pressure of oxygen on both sides of the membrane, which induces a chemical potential gradient across the membrane (Figure 14). To maintain electroneutrality, there is also transport of electrons and/or electron holes (Świerczek et al. 2019).

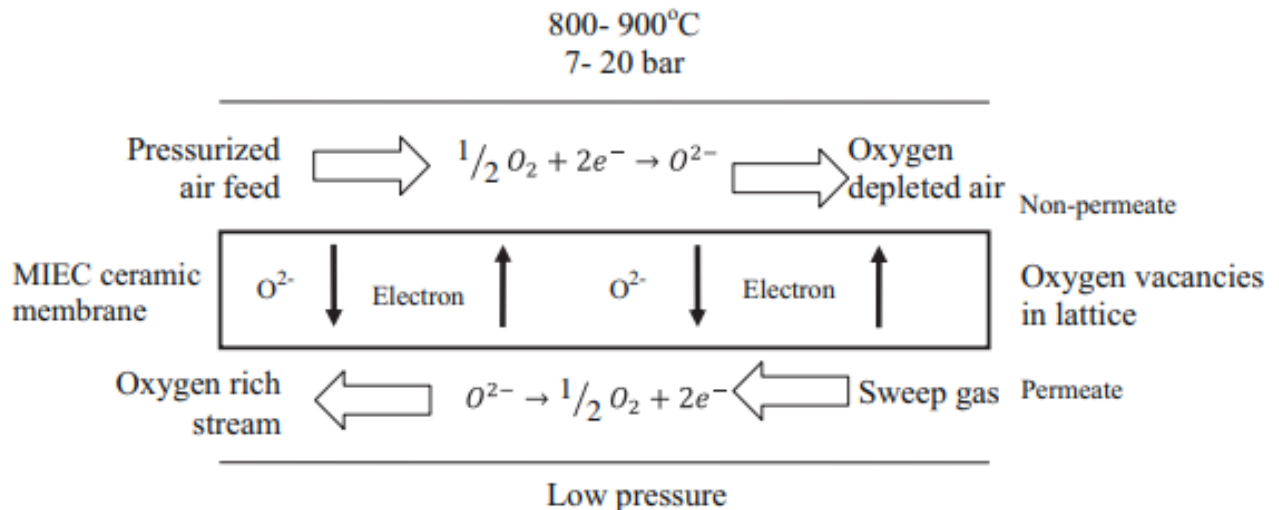


Figure 14 - Oxygen separation on MIEC-type membrane (S.S. Hashim, Mohamed, and Bhatia 2011).

As can be seen in Figure 15, there are different types of membrane modules, such as Plate-and-Frame Module, Spiral-Wound Module, Tubular Module, Hollow Fiber Module.

These different geometries allow the generation of a higher membrane surface area in a small volume, resulting in better and more efficient separation.

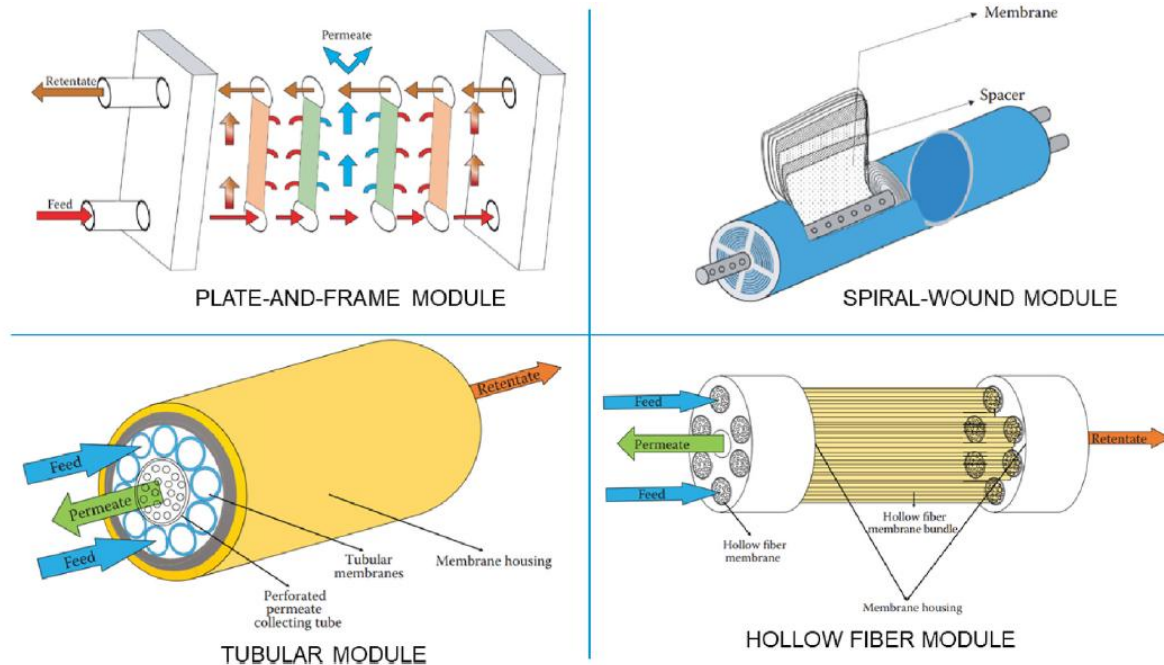


Figure 15 - Schematic representation of different module types (Singh, Prasad, and Ahn 2024).

For the studied situation, the commercially available membranes for gas separation are summarized in Table 2 (Sidhikku Kandath Valappil, Ghasem, and Al-Marzouqi 2021).

Table 2 - Commercially available membranes for O₂/N₂ separation.

Membrane	Supplier	Material	Gas Separation	Module Type
IMS	Praxair	Polyimide	O ₂ /N ₂	Hollow fiber
UBE	Ube Industries	Polyimide	O ₂ /N ₂	Hollow fiber

The working principle of membrane separation is based on the fact that the permeability of the membrane materials to different molecular gases is different: the gas with high permeability is more suitable to pass through the membrane, and the original gas mixture can be divided into two different streams (Figure 16).

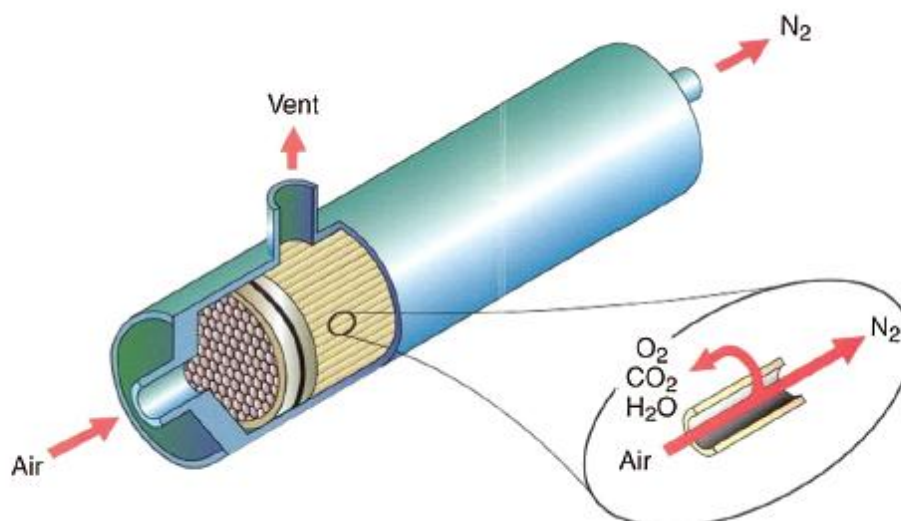


Figure 16 - Schematic of a hollow fibre membrane module (Tu and Zeng 2021).

2.4.4 Advantages and disadvantages

All oxygen separation methods, available in the market, have advantages and disadvantages, as detailed in Table 3.

Table 3 - Advantages and disadvantages of oxygen separation methods (Sidhikku Kandath Valappil, Ghasem, and Al-Marzouqi 2021).

Cryogenic Oxygen Production	
Advantages	Disadvantages
• Very high purity product. • Produces a product that is ready for pipeline transport. • Eco-friendly, as no chemical reagents are required. • Suitable for high-pressure gas stream.	• Uneconomical, as it can only be used for separating high concentrations of the target gas. • Highly energy-intensive for regeneration. • Overall decrease in plant efficiency when applied to gas streams with a low concentration of the target gas.
Adsorption Processes	
• Simple operation. • Economic. • Adsorbents resist mechanical degradation.	• Low recovery of the product. • Limited availability of adsorbent materials.

• High transfer rates, renewability, and capacity for ideal adsorbents	• Adsorbents are sensitive to the presence of moisture in the flue gas stream.
Membrane Separation Technology	
• Low maintenance. • Low cost. • Allows the separation of gases at low temperature and pressure. • Can be coupled with other separation methods to achieve more efficient gas separation.	• The process requires additional energy to compress the feed gas, since the separated gas is at low pressure. • Plugging and clogging of membrane pores in the presence of impurities. • Moderate purity.

2.6 Oxy-combustion in IC engines

2.6.1 Combustion process and control in oxy-fuel IC engines

To optimize power performance, thermal efficiency, and emissions in IC engines with oxy-fuel combustion, combustion process control strategies are vital.

The following sub-section presents a summary of typical parameters that can affect combustion in oxy-fuel spark combustion (SI) and compression ignition (CI) engines.

Oxygen concentration

The heat capacity and thermal diffusivity of CO₂ differ significantly from nitrogen, leading to lower combustion temperatures under the same operating conditions. Thus, oxy-combustion probably results in a more substantial heat loss than conventional air combustion.

It is necessary to optimize the oxy-combustion process, oxy-fuel combustion by controlling the oxygen concentration.

To understand the influence of oxygen concentration in an SI engine, the concept of R_{OF} was introduced, which represents the volume percentage of oxygen. Studies show that a higher R_{OF} accelerates the combustion process and improves the cycle performance (Li et al. 2021).

EGR strategy

In conventional internal combustion engines (ICEs), using the recirculation of part of the exhaust gases back to engine cylinders, EGR (Exhaust Gas Recirculation) technology was first adopted in CI engines to control NO_x emissions by reducing combustion temperature. More recently, EGR technology has also been applied in SI engines due to restrictive emissions regulations and fuel economy requirements. The recycled CO₂ can also be used to control the combustion process in-cylinder, improving flame stability and thermal efficiency, as well as limiting combustion roughness.

The EGR ratio is usually used to represent the recirculated exhaust gases, and it is calculated using Equation 48.

$$EGR(\%) = \frac{[CO_2]_{Intake} - [CO_2]_{Ambient}}{[CO_2]_{Exhaust} - [CO_2]_{Ambient}} \quad (48)$$

where $[CO_2]_{Ambient}$, $[CO_2]_{Intake}$ and $[CO_2]_{Exhaust}$ are measured in the environment, in the intake manifold and in the exhaust gases, respectively (Li et al. 2021).

Water injection

In order to improve power performance and economy in ICEs, the compression ratio should be increased. However, under this condition, an abnormal combustion phenomenon named knock occurs, which can happen under low speed and high load engine conditions. This phenomenon normally occurs when the combustion of part of the air/fuel mixture in the cylinder does not result from the propagation of the flame front, ignited by the spark plug, Instead, and explodes outside the regular combustion front envelope. There is a rapid release of chemical energy in the end-gas, causing the propagation of powerful waves with substantial amplitude across the combustion chamber.

Water injection technology is used to reduce engine knock by controlling the temperature inside the cylinder, and can achieve the target of maximum engine performance while preventing damage due to knocking.

For ICEs using oxy-fuel, water injection technology, including different water injection strategies, such as varying timing, duration, pressure, mass, and injection temperature, has been studied in order to optimize combustion (Li et al. 2021).

2.6.2 Benefits and potential problems

In a normal combustion, air is approximately 79 % N_2 and 21% O_2 , but only oxygen is necessary for combustion, and by removing N_2 , many benefits can be achieved, such as energy efficiency, turndown ratio, and flame stability with a lower volume of exhaust gases and pollutants.

Higher thermal efficiency

Using oxygen instead of air, more energy goes into the load, instead of being lost in heating up N_2 . Overall, the process uses less energy for a given amount of production due to the higher available heat. An important reason to use an oxygen-enhanced combustion (OEC) is the reduction of the specific fuel consumption, where less fuel is required for a given unit of production due to the improvement in available heat (Baukal Jr 2013).

Improved flame characteristics

As the oxygen concentration in the oxidizer increases, the flammability limits for the fuel increase. One consequence of this is the increase in turndown ratio for the combustion system.

Oxygen-enhanced flames have higher flame speeds than air/fuel flames. The minimum gas exit velocity for OEC must be higher than that in an air/fuel flame to prevent flashback

or flame extinguishment. Thus, much higher velocities can be used in OEC without blowing off the flame, and these higher velocities normally produce more stable flames that are not easily disturbed by the flow patterns in the combustion chamber.

Compared to air, OEC requires less ignition energy than air/fuel combustion, which occurs at a lower temperature, and for this reason, it is easier to ignite flames with OEC. It is also easier to ignite inadvertently with OEC, so it is important to take safety precautions.

Oxygen-enriched combustion can also be used to control flame shape. This control allows preventing the overheating of the refractory in a specific location or changing the heat flow and temperature profile in the combustion chamber (Baukal Jr 2013).

Lower exhaust gas volumes

Eliminating N_2 from the air can reduce the exhaust flow rate by around 96 %. With these reductions in flue gases, in a given combustion chamber, it is possible to reduce the average gas velocity, and lower gas velocities carry fewer fine particles from the residues, reducing particulate emissions.

Potential problems may arise in the implementation of an OEC system if it is not properly designed. Many of these issues are related to the increased intensity of combustion (Baukal Jr 2013).

Materials damage and corrosion

With higher flame temperatures, if the heat is not distributed properly, the intensified radiation from the flame can cause material damage. This principle is suitable for furnaces, but the same logic can be applied to ICEs, where high heat flows lead to material degradation and abnormal combustion (Baukal Jr 2013).

Another problem is associated with the material corrosion. This material destruction phenomenon, exemplified in Figure 17, is caused by the environment to which the material is exposed and is widely observed during the operation of engine components. The ablation phenomenon is strongly associated with high-temperature oxidation

corrosion, meaning that the corrosion process in metal components of the engine is due to the chemical reaction with the surrounding high temperatures and a strong oxidizing gaseous environment.

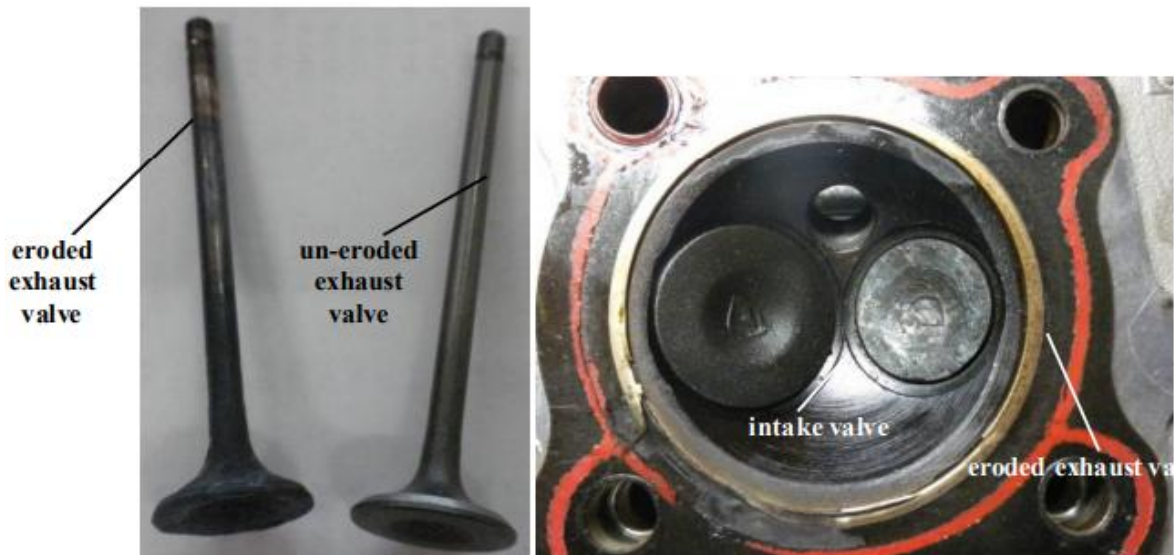


Figure 17 - Comparison between eroded and un-eroded engine components (Han et al. 2015).

With OEC, the combustion rate increases, ignition occurs more rapidly, the ignition delay is reduced, and more complete combustion is achieved.

The combustion temperature can be improved, and combustion efficiency increased, although this ablation phenomenon affects a wide range of crucial engine components, such as exhaust valve, cylinder head, liner and walls, piston and piston rings, resulting in a reduction of the engine's life cycle under this environment.

To reduce this effect, it is possible to apply anti-corrosion coatings, therefore ensuring stable and reliable operation and extending the technical and economic life of the engine.

2.6.3 Applications

OEC has been widely used in industrial heating applications. In general, it is used in high-temperature heating and melting processes that are either inefficient or impossible with air/fuel combustion.

OEC is used in several industries, but it is important to highlight the metallurgical industry, the mineral industry, and incineration.

In the metallurgical industry, oxy-combustion is used to heat and melt metal, being one of the first industrial applications in this sector. It is also used in the production of non-ferrous metals, such as aluminium, brass, copper, and lead.

The mineral industry refers to glass, cement, lime, bricks, and other minerals that require high-temperature heating and melting during their manufacture.

In incineration, OEC is used to improve performance and to clean contaminated soil. It is also used in municipal solid waste incinerators and in boilers that burn residual fuels.

Other applications include gasification of organic materials and vitrification of residual ashes, removal of unburned carbon from fly ash, oxygen enrichment in fluid catalytic crackers, oxygen enrichment in steam-methane reformers, and low-level air oxygen enrichment in sulfur recovery units using the Claus process, and a final application is its use in diesel engines (Baukal Jr 2013).

2.6.4 Oxy-Combustion applied to ICEs and UAVs

Oxy-combustion applied to UAVs is not a very explored topic; researchers are more focused on finding solutions, mostly new propulsion systems. Improved battery technologies, hybrid systems, the combination of fuel and electric engines, and the application of hydrogen fuel cells are some of the technologies that researchers intend to implement in the future (Jobs 2025).

However, there are some studies and research on oxy-combustion applied to internal combustion engines. For example, some studies were performed on a spark ignition engine with a coupled MIEC (Mixed Ionic Electronic Conducting) membrane. By varying

the O_2 mass fraction, compression ratio, engine load, and speed, some improvements in engine performance were made. The researchers conclude that a 30 % O_2 mass fraction allows the compression ratio to be increased up to 20, thus achieving the best engine performance parameters in the study. Particular attention must be given to some operational limits found in the study. For high oxygen concentration and low compression ratios, good performances were found, as well as good fuel consumption. However, in some cases, high temperatures (above 1000 °C) could compromise the integrity of the engine parts (Serrano et al. 2023).

Another study was conducted in order to evaluate the effect of oxygen-enrichment in diesel engines. Using a single cylinder, direct injection diesel engine with different oxygen concentrations, some conclusions were made. Engine performance improved significantly, brake thermal efficiency increased, and brake specific fuel consumption was reduced. This occurs due to a higher combustion rate, which in turn is due to higher flame temperature and burning speed. Oxygen-enrichment is also a good method to reduce the formation of carbon monoxide (CO) and hydrocarbons. One disadvantage of this study is that NO_x emissions were not reduced, and some developments need to be made in order to study a technology that allows reducing these emissions (Baskar and Senthilkumar 2016).

2.6.5 Emissions

Nitrogen oxides

NO_x refers to nitrogen oxides, which include nitrogen monoxide, also known as nitric oxide (NO), and nitrogen dioxide (NO₂).

In high-temperature heating applications, most of the NO_x emitted in the exhaust is in the form of NO, which quickly combines with atmospheric O_2 and forms NO₂. Both NO and NO₂ are harmful to humans; however, a major concern is their effect on the environment and man-made structures. It is destructive due to the reaction between NO₂ and the rainwater, forming nitric acid (HNO₃), a highly corrosive acid.

Overall, the main purpose of increasing the oxygen concentration in combustion and decreasing nitrogen concentration is to reduce NO_x formation. However, a high flame temperature leads to a high NO_x concentration. Therefore, it is important to apply temperature control strategies to reduce NO_x concentrations (Baukal Jr 2013).

Carbon Dioxide

Carbon Dioxide is a colourless, odourless and inert gas that is naturally found in the atmosphere at low concentrations, around 0.03 %. Higher concentrations can have consequences for humans, and concentrations above 10 % can be fatal.

CO_2 emissions are produced when a fuel containing carbon is burned near or above stoichiometric conditions and are one of the main causes of the greenhouse effect.

Many methods have been suggested to reduce CO_2 emissions, including carbon sequestration technologies, referred several times above. In some cases, CO_2 emissions are expected to be reduced by 55 % (Baukal Jr 2013).

Carbon monoxide (CO)

CO is a flammable non-irritating gas, colourless, odourless, tasteless, and normally non-corrosive. For humans, CO is highly toxic and can act as a chemical asphyxiant when it combines with blood hemoglobin, which usually transports oxygen in the body. Since it can be a dangerous pollutant, CO emissions are regulated by specific guidelines depending on the application and the geographical location.

Carbon monoxide is generally produced in extremely small amounts in combustion processes, as a product of incomplete combustion, and the combustion system normally operates slightly fuel lean (excess O_2), to ensure complete combustion and minimize CO emissions.

There is an increasing tendency for CO concentration to increase with rising oxygen concentration, and when the flame temperature decreases, CO concentration also decreases (Baukal Jr 2013).

Unburnt hydrocarbons (UHCs)

Hydrocarbons (HCs) emissions occur due to unburned and partially burned HCs. The origin of these components can be from fuel or the engine lubricants. Several mechanisms can generate these emissions, for example, incomplete combustion of HCs due to partial ignition of the overall combustion chamber volume, and fuel deposits on the walls. Other reasons can be residual fuel in the dead spaces, such as gaps in the cylinder head seal, valve seats, piston rings, etc. Other causes of increased HC emissions are misfiring, emissions from the lubricants HCs, absorption of fuel molecules into the cylinder lubricant film, and impurities.

With lower fuel/air ratios, HC emissions increase, since there are reduced amounts of oxygen to complete combustion (Basshuysen and Schaefer 2016).

Volatile organic compounds (VOCs)

VOCs are usually aliphatic and aromatic hydrocarbons such as alcohols, ketones, esters, and aldehydes. Typical VOCs include benzene, acetone, acetaldehyde, chloroform, toluene, methanol, and formaldehyde. These compounds are regulated pollutants, since they can cause photochemical smog and destruction of the ozone layer.

Using OEC technologies, it is expected that VOCs emissions decrease, due to higher flame temperatures and reduced dilution (Baukal Jr 2013).

2.7 Materials

If an engine is operating under oxy-combustion conditions, the adiabatic flame temperatures are higher than in normal combustion, and since the environment created inside the engine is highly oxidizing, the working conditions are severe and materials are subject to accelerated corrosion, hot corrosion, creep, and thermal fatigue, making the material selection a critical aspect of design.

2.7.1 Superalloys

Metallic superalloys, and more specifically nickel based superalloys, are materials widely used in components subject to high temperatures or very oxidizing atmospheres. These alloys were created to maintain mechanical resistance and microstructural stability at temperatures above 600 °C, and when combined with elements such as Chromium (Cr), Aluminium (Al), Titanium (Ti), and Niobium (Nb), provide resistance to oxidation and fluence.

Nickel superalloys have an excellent performance in combustion environments because they form a stable protective oxide layer, such as Cr_2O_3 and Al_2O_3 . These protective coatings help to retard the oxidation of the material.

Inconel 718, Inconel 625, René 80, and Hastelloy X, are examples of superalloys that have these characteristics and are particularly suitable for combustion chambers, valves, and injectors (Reed 2006).

2.7.2 Thermal Barrier Coatings

Although superalloys have high thermal resistance, their operational limits are often exceeded under oxy-combustion conditions. To mitigate this problem, thermal barrier coatings (TBCs) are widely used.

TBCs systems typically consist of a top ceramic layer, commonly yttria-stabilized zirconia (YSZ), with a melting point around 2700 °C, is deposited over a metallic bond coat of MCrAlY type (M=Ni, Co or both). These systems significantly reduce heat flow to the metallic substrate while enhancing resistance to oxidation and hot corrosion.

To high intensity combustion applications, TBC are currently an indispensable technology because they allow the operational temperatures of components to be increased.

Recent studies show that this technology is relevant in highly oxidizing environments, such as under oxygen-enriched conditions (Vaßen et al. 2010) (Padture, Gell, and Jordan 2002).

2.7.3 Advanced Ceramics and Ceramic Matrix Composites (CMCs)

Advanced ceramic and ceramic matrix composites (CMCs) are a class of materials with significant potential in oxy-combustion applications, due to their ability to operate at temperatures above 1200-1400 °C. Among these, SiC/SiC composites stand out, combining high thermal resistance with lower density compared to metallic superalloys.

CMCs exhibit excellent creep resistance and thermal shock resistance, making them promising candidates for components in the hot-section of engines. However, in environments enriched with oxygen and water vapor, these materials undergo chemical degradation, requiring the application of environmental barrier coatings (EBCs). EBCs are a way to protect CMCs when operating under severe conditions and are typically categorised into different generations according to their composition (Naslain 2004); (Kiser et al. 2005; Opila and Hann Jr. 1997; Tejero-Martin, Bennett, and Hussain 2021).

Chapter 3

Methodology and Numerical Setup

3.1 Combustion Numerical Modelling

Combustion plays an important role in global energy production and in engineering systems, such as internal combustion engines, turbines, and other industrial combustion devices, being directly associated with energy efficiency and pollutant formation (Turns 2000).

During the combustion process, several complex phenomena occur – such as turbulent flows, highly nonlinear chemical reactions, and heat transfer – making experimental analysis both costly, and in some cases, limited (Heywood 1998).

In this context, computational fluid dynamics (CFD) has become an essential tool for investigating and understanding combustion processes, allowing detailed analysis of physical and chemical processes under controlled conditions (Versteeg 2007).

Over the last few decades, numerical and combustion models have been developed, leading to a very significant increase in the use of CFD simulations to support the development and optimization of existing systems.

Among specialized tools available, Ansys Forte stands out for being specifically designed to simulate transient flows, integrating advanced turbulence, combustion, chemical kinetics, and pollutant formation models (ANSYS 2024a).

The detailed equations and methods used by the CFD software, particularly by ANSYS Forte, are described in Appendix A (ANSYS 2024a; Design 2015; Versteeg 2007).

3.2 Geometry Modelling

3.2.1 Two-stroke engine

TEKEVER UAS, provided a two-stroke engine from Ekarus Engines GmbH for the analysis. The engine, named E-34 (Figure 18), is intended for UAV up to 25 kg. Table 4 summarizes the engine's characteristics.

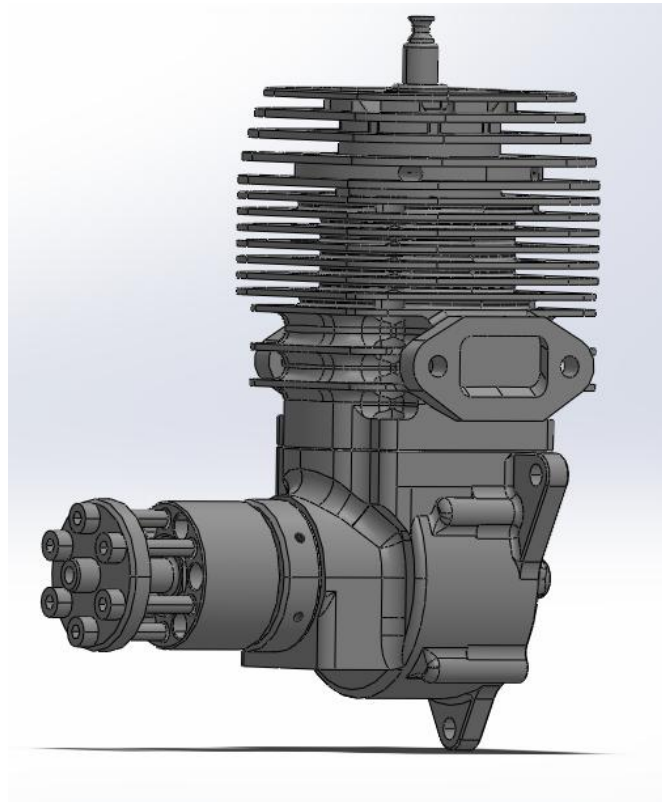


Figure 18 - E-34 engine. (This image was provided by TEKEVER).

Table 4 - E-34 characteristics. (Engines 2026)

E-34	
Weight	1.16 kg
Displacement	34 cc
Bore	38 mm
Stroke	30 mm
Max. continuous speed	9800 rpm
Rated power at 8300 rpm	2.2 kW

All interior and internal components of the engine were measured, and the parts and the entire assembly are shown in Appendix B.

Two different engine models were designed. One with the transfer ports incorporated in the piston skirt and with the crankshaft, and the other without the transfer ports and with the bottom cylinder closed (Appendix B). The model designed to be used in ANSYS Forte is represented in Figure 19.

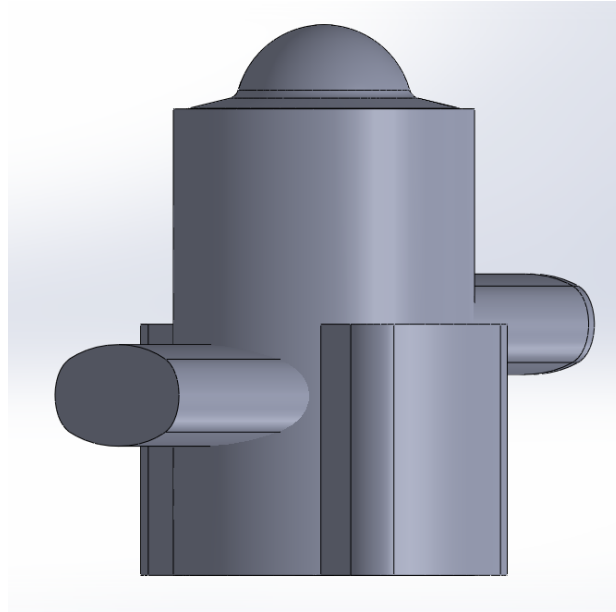


Figure 19 - Assembly of the design engine.

3.2.2 Four-stroke engine

The four-stroke engine used in the simulations (Figure 20), and its characteristics are summarized in Table 5. More information can be found in Appendix B.

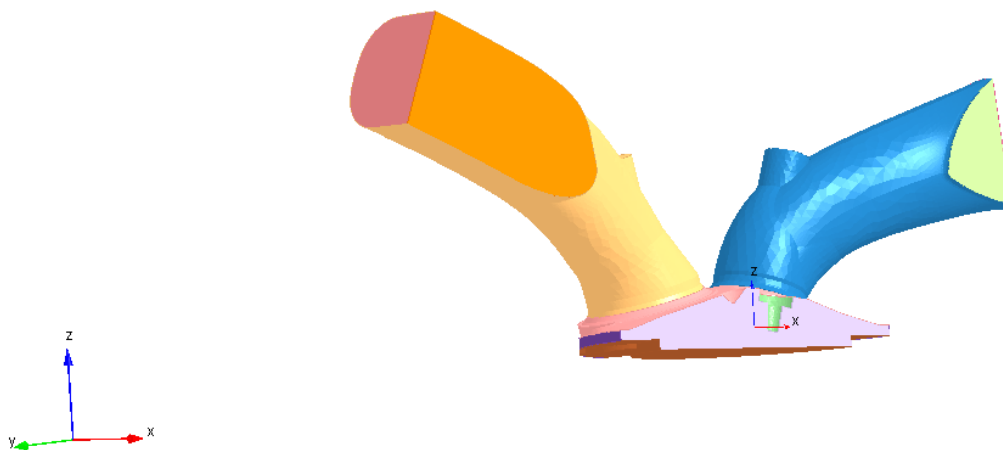


Figure 20 - Four-Stroke engine from ANSYS Forte.

Table 5 - Characteristics of ANSYS Forte four-stroke engine.

Four-stroke engine from ANSYS Forte	
Displacement	332.85 cc
Bore	72.2 mm
Stroke	81.3 mm

3.3 Mesh Controls

In ANSYS Forte, before starting the simulations, it is necessary to perform a mesh refinement. ANSYS Forte uses automatic-mesh generation, and for this option, some mesh-size criteria and refinement must be specified, as well as a material point. Based on these parameters and the boundary conditions specified later, the mesh-generation is performed automatically during the simulation.

Appendix C presents several constraints to be considered, about mesh controls for automatic meshing and the values used in those parameters.

3.3.1 Material Point and Global Mesh Size

The material point and the global mesh size considered for this simulation are described in Table 6.

Table 6 - Material Point Coordinates and Global Mesh Size parameters.

Material Point		
x [cm]	y [cm]	z [cm]
0.2175	2.8275	0.2175
Global Mesh Size		
Mesh Size	0.2 cm	
Small Feature Deactivation Factor	0.25	

3.3.2 Mesh Refinements

Appendix C provides the description of the mesh refinements used in this simulation, as well as all the setup for mesh refinements applied in the simulation.

3.4 Models Setup

In the Models node, it is possible to configure the simulation by specifying which physical models to apply and defining options related to these models. The models are selected using check boxes, and after that, some parameters can be defined as necessary.

3.4.1 Chemistry

The first step is to import a species library from ANSYS Forte data, named *Gasoline_1comp_49sp.cks*, where information about the physicochemical properties of the fuel can be seen.

Then an option appears: Flame Speed Model. And in the field “Laminar Flame Speed”, the option “Table Library” is selected. Here, it is possible to configure the fuel species, in this case ic8h18 (iso-Octane). All the values below, in the Flame Speed Model setup, remain as default, except for the Turbulent Flame Speed Ratio (b1), which should be set to 2.0.

3.4.2 Transport

The model used is the default RNG $k - \varepsilon$ (k-epsilon) model. In the editor's panel, in Transport, then Turbulence, there are used the default fluid properties. The values set as default are shown in Figure 21, and the definition of each parameter is described in Appendix C.

Transport

Models

Turbulence

Fluid Properties

Prandtl Number	0.74	
Recip. Turb. Prandtl No.	1.11	
Recip. Turb. Schmidt No.	1.78	
Air Mu Coef. 1	1.457E-5	
Air Mu Coef. 2	110.0	
Air Lambda Coef. 1	252.0	
Air Lambda Coef. 2	200.0	

Body Acceleration

X Direction	0.0	cm/sec2
Y Direction	0.0	cm/sec2
Z Direction	0.0	cm/sec2

☐ Transport Total Energy

Figure 21 - Values for the Transport Equations.

3.4.3 Spray Model

First, an Injector is created, then Injection events and Nozzles are added to the Injector. ANSYS Forte allows multiple injectors with different fuels.

For this simulation, a Solid Cone Injector named Solid Injector was used. Then, an Injection was added to the Solid Injector. Finally, three nozzles were added and placed in different positions. All configurations used to define Spray Model are detailed in Appendix D.

3.4.4 Spark Ignition

A Spark Ignition Model must be added, which, when activated, the setting remains as the default. Afterwards a new Spark is added, and configurations are described in Appendix D.

3.5 Boundary Conditions

3.5.1 Inlet

To create the inlet boundary conditions, it is necessary to select “new inlet” and the configure as summarized in Table 7.

The composition of the inlet air is described as presented in Figure 22.

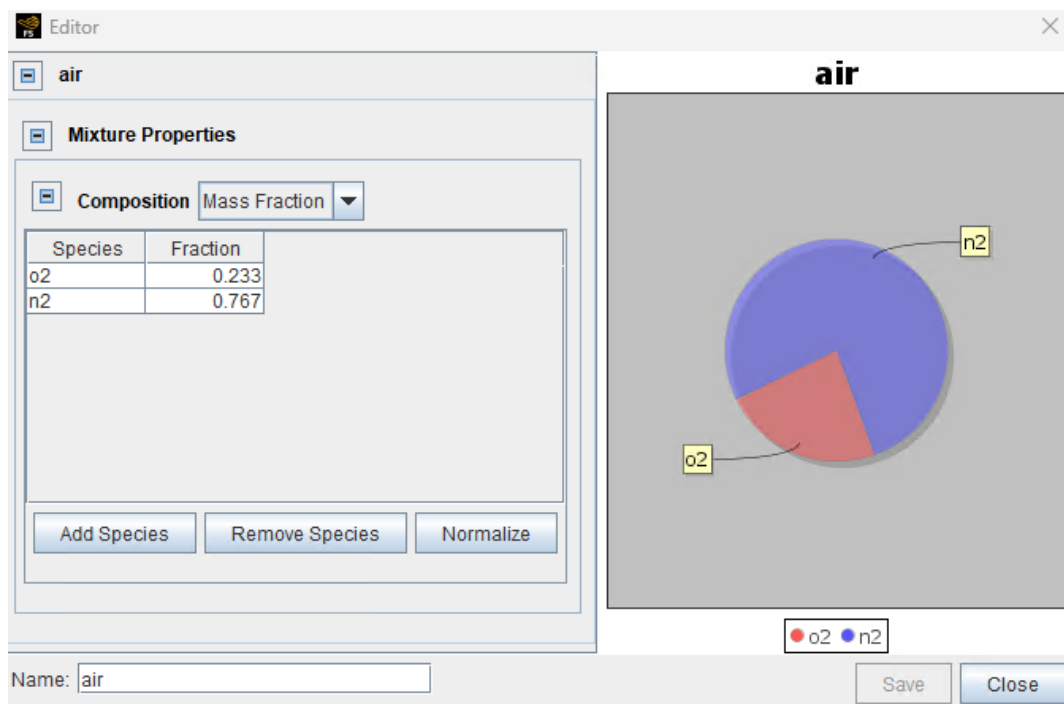


Figure 22 - Air composition for the inlet boundary condition.

Table 7 - Parameters for inlet boundary condition.

Inlet	
Location	Inlet
Inlet	Total Pressure Pressure = 2.54 bar
Turbulence	Turbulent Kinetic Energy and Length Scale Turbulent Kinetic Energy = 10000.0 cm ² /sec ² Turbulent Length Scale = 1.0 cm
Temperature	Assume Isentropic

3.5.2 Outlet

The characteristics of the created outlet boundary condition are described in Table 8.

Table 8 - Parameters for the outlet boundary condition.

Outlet	
Location	Outlet
Outlet	Total Pressure Pressure = $1.0 \times 10^5 \text{ Pa}$ Offset Distance to apply Pressure = 0.0 cm
Turbulence	Turbulent Kinetic Energy and Length Scale Turbulent Kinetic Energy = 10000.0 cm ² /sec ² Turbulent Length Scale = 1.0 cm

3.5.3 Wall

Regarding the boundary conditions of the walls, only three situations will be described.

The boundary conditions of the other walls are detailed in Appendix E.

Piston

This boundary condition is a wall, and the first step is to create a new Wall, named piston, and change all the parameters according to Table 9.

Table 9 - Parameters for piston wall boundary condition.

Piston	
Location	Piston
Thermal Boundary Condition	Wall Temperature, Constant Temperature = 485 K
Wall Motion – ON	Motion Type: Slider Crank Stroke = 81.3mm Connecting Rod Length = 13.0cm Piston Offset = 0.0cm Direction: (0;0;1) cm Movement Type: Moving Surface

Intake

For the intake, a new wall named intake-port was created. The parameters changed in Wall Boundary Condition setup are in Table 10. For exhaust, liner, and head, the parameters are described in Appendix E.

Table 10 - Parameter for the intake-port wall boundary condition.

Intake-port	
Location	Intake-port
Thermal Boundary Condition	Wall Temperature, Constant Temperature = 313 K

Intake Valves

Create a new wall named intake-valve. The specifications are a little more complicated than stationary walls, and they are specified in Table 11. For the exhaust valve, the procedure is the same, and it is described in Appendix E.

Table 11 - Parameters for the intake-valve wall boundary condition.

Intake-valve	
Location	Intake-valve
Thermal Boundary Condition	Wall Temperature, Constant Temperature = 400 K
Wall Motion – ON	Motion Type: Offset Table
Direction	$x = 0.241922 \text{ cm}$ $y = 0.0 \text{ cm}$ $z = -0.970296 \text{ cm}$
Time Option	Crank Angle Lift Profile – Figure E1 - Appendix E
Moment Type	Valve
Multi Select the Valve Seat and the Surface it Contacts	head intake-valve
Valve Motion Activation Threshold	0.02 cm
Approx. Cells in Gap At Min. Lift	1.5

3.5.4 Symmetry

A new symmetry was added, and the only parameter that was modified was in the Location list, with the following were added: cylinder-symmetry, exhaust-symmetry, and intake-symmetry.

3.6 Initialization

The domain is initialized with the operating conditions, species concentrations, and temperatures. The Default Initialization is with the expected composition of the exhaust gases, assuming complete combustion. The intake and exhaust must also be initialized with the values of the boundary conditions.

3.6.1 Default Initialization

Set the Initialization Order to 2. The flow generally goes from the intake to the cylinder and then to the exhaust, which indicates that, by the default, the cylinder area will be second in the initialization order precedence list.

To calculate the exhaust gas composition, the Ansys Forte Composition Calculator was used, IVC Calculation command.

In the composition calculation, the fuel mass value was specified, in this case is 50.85 mg. The parameters filled in the IVC Calculator are specified in Table 12.

Table 12 - Parameters for IVC calculation command.

Fuel Mass	50.85 mg
Fuel	Liquid
Fuel Composition	E5
Air Flow	Phi
Phi	1.0
EGR	0.0
Internal EGR	Estimate from CR
CR	1.0

The name given to this mixture was “50.85mgE5”, and its composition is shown in Figure 23.

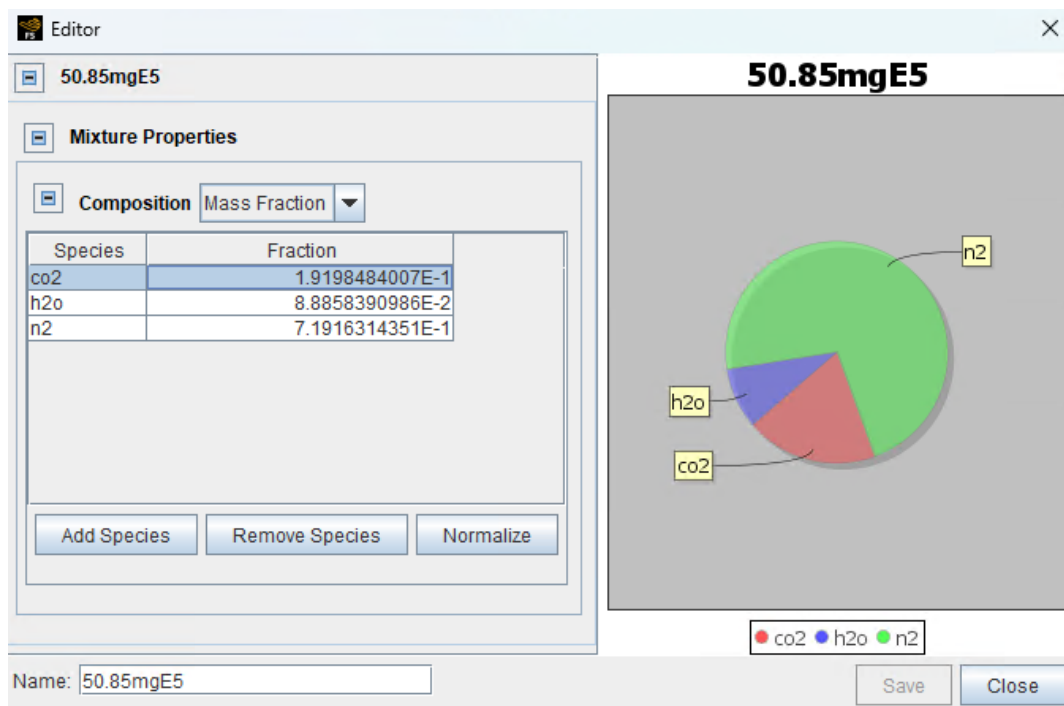


Figure 23 - Initial composition for the exhaust gas.

Still in the Default Initialization menu, the remaining parameters were presented in Table 13

Table 13 - Parameter for the Default Initialization.

Temperature	1070 K
Turbulence	Turbulent Kinetic Energy and Length Scale Turbulent Kinetic Energy = $10000\text{cm}^2/\text{sec}^2$ Turbulent Length Scale = 1.0 cm
Velocity	Velocity Components – all values set as zero.

3.6.2 Intake Initialization

In the Initial Conditions menu, a Secondary Region was created from a Material Point, named intake.

To identify this region, a point was defined for the Location (Figure 24) under the Reference Frame, and in this case, this point should always be inside the intake-port (Table 14).

Intake

[Initial Conditions](#)

Location

Ref. Frame: Global Origin

Coord. System: Cartesian

X: -4.94491 cm

Y: 1.243665 cm

Z: 3.728646 cm

Initialization Order: 1

Figure 24 - Location of the point for Intake Initialization

Table 14 - Coordinates for the intake secondary region point.

x [cm]	y [cm]	z [cm]
-4.94491	1.243665	3.728646

The Initialization Order should be set as 1. It is expected to go from the intake to the main region, and for this reason, this initialization order was assigned.

The fuel composition was set as being $O_2=0.21$ and $N_2=0.79$ (mass fraction), and during the work, this composition was varied, to obtain the desired results for analysis.

The intake temperature considered was 313 K, and the pressure was 2.54 bar, for 4000 rpm engine speed. These values, along with the composition values, will also be varied during the simulations.

For Turbulent Kinetic Energy and Length Scale, the default values were $10000 \text{ cm}^2/\text{sec}^2$ and 1.0 cm, respectively.

3.6.3 Exhaust Initialization

The procedure to create the exhaust initialization is the same as in intake initialization (Figure 25).

The chosen point is defined in Table 15.

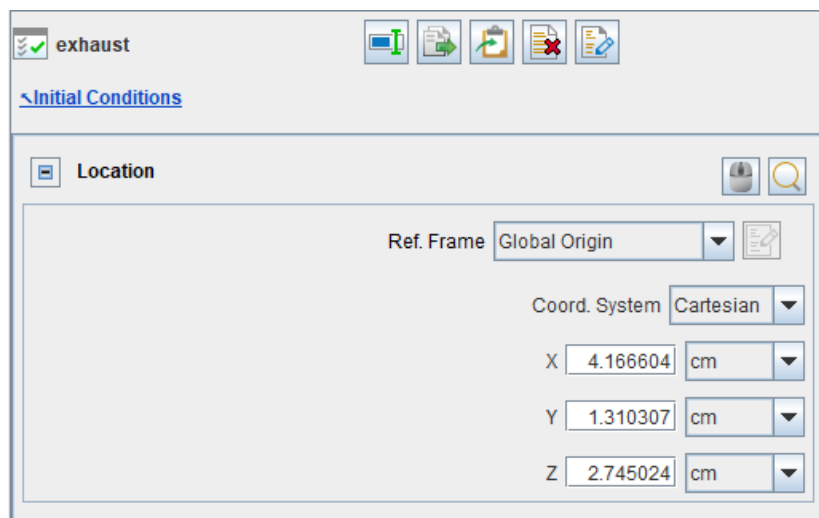


Figure 25 - Location of the point for Exhaust Initialization

Table 15 - Coordinates for the exhaust secondary region point.

x [cm]	y [cm]	z [cm]
4.166604	1.310307	2.745024

The Initialization Order should be set to 3. It is expected to go from the cylinder to the exhaust port.

The composition was set to be the same as that used in Default Initialization, “50.85mgE5”.

The exhaust temperature considered was 1070 K, and the pressure was 1×10^5 Pa. These values along with composition values, will also be varied during the simulations.

For the Turbulent Kinetic Energy and the Length Scale, the default values were 10000 cm^2/sec^2 and 1.0 cm, respectively.

3.7 Simulation Controls

This section defines the simulation limits, RPM, time step, chemistry solver, and transport terms.

In the Simulation Limits menu, the parameters were defined as shown in Table 16.

Table 16 - Parameters for Simulation Limits.

Simulation Limits	
Simulation End Point Option	Crank Angle Based
Initial Crank Angle	328 °
Final Simulation Crank Angle	880.2 °
RPM	4000 rpm
Cycle Type	4-Stroke
Engine Bore	User Specified Bore = 72.2 mm

This is the point at which the engine’s velocity varied, which will be required for further simulations.

Note that simulation occurs between 328 ° and 880.2 °, and this interval is where the actual combustion occurs. The simulation finishes when the exhaust valves open.

Chapter 4

Results and Discussion

4.1 Influence of Oxygen Concentration on Engine Performance

For this first group of simulations, all parameters described in Chapter 4 were kept constant, with the only variation being the oxygen concentration, as detailed below.

In the Initialization menu, the oxygen concentration was modified. Thirteen different gas mixtures were created as described in Table 17. For each oxygen concentration, the nitrogen concentration was adjusted accordingly, corresponding to the difference between 100 % and the oxygen concentration. Figure 26 illustrates the menu in which the O₂ and N₂ concentrations were modified to perform the simulations.

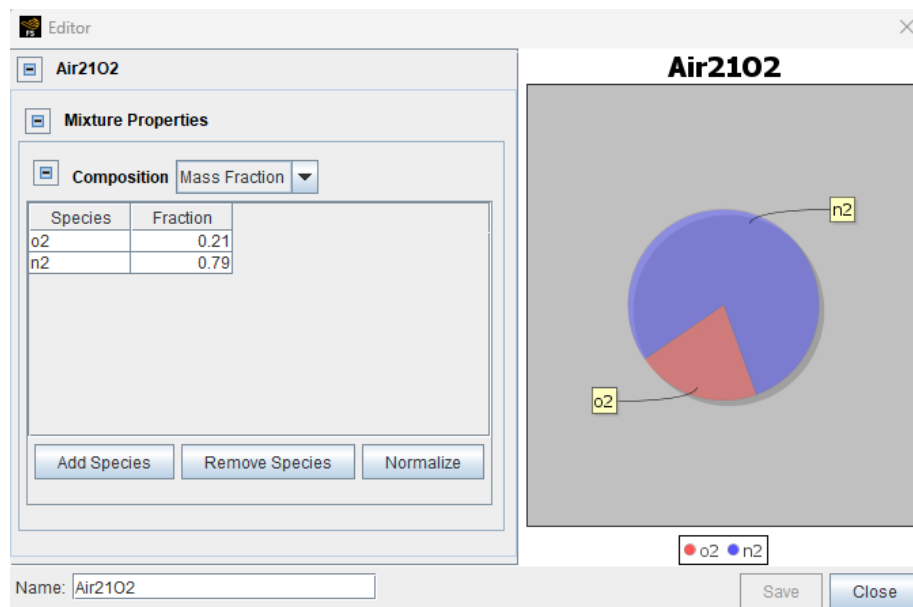


Figure 26 - Example of the setup of air composition for a simulation.

Table 17 - Oxygen and nitrogen concentrations used in simulations.

O₂(%)	21	25	30	35	40	50	60	70	80	90	95
N₂(%)	79	75	70	65	60	50	40	30	20	10	5

Besides the concentration as input, there are other relevant parameters for the combustion process, like the injection time, spark, and the start and end points of the simulation.

For the engine under analysis, the reference parameters for the engine operation at 4000 rpm, are:

- The simulations only consider the combustion process, starting at 328.0°, with the opening of the intake valves, and ending at 880.2°, with the opening of the exhaust valves.
- The injection starts at 380° and lasts for 40°.
- The spark ignition starts at 698° and lasts 18°.
- The volume at Top Dead Centre is 35.3 cm³ and occurs around 720°.

The reference simulation was conducted using conventional atmospheric air concentrations, namely 21 % O₂ and 79 % N₂, and the resulting power output was used as a reference for evaluating the results of the other simulations.

After each simulation, the data from the file named *engine_summary* were analysed, including the engine characteristics and parameters related to engine and combustion efficiency, can be seen in Table 18.

Table 18 - Engine performance and combustion parameters for 21 % oxygen simulation.

P_{max}	18.09 MPa
T_{max}	2736.43 K
Compression ratio	10.42
IMEP	2.94 MPa
Combustion Efficiency	1.00
Thermal Efficiency	0.44
Power (for one cylinder)	32.63 kW
Fuel mass	50.85 mg

n	4000 <i>rpm</i>
----------	-----------------

The following notes should be considered:

- P_{max} and T_{max} are instantaneous values, recorded at the specific engine crank angle at which the maximum values occur.
- Compression ratio indicates how many times the mixture must be compressed to fit inside the combustion chamber. In this case, the air-fuel mixture must be compressed 10.42 times.
- IMEP represents the work per unit volume applied to the piston under ideal conditions.
- Combustion efficiency is defined as the ratio between the heat release rate during combustion and the heating value, indicating how effectively the chemical energy of the fuel is converted into thermal energy. When the value is close to or equal to 100 %, that indicates the complete conversion of the fuel's heating value into heat.
- Thermal efficiency is defined as the ratio between the work performed by the working substance, in this case fuel, in a cylinder and the thermal energy supplied by the fuel during the same period of time.
- The value for mass fuel is a manufacturer's specification for an air-fed engine.
- The angular speed considered corresponds to the normal operating angular speed of the engine.

4.1.1 Effect on Temperature and Pressure

After completing all the simulations, several values related with engine performance were compared to determine the most suitable oxygen concentration for the intended application, in this case, a four-stroke engine working under oxy-combustion conditions.

Temperature Comparison

To understand the temperature variations, Figure 27 shows the maximum temperature as a function of oxygen concentration.

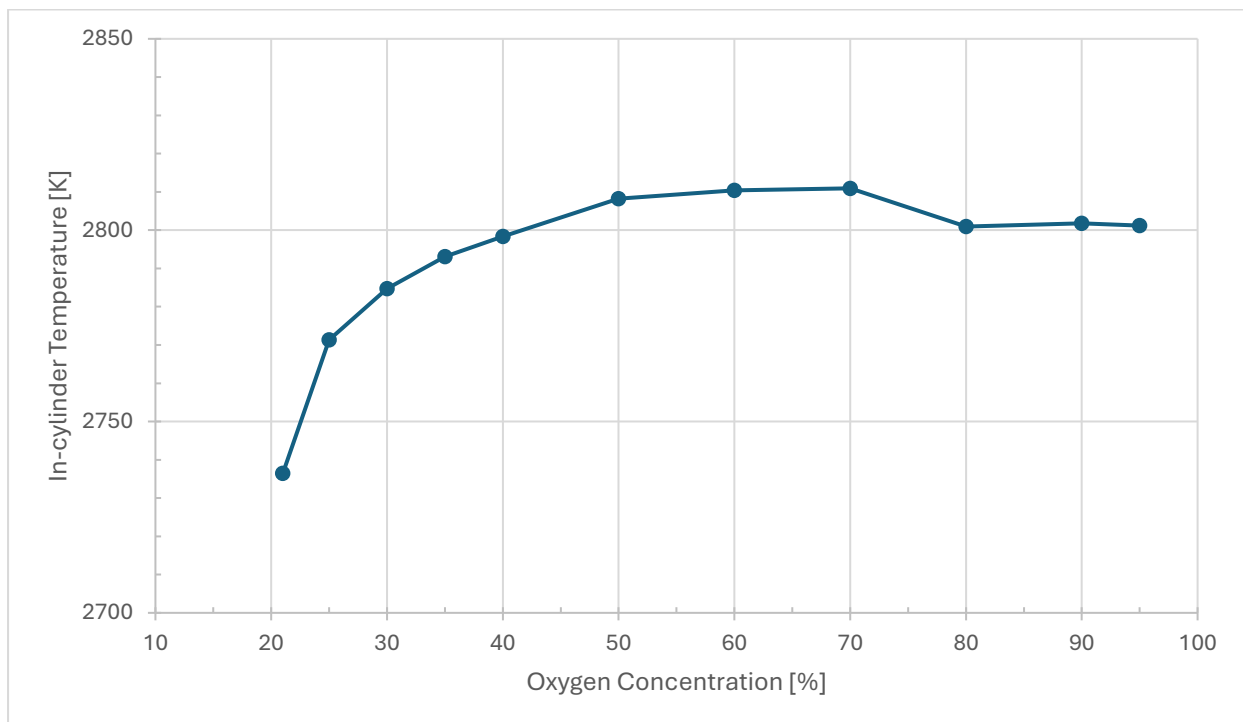


Figure 27 - Maximum in-cylinder temperatures for all simulated oxygen concentrations.

A pronounced increase in temperature was observed between 21 % and 50 % oxygen, remaining practically constant between 50 and 70 %, followed by a slight decrease between 70 % and 80 %, and finally stabilizes between 80 and 95 %.

The initial fast temperature increase is due to the diluent effect of the nitrogen. Nitrogen is an inert gas, and decreasing its concentration reduces the mixture's heat capacity. As a result, the same amount of released combustion energy produces a higher temperature, leading to an increase in the adiabatic flame temperature and, consequently, the overall combustion temperature. At oxygen concentration above 70 %, the temperature remains relatively stable.

a slight temperature decrease is observed, followed by stabilization. This behaviour is caused by chemical dissociation, which becomes significant at temperatures above 2800 K. Stable molecules such as CO_2 and H_2O decompose into simpler species and radicals, including CO, OH, and H. These dissociation reactions absorb part of the combustion energy, limiting further temperature increases despite the higher oxygen availability.

Pressure Comparison

Figure 27 shows the variation of in-cylinder pressure as a function of crank angle, using the concentration of 21 % O_2 as a reference.

As can be seen, the maximum pressure of 18.09 MPa was reached right after the angle of 698° time when ignition occurs, which will be used as a reference for comparison with the other simulations.

Values from 328° to around 690° are not shown in the figure, since, until 690° , for all oxygen concentrations, the pressure in-cylinder does not appear to vary. For a better understanding of the results, the evolution of the pressure in-cylinder with crank angle (θ), will be presented in two figures, one showing the evolution for 21 %, 25 %, 30 %, 35 %, 40 % and 50 % oxygen (Figure 28) and the other for 60 %, 70 %, 80 %, 90 % and 95 % (Figure 29).

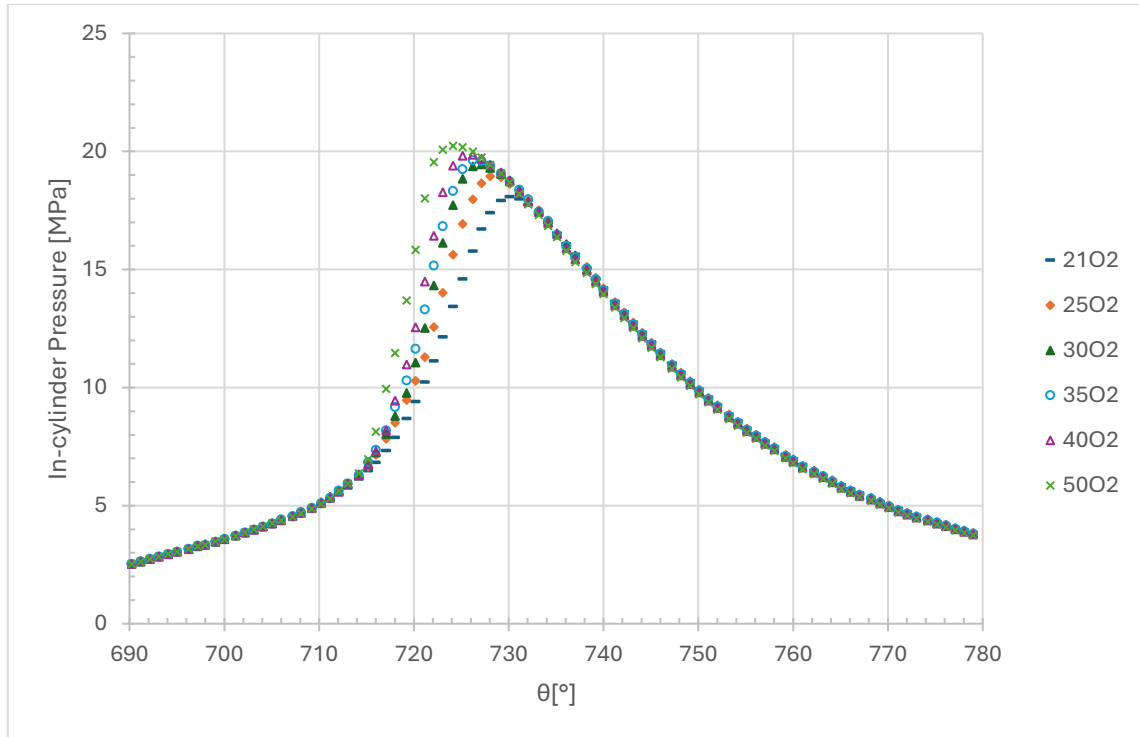


Figure 28 – Cylinder pressure as function of crank angle for 21 % to 50 % O₂.

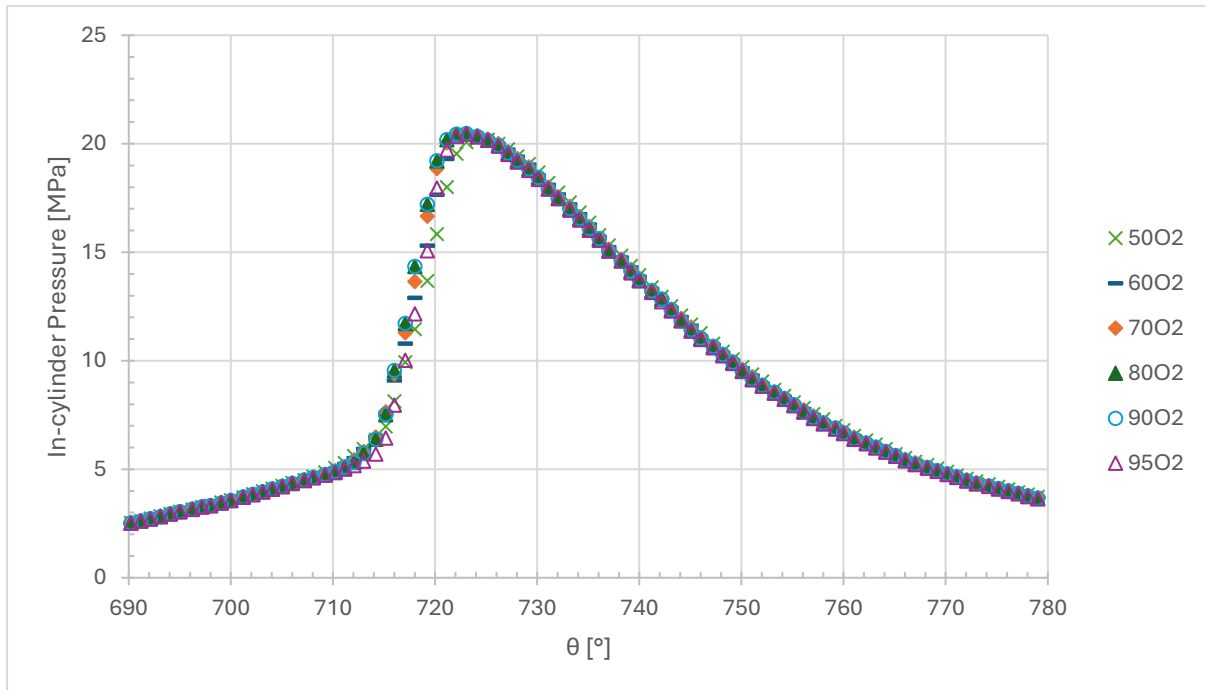


Figure 29 - Cylinder pressure as function of crank angle for 50 to 95 % O₂.

Figure 28 shows that increasing the oxygen concentration from 21 to 50 % causes the peak pressure to shift to the left, meaning that the maximum pressure is reached earlier, compared to the reference case with 21 % oxygen. For higher oxygen concentration

between 60 to 95 % (Figure 29), the peak pressure occurs at almost the same crank angle, without any significant shift being observed.

Figures 30 and 31 show that with the increase in oxygen concentrations, the pressure peak also increases. To confirm that effect, Figure 29 shows the maximum pressure for each simulated oxygen concentration.

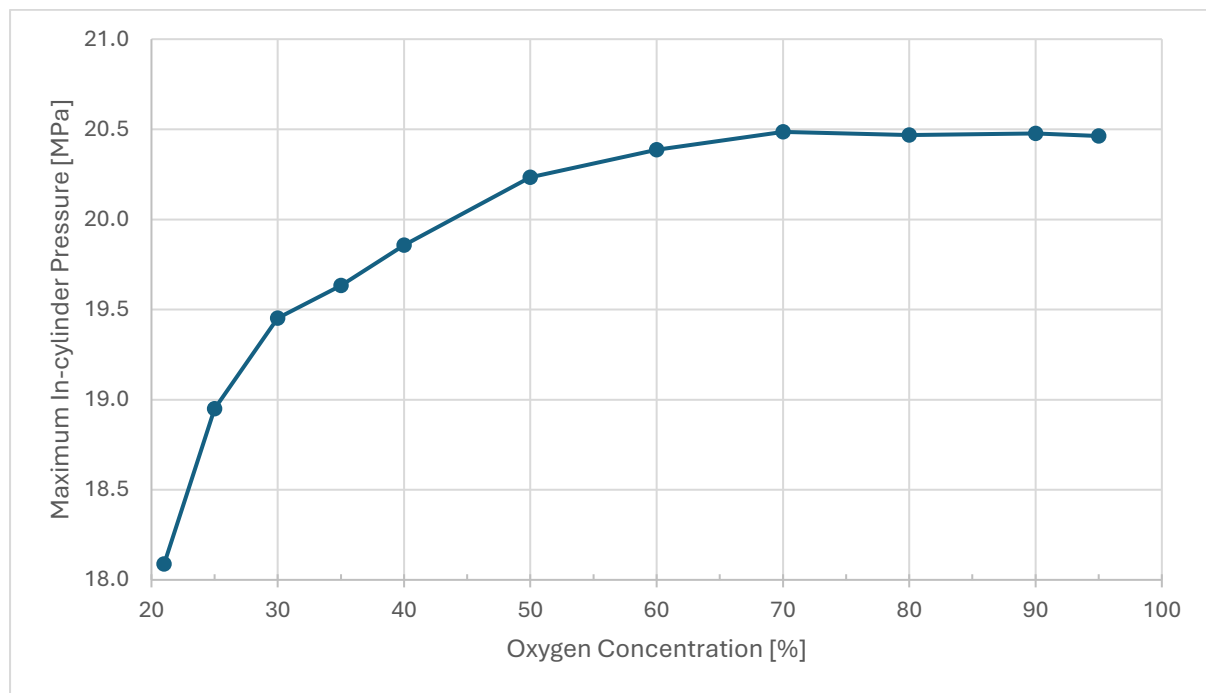


Figure 30 - Maximum in-cylinder pressures for all simulated oxygen concentrations.

As can be seen in Figure 30, the peak pressure increases with increasing oxygen concentrations (up to 60 %) and tends to stabilize for high oxygen concentrations (above 60 %).

As mentioned above, Figure 30 confirms that as the oxygen concentration increases from 21 % to 70 %, the pressure rises, and from 70 % to 95 %, it begins to stabilize.

The increase in peak pressure observed between 21 and 70 % oxygen can be attributed to combustion occurring closer to the TDC (720°). The higher oxygen concentration traduces the need of advancing the ignition time, since it is observed that with increasing oxygen concentration, the peak shifts to the left. Another reason for this difference is the flame speed, which increases drastically with oxygen enrichment, leading to an increase in pressure.

When the pressure stabilizes from 60 % to 95 %, this suggests that oxygen is no longer a combustion enhancer.

Temperature Behaviour inside the Combustion Chamber

Using EnSight, an ANSYS tool, it is possible to develop images of each variable studied during simulations. In this case, some images of the temperature behaviour inside the combustion chamber. For oxygen concentrations of 30 %, 70 %, and 90 %, the behaviour was slightly different, as can be seen in Figures 30b, 30c, and 30d. It should be noted that in these images, the temperature shown is not the maximum temperature previously obtained, but an average of the temperature values registered in the mesh.

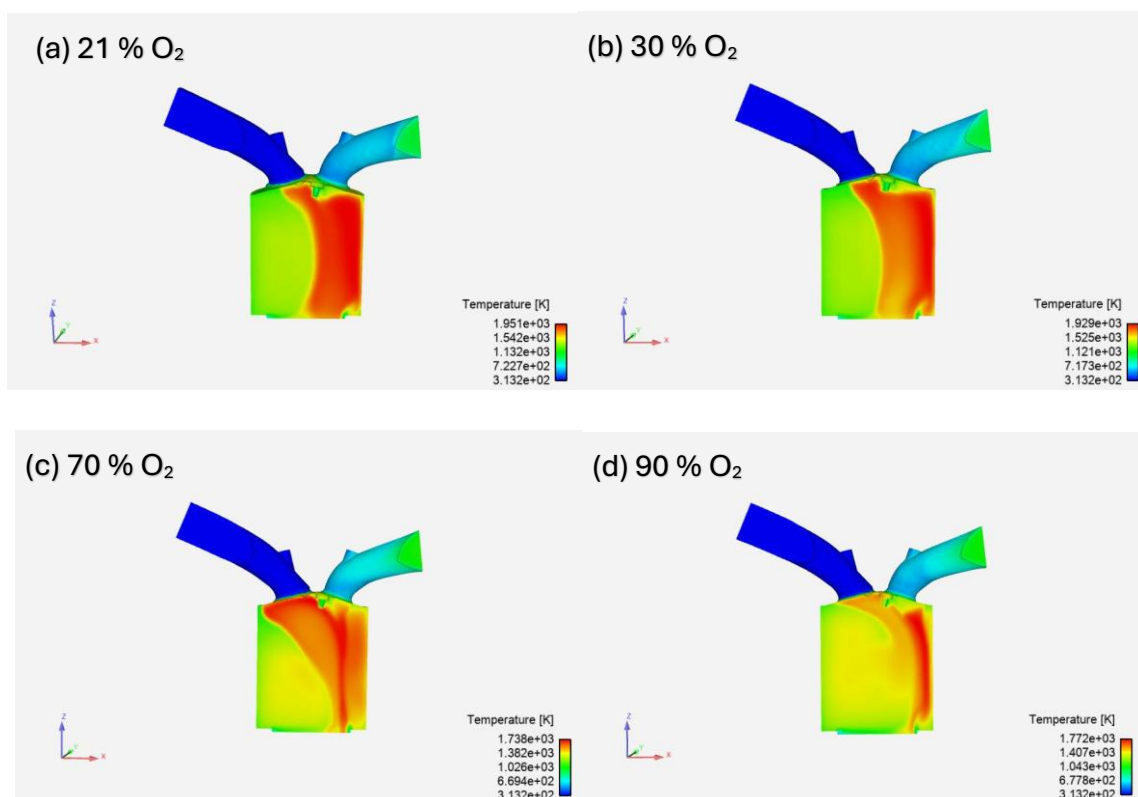


Figure 31 - Temperature gradients for: (a) 21 % oxygen; (b) 30 % oxygen; (c) 70 % oxygen and (d) 90 % oxygen.

Figure 31 shows the end of the combustion cycle, and it is possible to observe that, with the increase in oxygen concentration, the temperature inside the combustion chamber decreases and spreads. This phenomenon can be explained by the velocity magnitude and the velocity scalar value and can be observed in Figure 32.

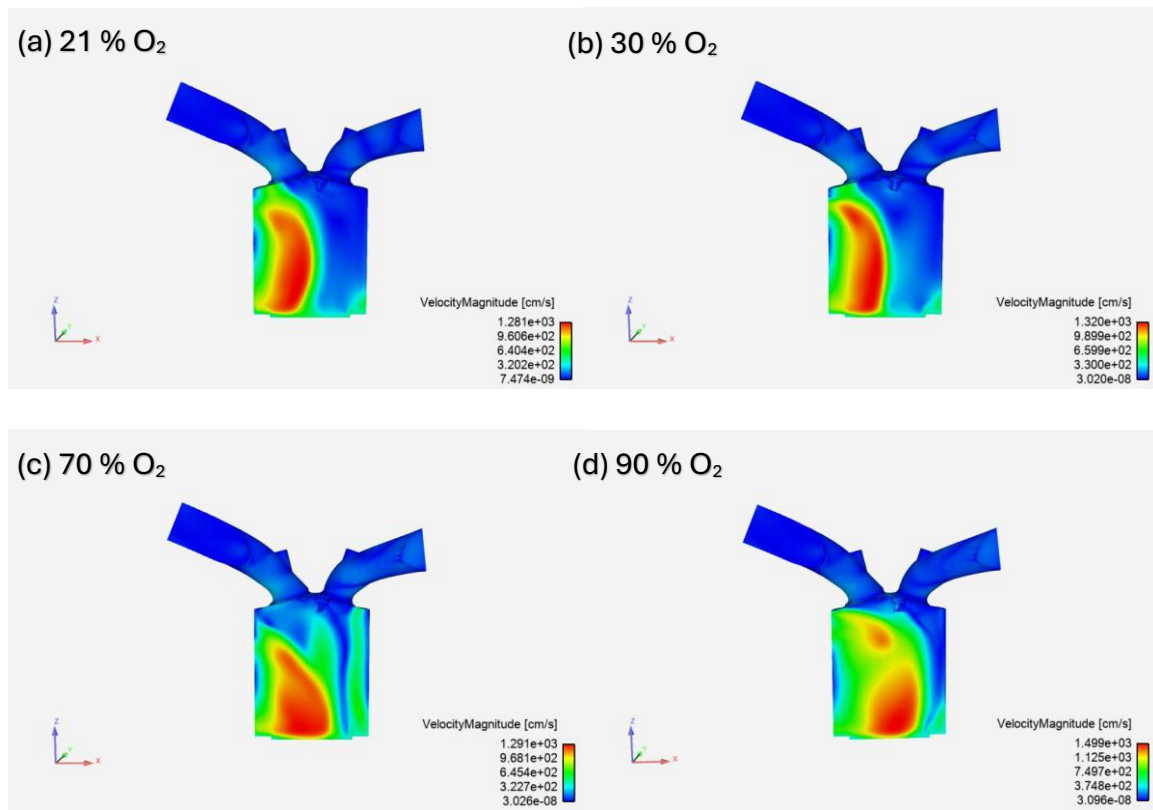


Figure 32 - Velocity magnitude gradients for: (a) 21 % oxygen; (b) 30 % oxygen; (c) 70 % oxygen and (d) 90 % oxygen.

Figure 32 shows that the velocity magnitude has the inverse behaviour of temperature and at low velocities, the temperature reaches higher values.

4.1.2 Effect on Pollutant Emissions

The pollutant emission results were classified into five main groups: CO (carbon monoxide), CO₂ (carbon dioxide), NO_x (nitrogen oxides), UHCs (unburnt hydrocarbons), and VOCs (volatile organic compounds). After analysing the pressures and temperatures results, it can be concluded that a suitable oxygen concentration lies between 25 % and

50 %. For this reason, the emissions analysis will be focused on this range, while the results for the remaining oxygen concentrations are presented in Appendix F.

To improve the readability of the figures, emission values between 328° and approximately 700° are not shown, as they were zero.

Regarding carbon monoxide (CO) emissions, a decreasing trend was observed (Figure 33) with the oxygen concentration increasing. According to Baukal et al., 2013, a peak in CO concentration occurs at 21 % O₂, when compared with other oxygen concentrations, while at higher oxygen concentrations, the CO levels remain low. This behaviour was expected, as the system operates with high oxygen levels, which promotes more complete combustion and reduces CO formation.

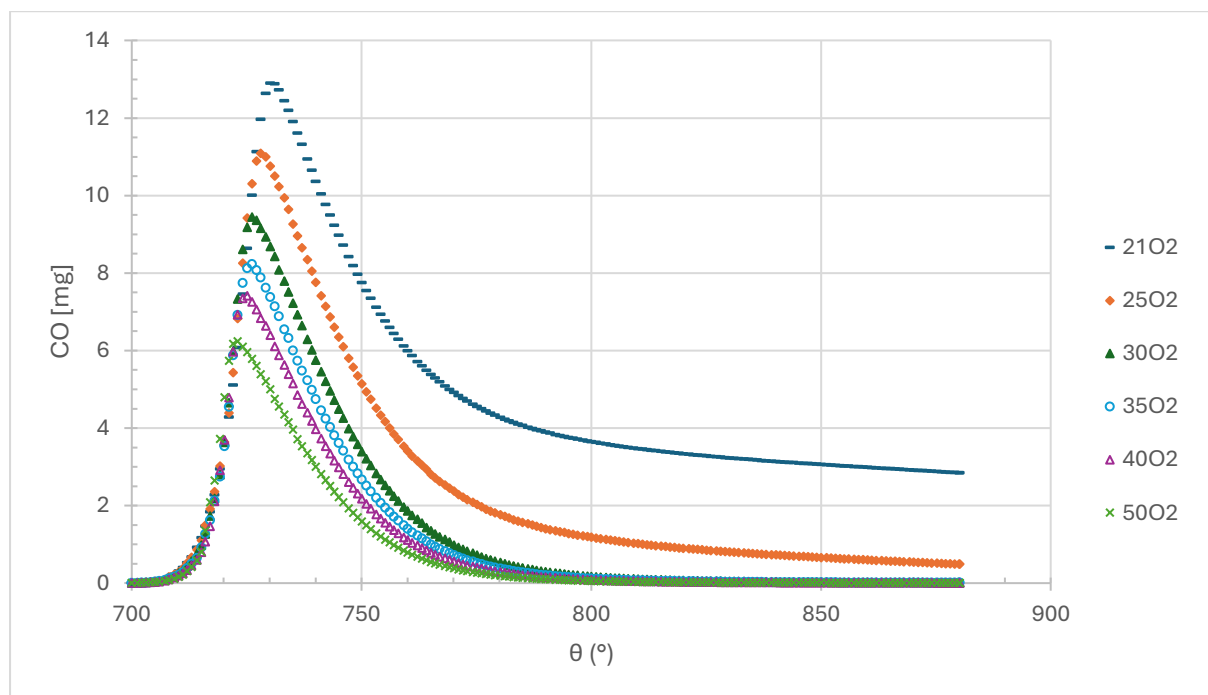


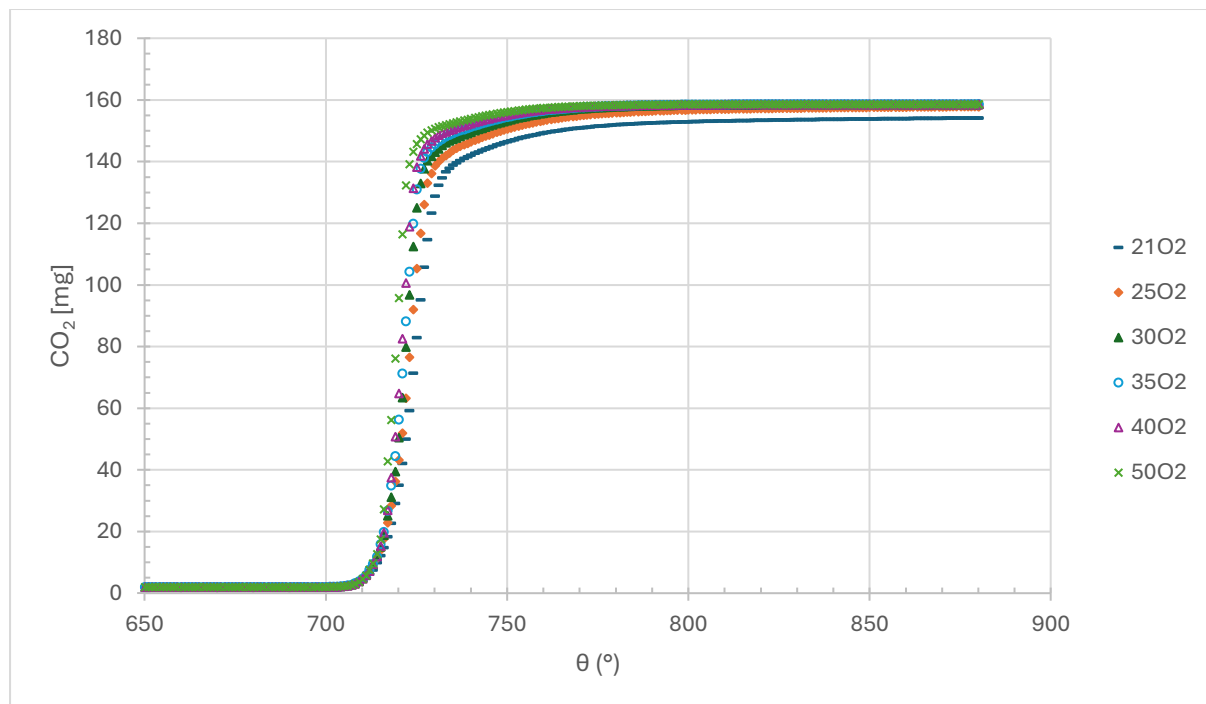
Figure 33 - Variation of carbon monoxide (CO) emissions with crank angle for different oxygen concentrations.

Although Figure 33 shows the evolution of CO inside the combustion chamber throughout the entire combustion process, the most relevant value for the emissions study is the amount of CO exiting the engine when the exhaust valves open (Table 19).

Table 19 – Carbon monoxide (CO) emitted when exhaust valves open.

O ₂ (%)	21	25	30	35	40	50
CO [mg]	2.84	0.49	0.01	0.01	0.01	0.00

Carbon dioxide (CO₂) emissions were evaluated based on the results presented in Figure 34. It was expected that CO₂ emission values would increase with higher oxygen concentrations, as more oxygen promotes more complete combustion; however, no significant difference was observed for concentrations between 21 % and 25 % O₂, and for the remaining oxygen concentrations, the difference is insignificant. As shown in Figure 35, for oxygen concentrations from 30 to 50 %, an approximation was made in Figure 34 to understand the small differences in CO₂ concentrations. To understand these differences, the CO₂ emissions values when the exhaust valves open are resumed in Table 20.

Figure 34 - Variation of carbon dioxide (CO₂) emissions with crank angle for different oxygen concentrations.

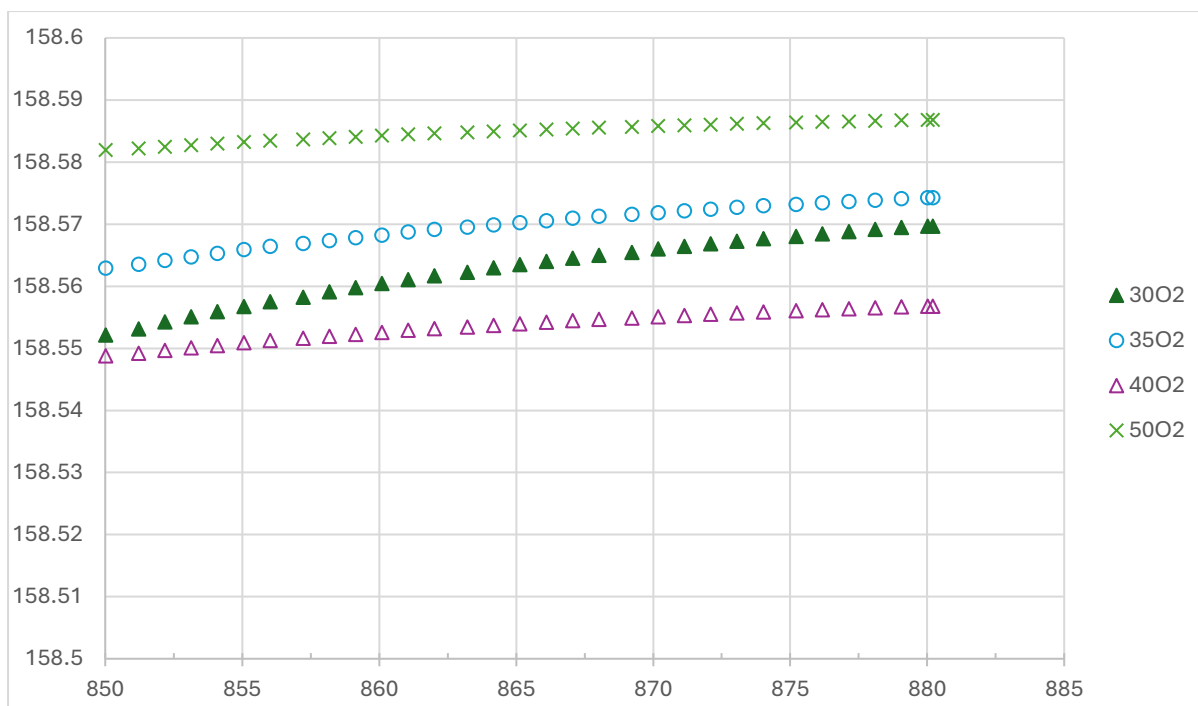


Figure 35 - Approximation of the CO₂ concentrations, for 30 %, 35 %, 40 %, 50 % O₂.

Table 20 - Carbon dioxide (CO₂) emitted when exhaust valves open.

O ₂ (%)	21	25	30	35	40	50
CO ₂ [mg]	154.12	157.83	158.57	158.57	158.56	158.59

Figures 36 and 37 show, respectively, the simulated NO and NO₂ emissions. For NO concentrations, Figure 36 shows an increase in NO concentrations with the oxygen concentration. The same trend is observed for NO₂ concentrations; there is an increase with oxygen concentration. Although an increase in oxygen concentration and a decrease in nitrogen concentration would be expected to reduce NO and NO₂ emissions, the high combustion temperatures, combined with the presence of excess O₂, promote the formation of these compounds.

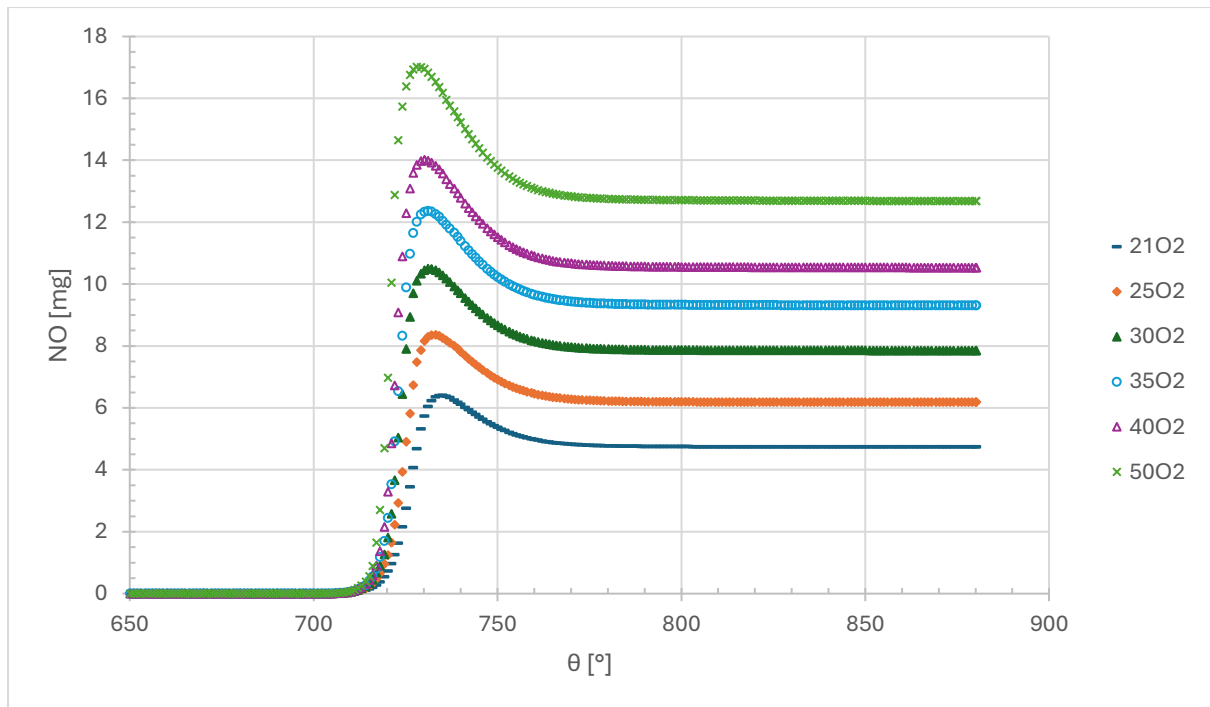


Figure 36 - Variation of nitrogen monoxide (NO) emissions with crank angle for different oxygen concentrations.

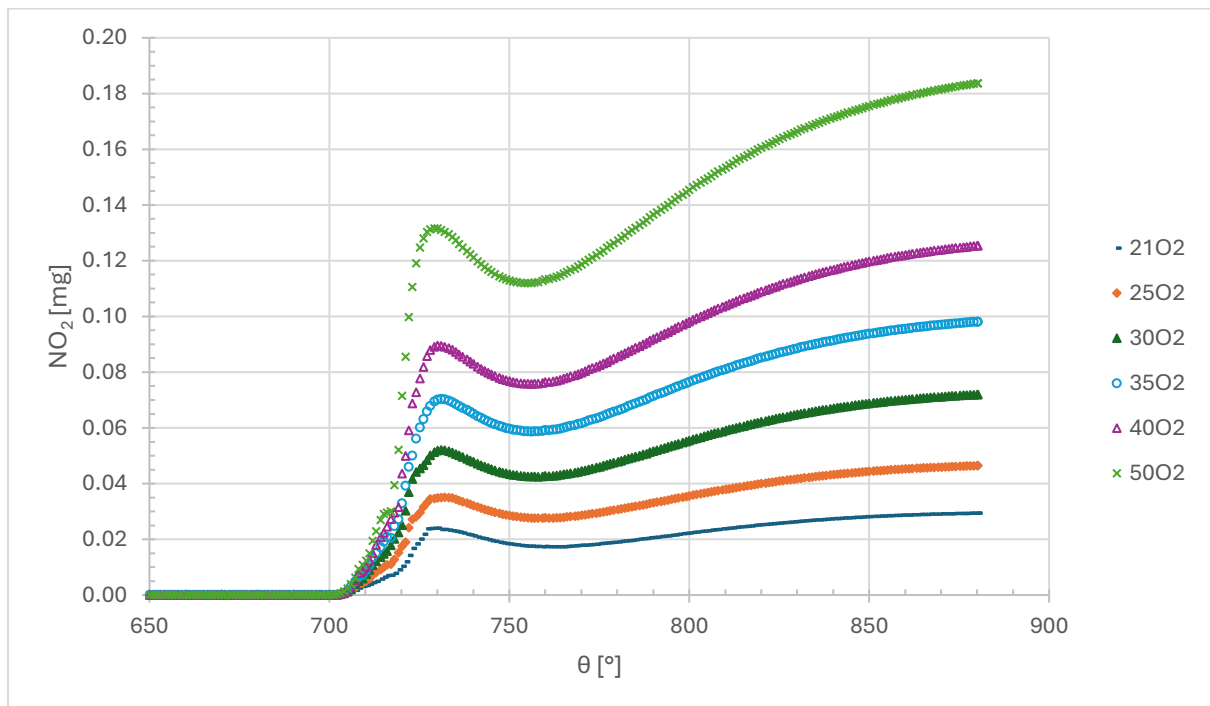


Figure 37 - Variation of nitrogen dioxide (NO₂) emissions with crank angle for different oxygen concentrations.

Figures 36 and 37 show that NO_x concentrations increase with oxygen concentrations. To evaluate the emissions, the values at the exhaust valves opening are resumed in Table 21, and it is possible to observe that between 21% and 50% oxygen, NO_x emissions almost triplicate. From 21 % to 50 % oxygen, there was a temperature increase, and the temperature is the main promoter of NO_x formation. With the oxygen concentration increase and consequent nitrogen decrease, the effect that nitrogen has in controlling combustion temperatures decreases lead to combustion temperature increase and consequently to NO_x formation.

Table 21 - Nitrogen oxides (NO_x) emitted when exhaust valves open.

O₂ (%)	21	25	30	35	40	50
NO [mg]	4.74	6.18	7.86	9.31	10.53	12.68
NO₂ [mg]	0.03	0.05	0.07	0.10	0.13	0.18

Figures 38 and 39 illustrate the evolution of Unburnt Hydrocarbons (UHCs) and Volatile Organic Compounds (VOCs) emissions, respectively. The first slope represents fuel injection, then the plateau represents the amount of fuel injected, that is, 50.85 mg, and the final slope corresponds to the combustion process. All the relevant points for interpreting these profiles are indicated in Figures 38 and 39.

The results indicate that no significant improvement was observed in UHC and VOC emissions.

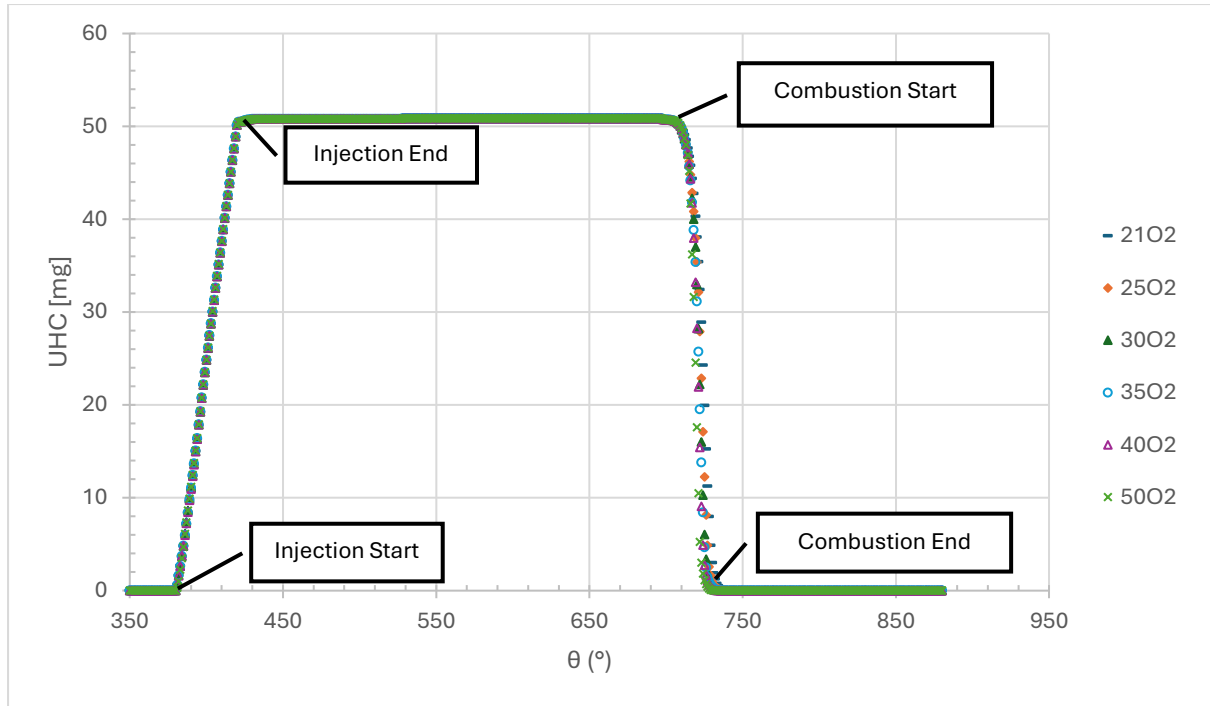


Figure 38 - Variation of unburnt hydrocarbons (UHCs) emissions with crank angle for different oxygen concentrations.

This behaviour can be attributed to the fact that these emissions depend on the fuel mass, which remained unaltered during the simulations; therefore, the final emission levels remain essentially unchanged.

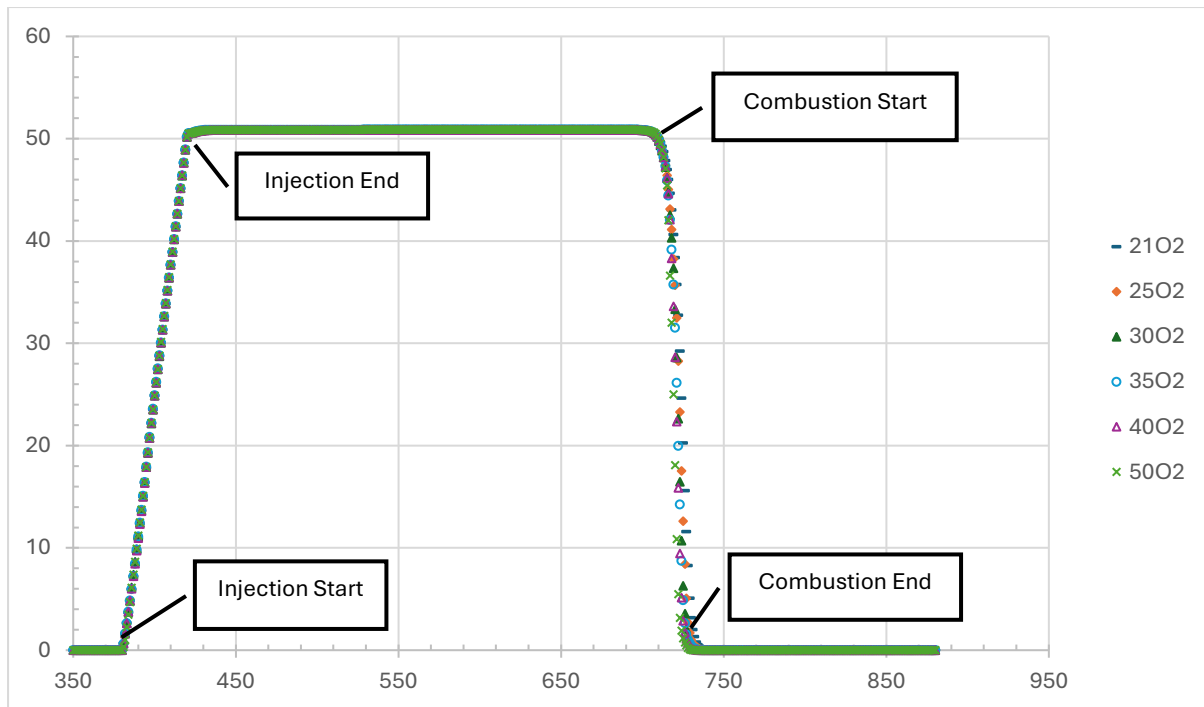


Figure 39 - Variation of volatile organic compounds (VOCs) emissions with crank angle for different oxygen concentrations.

4.1.3 Effect on Power and Combustion Efficiency

The final parameters studied were engine power, combustion efficiency, and thermal efficiency. These parameters are critical for evaluating engine performance and, in the case of combustion efficiency, for determining whether the combustion process was successful.

The reference power value corresponds to 21 % O_2 , which is 32.6 KW. However, to select the most appropriate oxygen concentration, all power values at different oxygen concentrations were assessed.

As can be seen in Table 22, power slightly increases from 21 to 25 % oxygen and then decreases. Although combustions remain efficient (efficiency ≈ 1), and all the fuel is burned, excess oxygen remains in the mixture. Thus, to achieve more efficient combustion, increase thermal efficiency to nearly 0.44, and restore power to around 32.6 kW, the reference value, it would be necessary to increase fuel mass.

Table 22 - Power and Combustion Efficiency values for simulated oxygen concentrations.

O₂ (%)	N₂ (%)	P (kW)	Combustion Efficiency (%)	Thermal Efficiency (%)
21	79	32.6	99.7	43.8
25	75	32.8	100	44.0
30	70	32.6	100	43.8
35	65	32.5	100	43.7
40	60	32.3	100	43.4
50	50	32.0	100	42.9
60	40	31.7	100	42.5
70	30	31.4	99.8	42.1
80	20	31.2	99.7	41.9
90	10	31.1	99.5	41.7
95	5	31.1	99.4	41.7

To evaluate if the remaining oxygen has any effect, these values were summarized in Table 6. Note that for each oxygen concentration, at the end of combustion, there is no fuel remaining, so iC_8H_{18} , C_2H_5OH , and CH_3OH are equal to zero milligrams.

Table 23 - Oxygen mass at the end of combustion cycles.

O₂ (%)	O₂ [mg]
21	9.64
25	15.59
30	25.53
35	35.60
40	46.18
50	67.83
60	90.48
70	113.78
80	138.09
90	163.09
95	175.89

Table 23 shows that as the intake oxygen concentration increases, combustion remains efficient, but at the end of the process, a high oxygen concentration is still present, and all the fuel mass was completely consumed.

Considering that the initial fuel mass in the simulations was 50.85 mg, this mass could be increased. However, since this engine is intended for drones, the fuel mass should not be significantly increased. For this reason, oxygen concentration above 60 % will be neglected and not considered in further studies.

Pressure, IMEP and Work correlation

In order to understand the correlation between mechanical performance and the cycle's energy efficiencies, this analysis highlights how increasing oxygen concentration affects the engine's ability to convert chemical energy into useful work.

Figures 40, 41, and 42 show the engine power, IMEP, and indicated work, respectively, for oxygen concentrations between 21 and 50 %, which, as previously concluded, correspond to the oxygen concentrations that will be used for further studies.

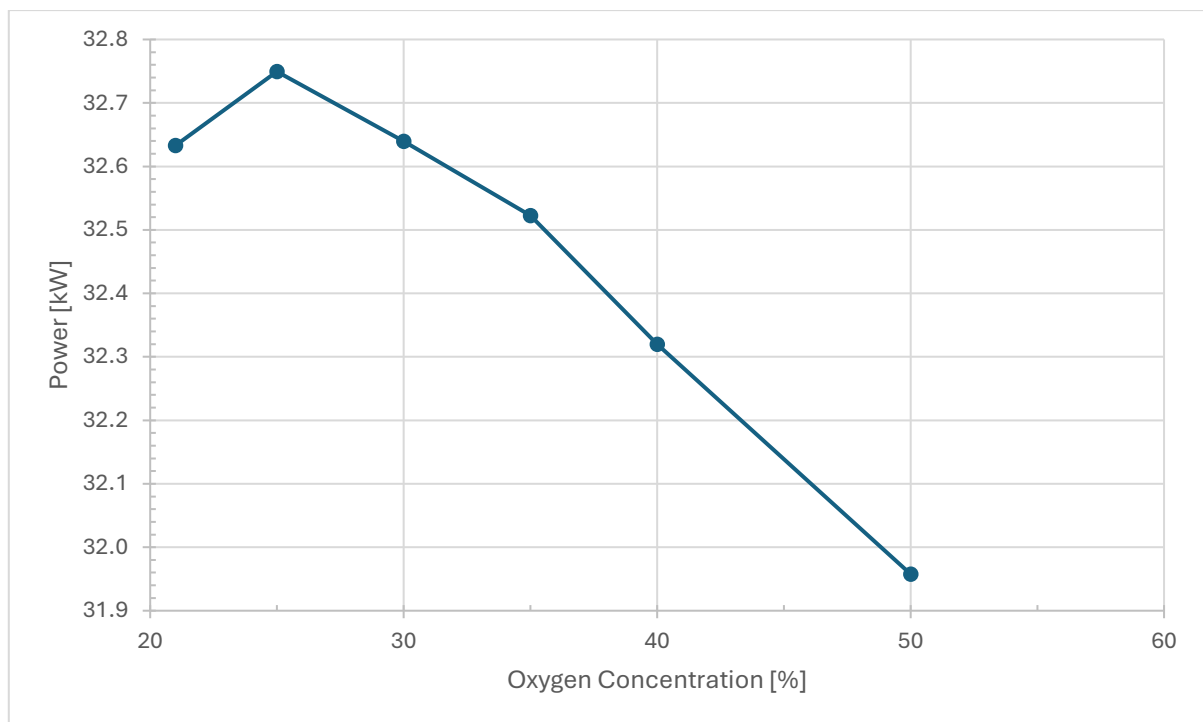


Figure 40 - Power for 21 and 50 % of oxygen.

Comparing power, IMEP and work, om Figures 39, 40 and 41, respectively, reveals a direct linear correlation, demonstrating that the engine's performance increase with oxygen enrichment, between 21 and 25 % O₂, improve combustion efficiency.

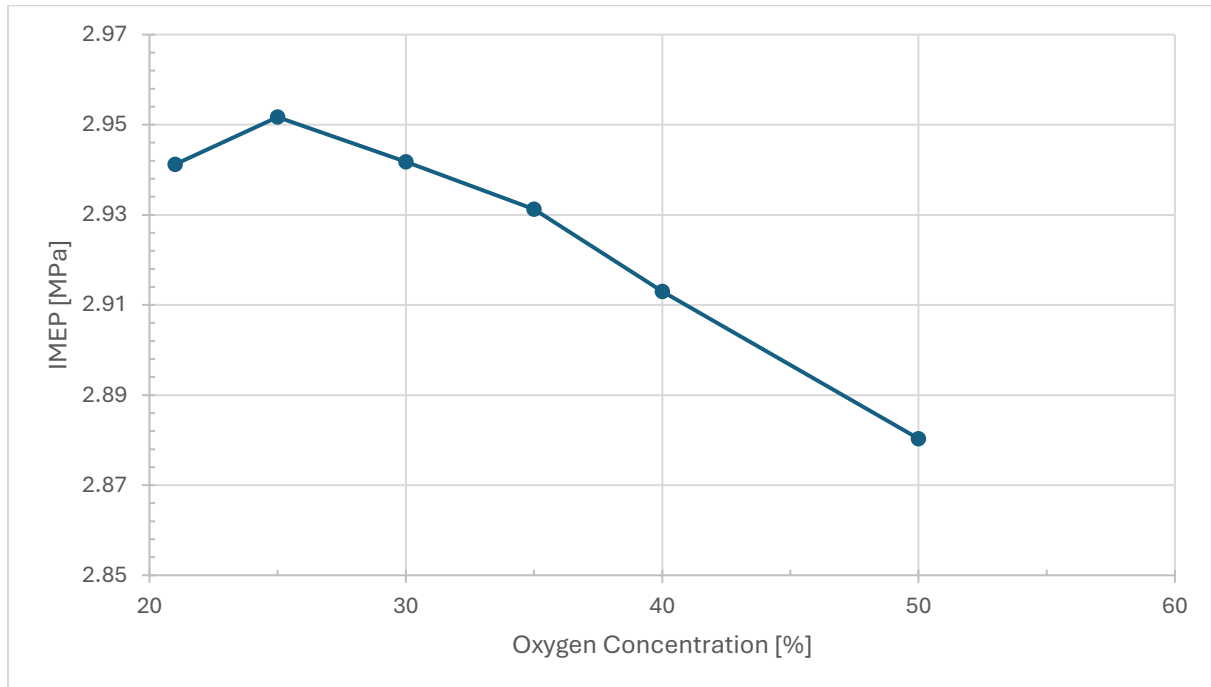


Figure 41 - IMEP for 21 and 50 % oxygen.

In an initial phase, the higher oxygen availability promotes complete fuel oxidation, effectively converting chemical energy into useful work. However, after 25 % O₂, a progressive degradation of both IMEP and power is observed, despite combustion being complete. This decrease is explained by a decrease in thermal efficiency: excess oxygen and high temperatures lead to higher heat losses to the cylinder walls, penalizing the work extracted from the cycle.

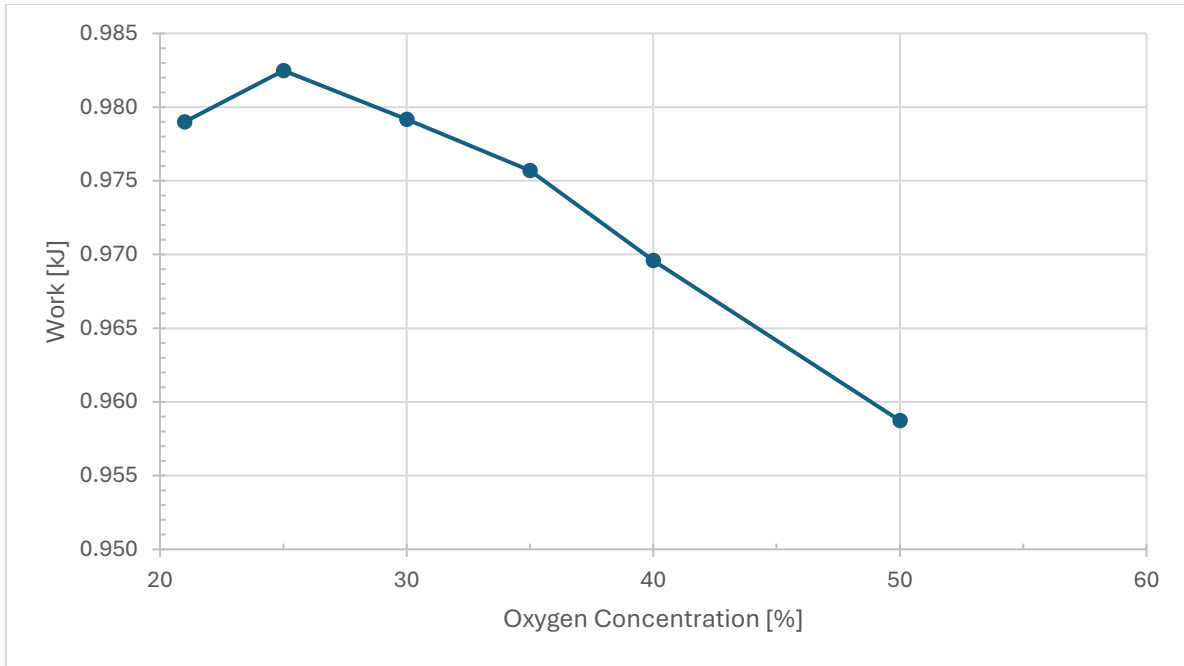


Figure 42 - Work for 21 and 50 % of oxygen.

Besides, the most promising oxygen concentration for performance was 25 %, which provides the best combination of power, combustion, and thermal efficiency. However, since it does not represent a significant difference between oxygen concentrations, the study will continue considering an oxygen point of 30 %. This concentration represents a good compromise when considering temperature and pressure.

4.2 Influence of Angular Speed Variation

After selecting an appropriate oxygen concentration, in this case 30 %, the influence of varying the angular speed was studied. The aim was to understand the effect of angular speed on engine performance and emissions, in this case reach an expected power of 32.6 kW, the power reference value for 21 % O_2 . For this, the angular speed was varied from 1500 rpm to 4500 rpm, and for the different speeds, the fuel mass, provided by the manufacturer, was also adjusted and the intake pressure remained the same as previously used: 2.54 bar. These parameters were configured for two different oxygen concentrations: 21 and 30 %. The values for angular speed and fuel masses used are summarized in Table 24.

Table 24 - Fuel masses (mg) for each oxygen concentration and angular speed.

	Angular Speed (rpm)				
	1500	2000	3000	4000	4500
21 % O₂	45.9 mg	56 mg	50.0 mg	50.9 mg	50.1 mg
30 % O₂					

The parameters were modified in the ANSYS Forte software. First, in the injection setup window, the fuel mass was changed (Figure 43).

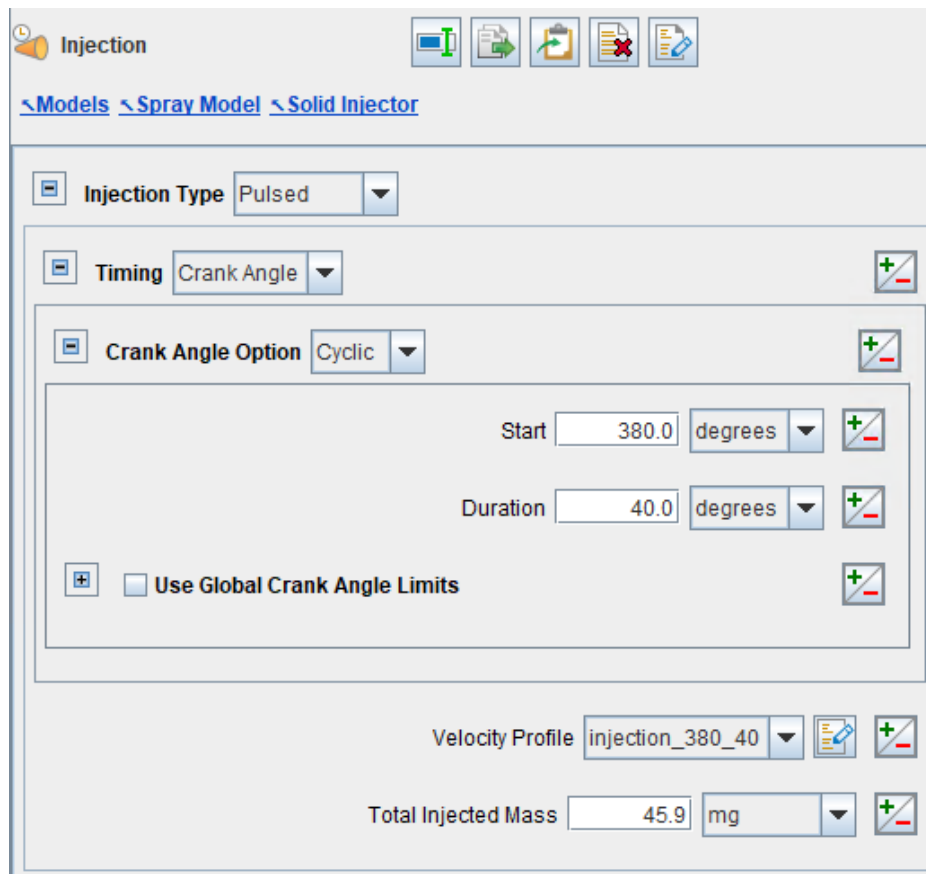


Figure 43 - Injection setup window.

Then, the air composition was also modified in the intake initial condition setup window (Figure 44), and finally, in the simulation condition setup window, the angular speed value was settled (Figure 45).

intake

[Initial Conditions](#)

Region Type Other

Composition Constant

Composition Air21O2

Temperature Constant

Temperature 313.0 K

Pressure Constant

Pressure 2.54 bar

Figure 44 - Initial Conditions setup window.

Simulation Controls

[Time Step](#) [Chemistry Solver](#) [Transport Terms](#) [System Coupling](#) [Detect Steady State](#)

Simulation Limits

Simulation End Point Option Crank Angle Based

Initial Crank Angle 328.0 degrees

Final Simulation Crank Angle 880.2 degrees

RPM 1,500.0 rpm

Cycle Type 4-Stroke

Engine Bore User Specified

Bore 72.2 mm

Figure 45 - Simulation Controls setup window.

4.2.1 Effect on Temperature and Pressure

A study on the effect of angular speed variation on temperature and pressure was developed to assess its impact on engine performance.

Temperature and Pressure Comparison

Figure 46 shows the evolution of temperature with angular speed variation. It is possible to observe that for 30 % oxygen, the temperature is higher than for 21 % oxygen. Although there is a significant increase in temperature between 1500 and 2000 rpm, at 3000 rpm the temperature decreases. After 3000 rpm, the temperatures rise and are followed by a reduction.

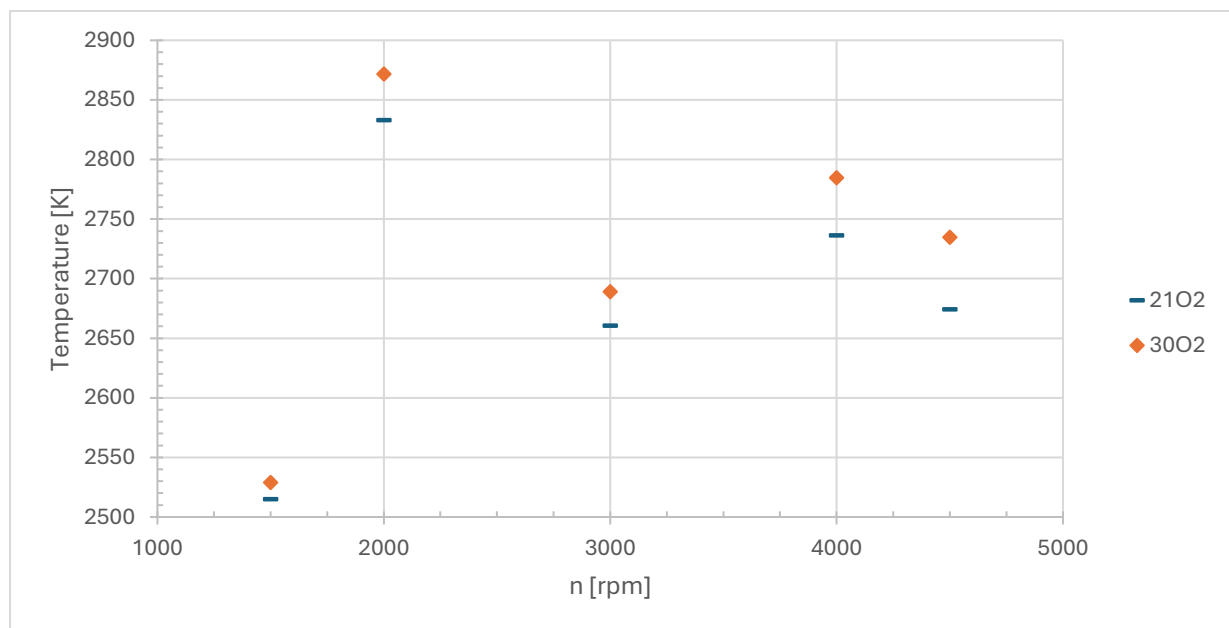


Figure 46 - Maximum in-cylinder temperatures for 21 and 30 % O₂.

At low speeds, the heat inside the combustion chamber has time to dissipate faster than at high speeds. To understand this phenomenon, the heat transfer parameter at the wall was studied, and a chart was created with the maximum heat transfer values at the wall (Figure 47). The maximum heat transfer at the wall was determined for a specific crank angle.

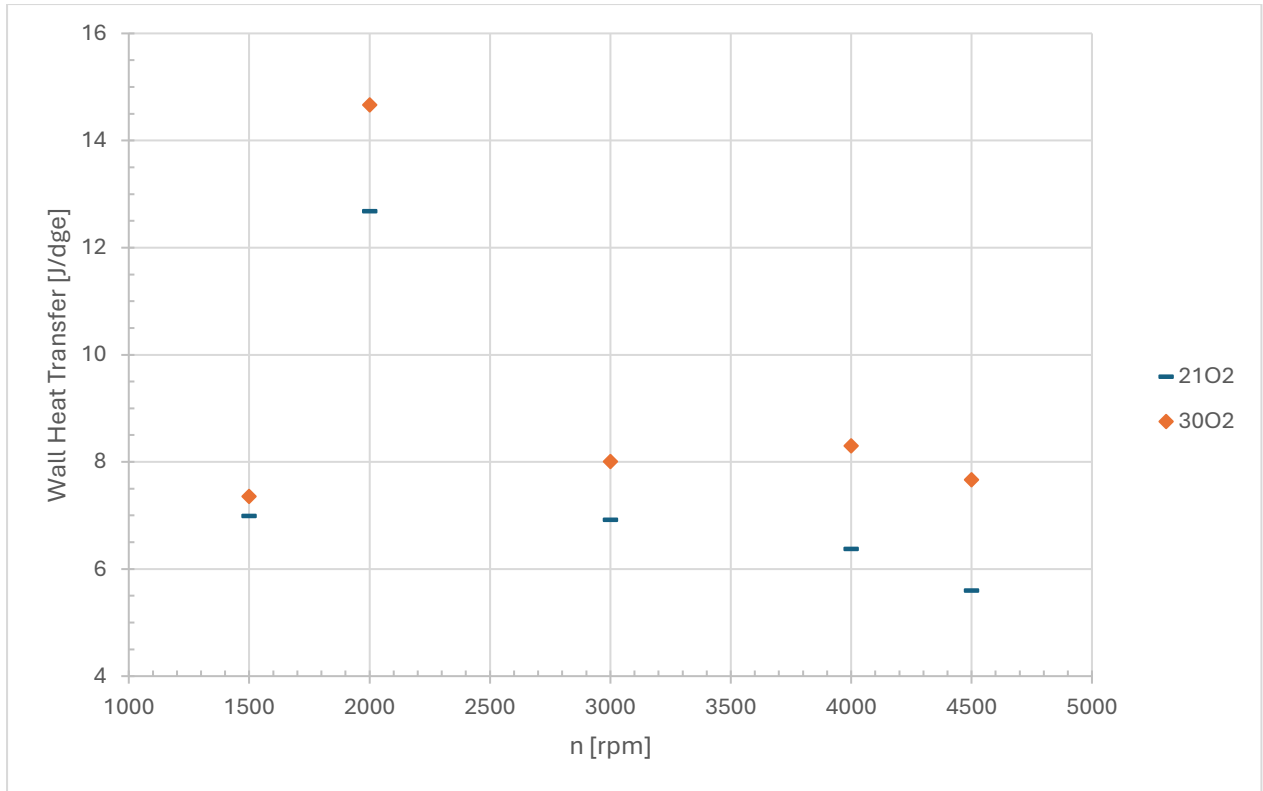


Figure 47 – Heat transfer at the wall for 21 and 30 % of oxygen.

As can be observed, the wall heat transfer has a similar behaviour to the temperature. There is a peak at 2000 rpm, almost double that obtained at 1500 rpm, which can be explained by the temperature peak at 2000 rpm. Although the engine was operating at low speed, the temperature reached very high values between 2800 and 2900 K. Since the wall heat transfer is proportional to the temperature difference between the gases and the wall, this results in a significant increase in heat transfer to the walls. The increase in temperature can also be explained by the pressure behaviour and is shown in Figure 48.

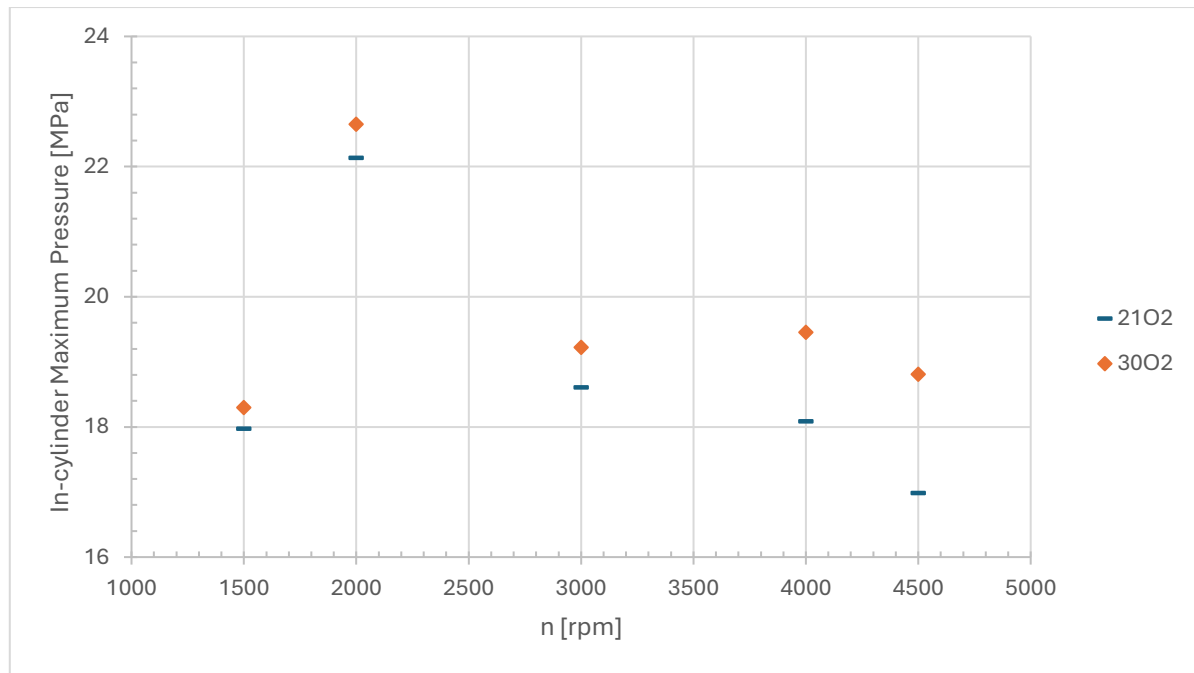


Figure 48 - Maximum in-cylinder pressures for 21 and 30 % oxygen.

Figure 48 allows to conclude, as observed in sub-section 4.1, that with the increase in oxygen concentration, the pressure also increases. It is also possible to observe that the pressure shows the same trend as the temperature with the angular speed variation.

The increase in pressure with variation of oxygen is explained by the combustion velocity: with the increase in oxygen concentration, combustion is faster, and there is a higher release of energy in a reduced period of time, and consequently, the pressure increases. To explain the similarity between pressure and temperature, it is necessary to resort to the Ideal Gas Law ($PV = nRT$), and in this case, as the volume and the ideal gas constant (R) are constant, the pressure is directly proportional to the temperature, so as the temperature increases, the pressure also increases.

4.2.2 Effect on Pollutant Emissions

As in sub-section 4.1.2, the results of the evolution of pollutant emissions, such as CO, CO₂, NO, NO₂, UHCs, and VOCs, were studied. The same procedure was adopted, the charts were developed considering the angular speed, and for each angular speed, each compound was studied.

Since the evolution of pollutant production during the combustion cycle is very similar to that observed in sub-section 4.1.2, in this sub-section only the pollutants at 2000 rpm were studied, as this is the point with the highest temperature and pressure, since is the angular speed value with high fuel mass (56 mg) and consequently more torque is obtained, and could be the point with the most pollutant variations.

To improve the readability of the figures, emission values between 328° and approximately 700° are not shown, as they were zero.

Regarding CO emissions, as expected, a decrease was observed at concentrations of 30 % O₂ (Figure 49). According to (Kuppusamy Rajkumar and Palanisamy Govindarajan 2011), carbon monoxide is produced during incomplete combustion, and if the system is operated with a high excess of air, it leads to complete combustion, consequently minimizing CO emissions. With oxygen enrichment, thermal dissociation occurs, and CO is converted into CO₂.

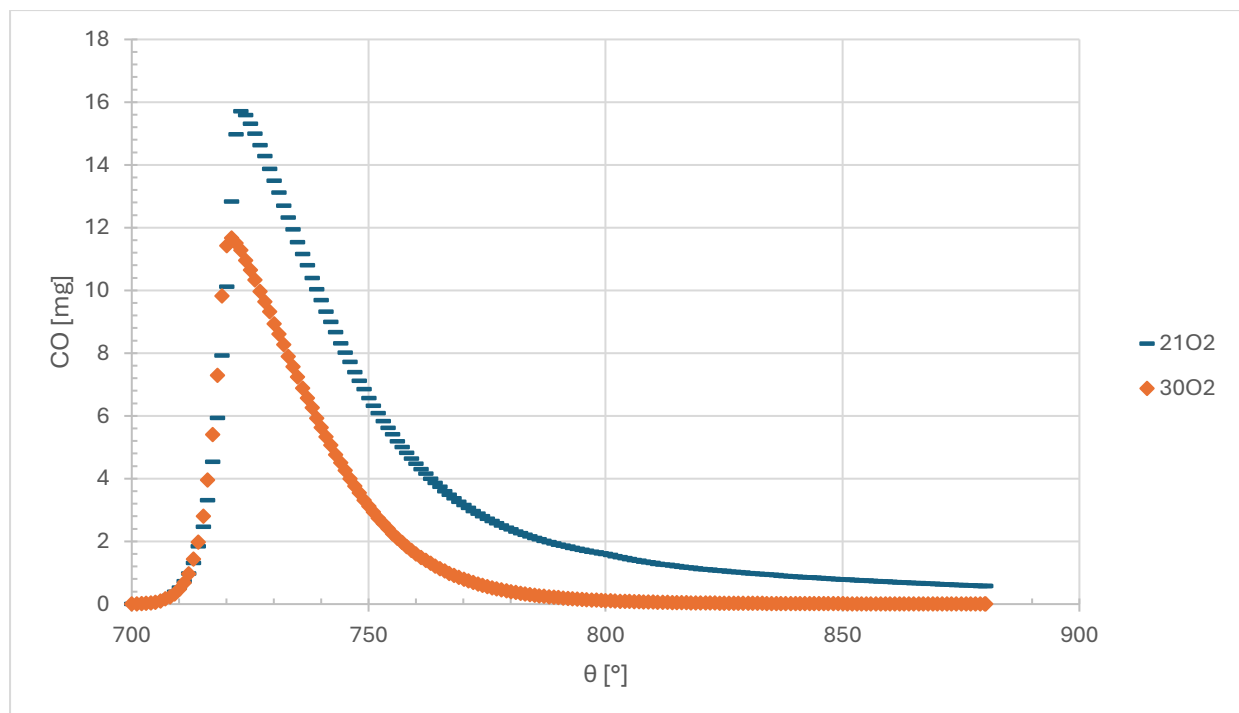


Figure 49 - Variation of carbon monoxide (CO) emissions with crank angle for 21 and 30 % oxygen, at 2000 rpm.

According to Figure 50, the CO_2 concentration was slightly higher for 30 % O_2 , however both tend to stabilize at around 173 mg of CO_2 . The observed difference, although small, was due to the previously described effect: thermal dissociation occurred and promoted the conversion of CO into CO_2 .

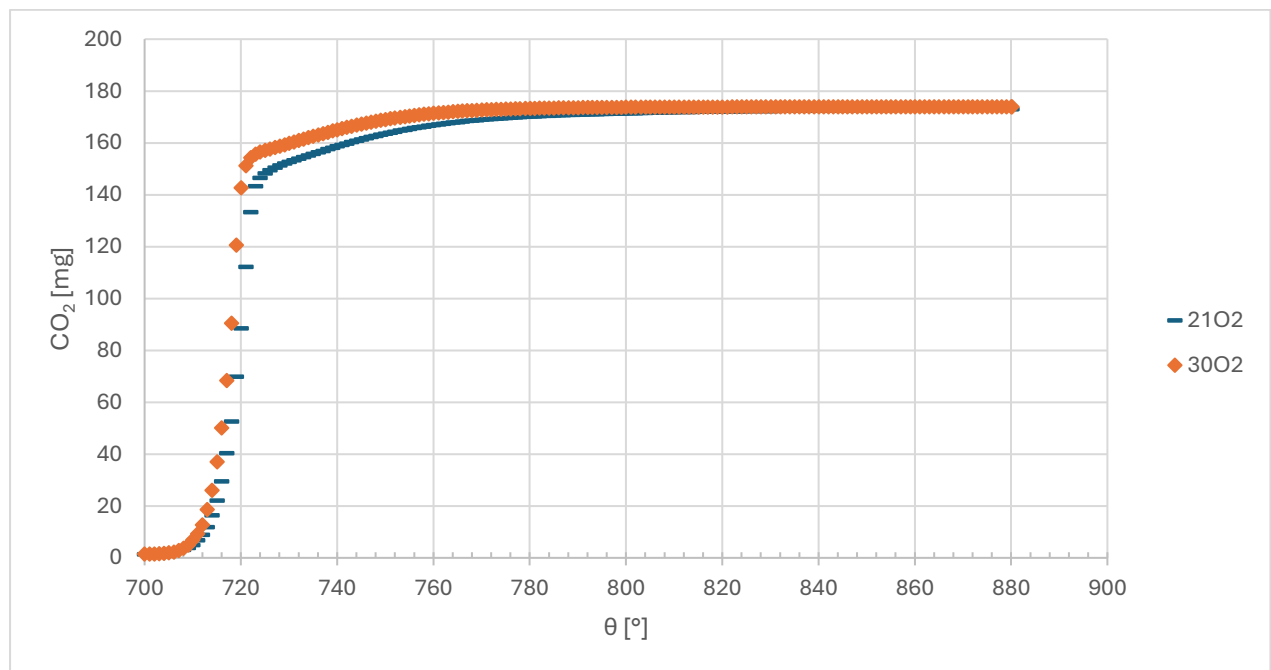


Figure 50 - Variation of carbon dioxide (CO_2) emissions with crank angle for 21 and 30 % oxygen, at 2000 rpm.

Figures 51 and 52 show the evolution of NO and NO_2 concentrations, and as expected, there is an increase when the oxygen concentration increases. NO concentrations present a similar behaviour in both cases, tending to stabilize, with emissions at 30 % O_2 , are almost double those at 21 % O_2 . For NO_2 evolution, both curves present an increasing behaviour during the combustion cycle, and for 21 % O_2 , the NO_2 concentrations tend to stabilize. A different behaviour can be observed for 30 % O_2 , where, during the combustion cycle, the formation of this compound is continuously increasing and does not stabilize. Although at the final stage of the combustion cycle, it was possible to observe that NO_2 values quadrupled.

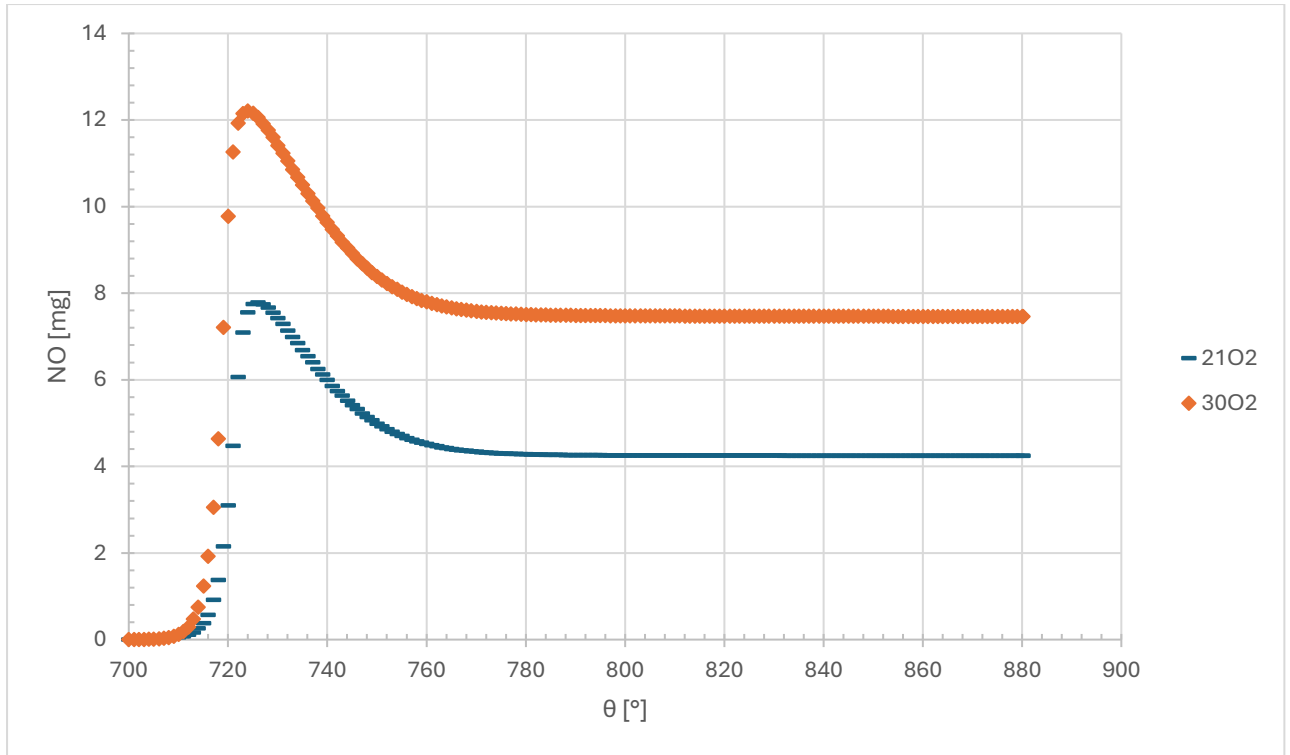


Figure 51 - Variation of nitrogen monoxide (NO) emissions with crank angle for 21 and 30 % oxygen, at 2000 rpm.

One of the formation mechanisms for NO_x formation is thermal NO_x , which is produced due to the high temperature reaction of nitrogen with oxygen. Another mechanism is the fast reaction between nitrogen, oxygen, and hydrocarbons. According to Kuppusamy Rajkumar and Palanisamy Govindarajan 2011, higher post flame temperatures and oxygen concentrations lead to high rates of NO_x formation, and NO_x emissions increase exponentially with increasing oxygen concentration.

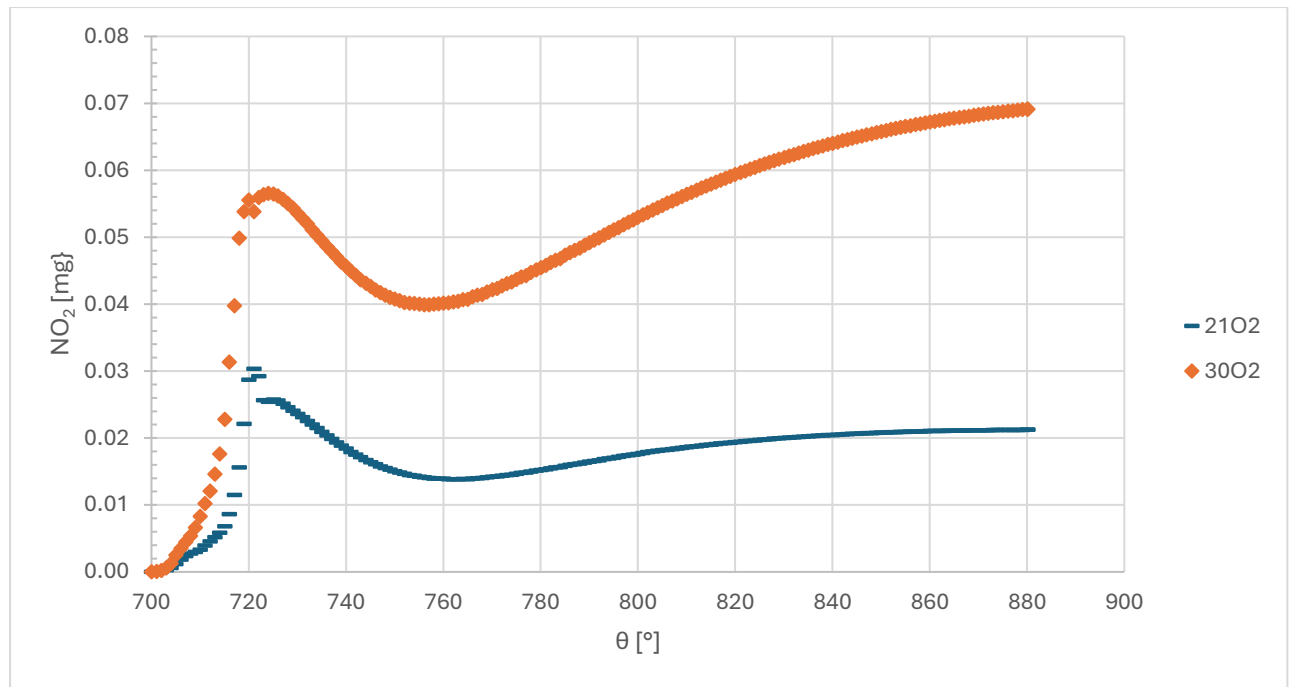


Figure 52 - Variation of nitrogen dioxide (NO_2) emissions with crank angle for 21 and 30 % oxygen, at 2000 rpm.

Figures 53 and 54 illustrate UHCs and VOCs emissions, respectively. In these figures, the slope represents the fuel injection, the plateau represents the amount of injected fuel, in this case, 56 mg, and the final slope is the combustion process, where it is possible to observe the fuel mass consumption. To understand these processes, all relevant points are represented in Figures 53 and 54.

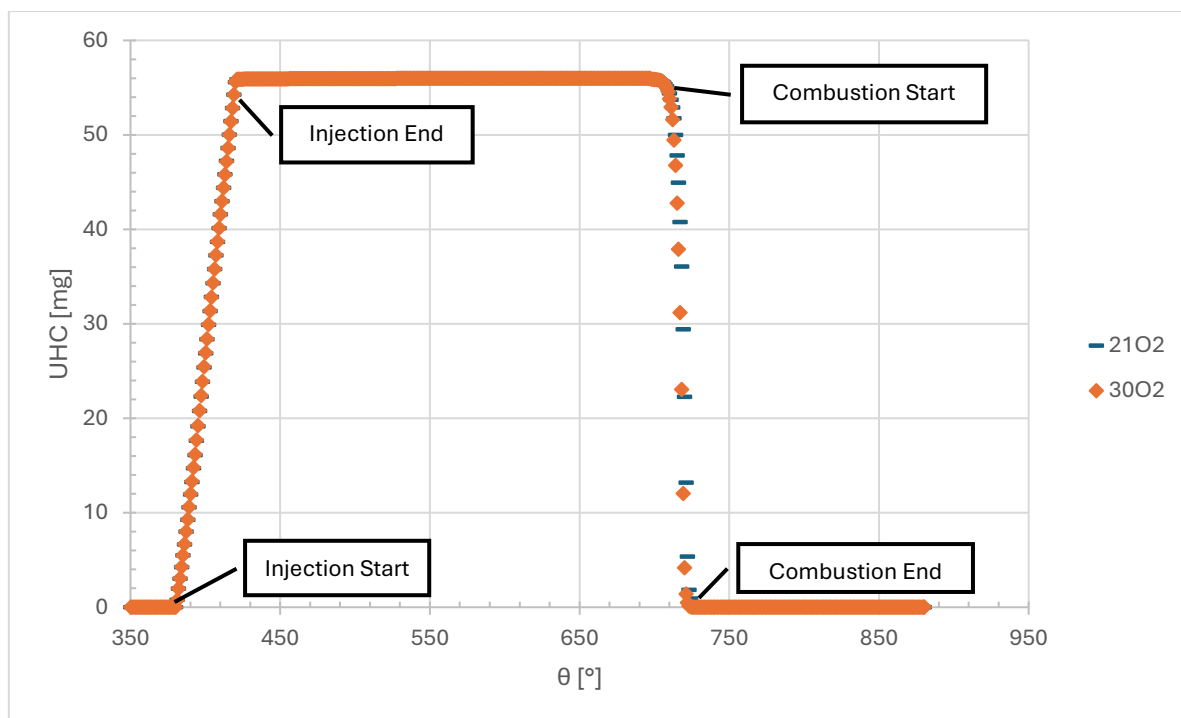


Figure 53 - Variation of unburnt hydrocarbons (UHCs) emissions with crank angle for 21 and 30 % oxygen, at 2000 rpm.

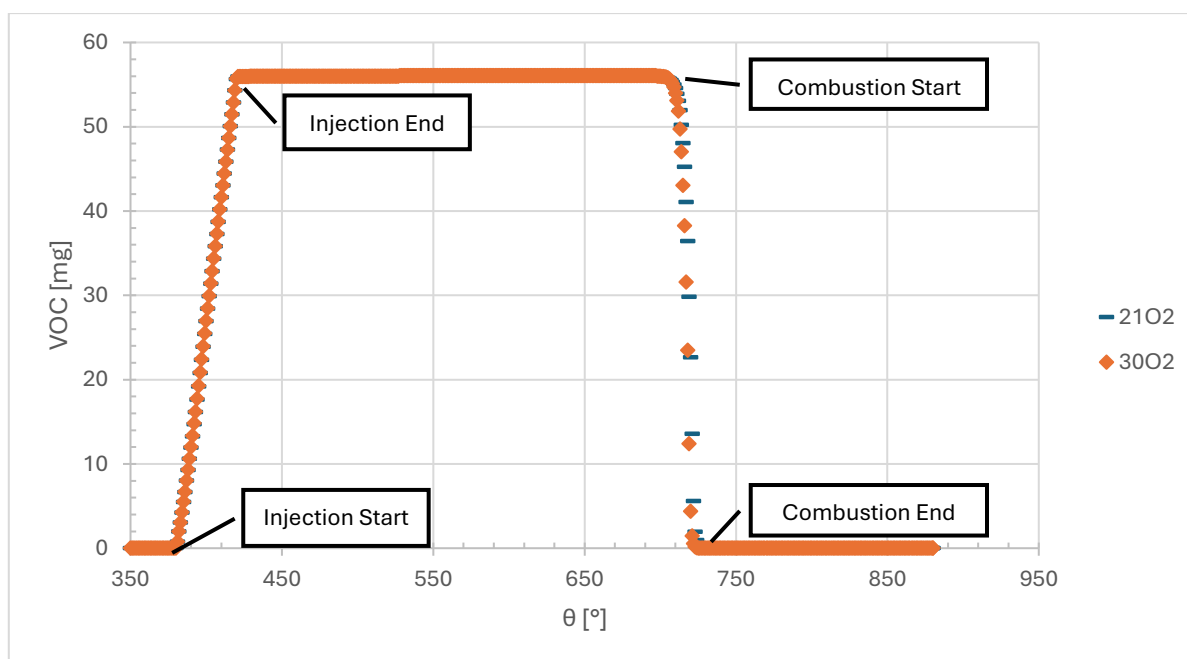


Figure 54 - Variation of volatile organic compounds (VOCs) emissions with crank angle for 21 and 30% oxygen, at 2000 rpm.

The behaviour observed was attributed to the fact that these emissions depend on fuel mass and consequently, on fuel consumption, which was maintained constant for each angular speed simulation.

Emission with the exhaust valve opening

Figure 55 shows the CO concentration at exhaust valve opening for different oxygen concentrations and angular speeds.

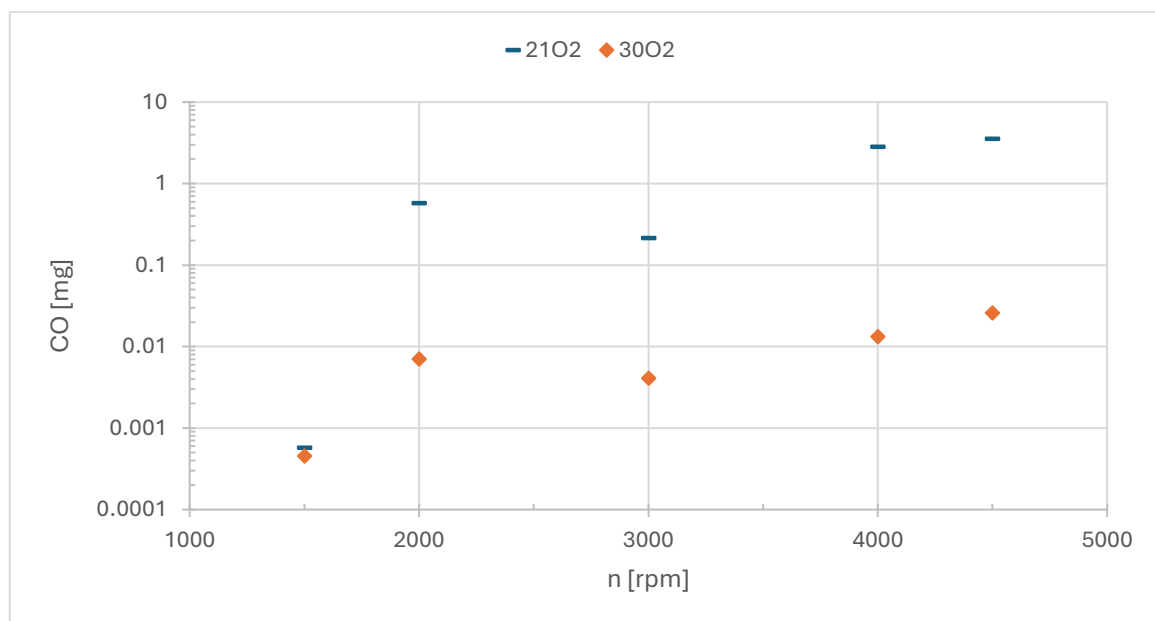


Figure 55 – CO concentrations at exhaust valve opening.

As can be seen in Figure 55, there is a decrease in CO emissions. According to literature (Man et al. 2016), CO emissions tend to increase with higher engine load or speed due to the increased of air/fuel ratio at high loads, associated with the higher fuel consumption at high loads.

Figure 56 summarizes the CO₂ emissions when the exhaust valve is open. As can be observed, at low speeds the CO₂ concentration does not show a considerable difference, but the inverse occurs at high speeds, where there is an increase of approximately 4 to 6 mg.

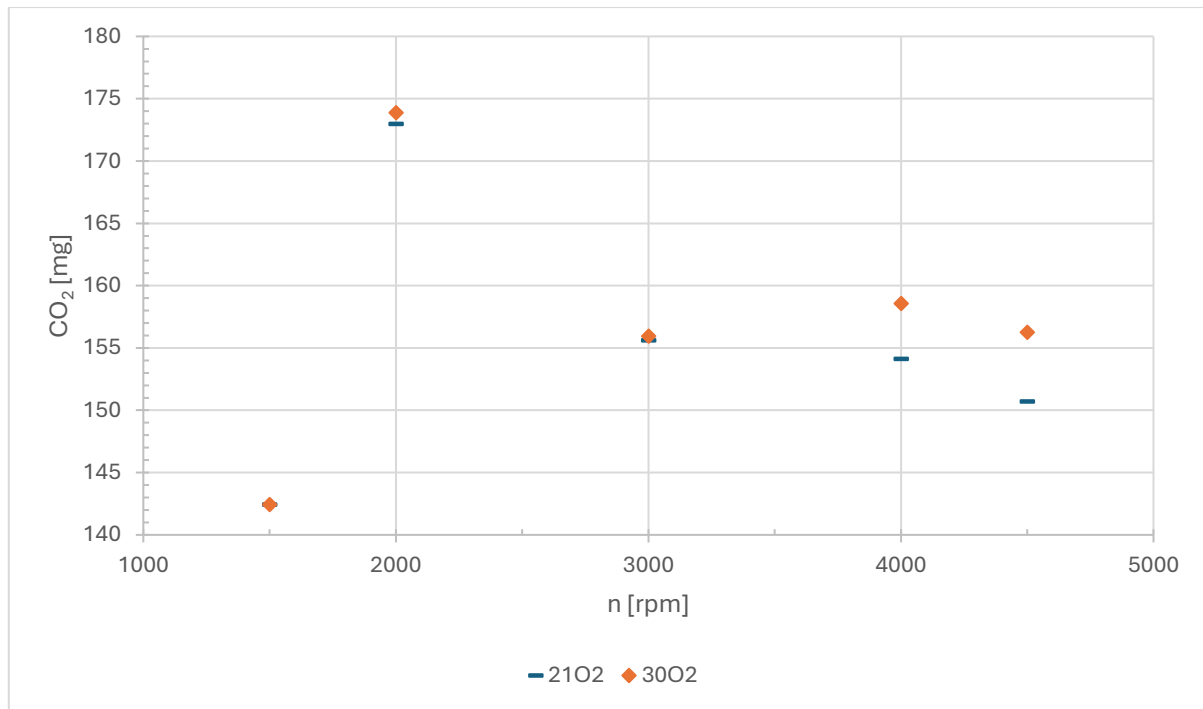


Figure 56 - CO₂ concentrations at exhaust valve opening.

A similar behaviour occurred for CO₂ concentrations, which increase with increasing engine load. For both CO and CO₂, the fuel mass plays an important role in the formation of these compounds. At 1500 rpm, the lowest fuel mass was used (45.9 mg), and for 2000 rpm, the highest fuel mass (56.0 mg) was used. The formation of these compounds is related to the fuel amount, since CO₂ and, consequently, CO formation depend on combustion efficiency, i.e., the extent to which complete combustion is reached.

Figures 57 and 58 present the exhaust valve emissions for NO and NO₂.

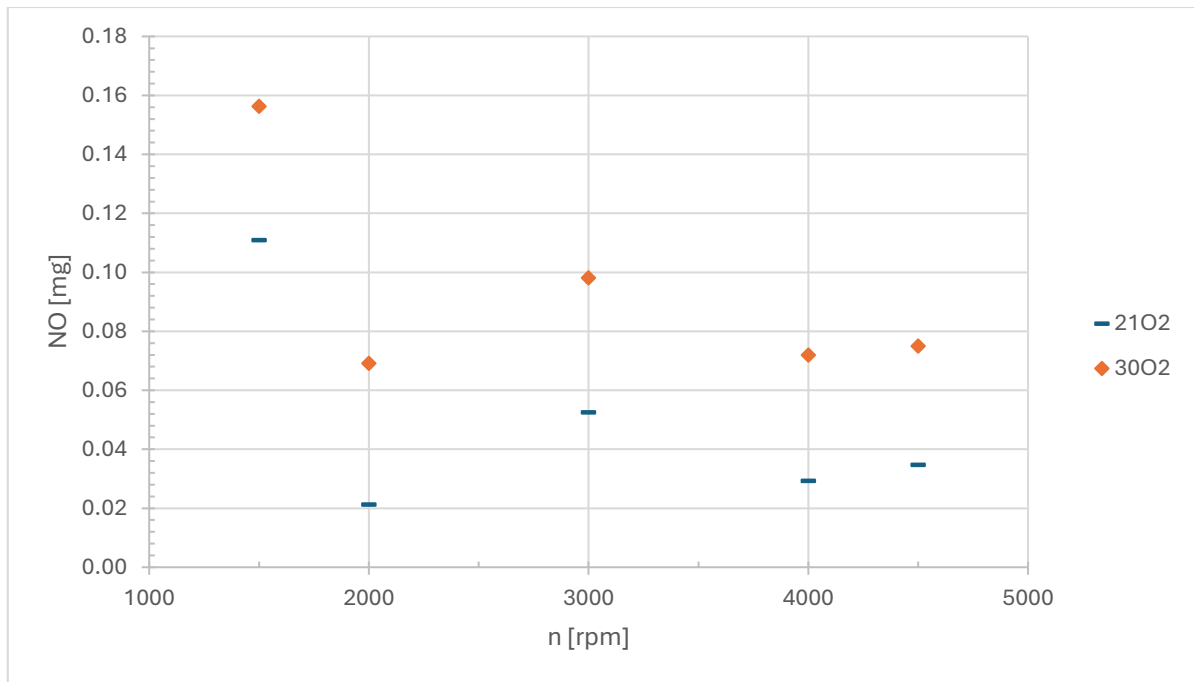


Figure 57 - NO concentrations at exhaust valve opening.

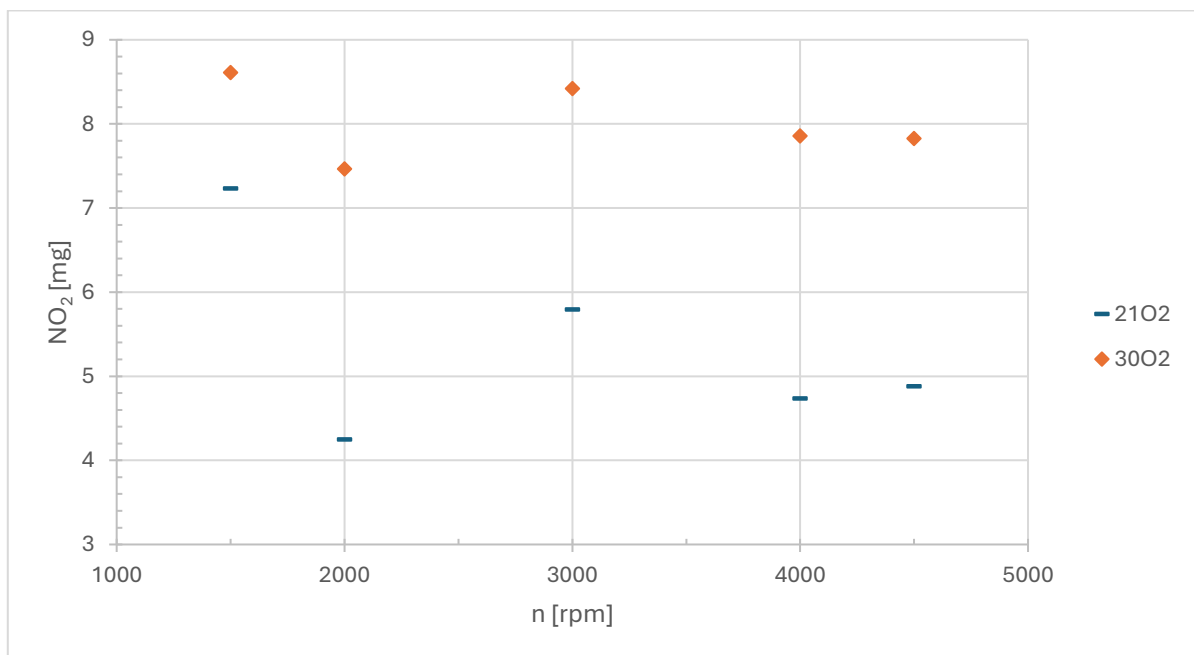


Figure 58 - NO₂ concentrations at exhaust valve opening.

As can be seen, NO and NO₂ concentration increases with higher oxygen concentration, and except for 1500 rpm, most values double when the oxygen rises from 21 to 30 %. The formation of these compounds is due to the high temperatures reached during the

combustion process, as well as the angular speed. It is proven that NO_x increases with the increase in load due to higher fuel consumption (Amirshekari 2012).

UHC and VOC concentrations at exhaust valve opening are approximately zero, since all the fuel was consumed.

4.2.3 Effect on Power, Combustion Efficiency and Thermal Efficiency

Finally, the effect of angular speed on power, combustion efficiency, and thermal efficiency was evaluated, as these parameters are critical indicators of engine performance.

Table 25 summarizes all the referred parameters, and it is important to note that, as was mentioned at the beginning of this chapter, the fuel mass was adapted for each simulated angular speed.

Table 25 – Power, combustion and thermal efficiency at different angular velocities and 21 and 30 % oxygen.

RPM	Power (kW)		Combustion Efficiency (%)		Thermal Efficiency (%)	
	21 % O_2	30 % O_2	21 % O_2	30 % O_2	21 % O_2	30 % O_2
1500	11.5	11.4	100	100	45.4	45.3
2000	17.6	17.3	100	100	42.8	42.3
3000	24.5	24.4	100	100	44.7	44.5
4000	32.6	32.6	99.7	100	43.8	43.8
4500	36.1	36.4	99.1	100	43.7	44.1

According to the results presented in Table 25, power, combustion efficiency, and thermal efficiency did not show significant changes across all angular speeds.

Regarding combustion efficiency, it is possible to observe that, for all oxygen concentrations and angular speeds, the combustion was successful, but this parameter is not enough to understand if all reactants were fully consumed during combustion. Therefore, the amounts of remaining oxygen and fuel at the end of combustion were analysed. Table x summarizes the results obtained; however, since the amounts of fuel species (iC_8H_{18} , $\text{C}_2\text{H}_5\text{OH}$, and CH_3OH) are all approximately zero, they are not represented in the table.

Table 26 - Oxygen and quantities at the end of combustion cycles.

RPM	Intake Oxygen Concentration (%)	Remaining Oxygen Mass (mg)
1500	21	44.19
	30	60.88
2000	21	4.74
	30	20.99
3000	21	19.77
	30	37.42
4000	21	9.64
	30	25.53
4500	21	13.97
	30	29.23

The data presented in Table 26 reveal that oxygen remained unconsumed in all conditions. This indicates that the engine thermal efficiency and power output were not yet optimized. To overcome this, the amount of fuel injected should be adjusted to consume all the supplied oxygen, thus increasing engine performance. Consequently, a 30 % oxygen enrichment appears to be a promising strategy for enhancing engine operation.

4.3 Influence of Oxygen Concentration and Intake Pressure and Temperature variation on Engine Performance

The first step in this analysis was to modify the intake temperature and pressure. For this, several assumptions were made:

- A four-stroke engine was used in a medium-sized UAV.
- Considering that the operational altitude range of a medium UAV is 3 to 9 km, it was assumed that the UAV would operate at 6 km (the midpoint).

- Based on this altitude and using ISO 2533 (Figure 59), the intake temperature and pressure were determined.

ISO 2533 is a standard that describes the characteristics of the standard atmosphere, calculated as a function of geometric and geopotential altitudes from 2000 to 50000 km. Figure 58 was extracted from the tables provided in this document and is presented in terms of geometric altitude.

H, m	h, m	T, K	$t, ^\circ C$	$p, mbar$	$p, mm\ Hg$	$\rho, kg \cdot m^{-3}$	$g, m \cdot s^{-2}$
6000	5994	249,187	-23,963	4,72176 +2	3,54161 +2	6,60111 -1	9,7882
6050	6044	248,862	-24,288	4,68955	3,51745	6,56462	9,7880
6100	6094	248,538	-24,612	4,65751	3,49342	6,52828	9,7879
6150	6144	248,214	-24,936	4,62565	3,46952	6,49210	9,7877
6200	6194	247,890	-25,261	4,59396	3,44576	6,45607	9,7875
6250	6244	247,565	-25,585	4,56246	3,42212	6,42019	9,7874
6300	6294	247,241	-25,909	4,53113	3,39863	6,38447	9,7872
6350	6344	246,916	-26,234	4,49997	3,37526	6,34890	9,7871
6400	6394	246,592	-26,558	4,46899	3,35202	6,31348	9,7869
6450	6443	246,267	-26,883	4,43818	3,32891	6,27821	9,7868
6500	6493	245,943	-27,207	4,40755 +2	3,30593 +2	6,24310 -1	9,7866
6550	6543	245,619	-27,531	4,37708	3,28308	6,20813	9,7865
6600	6593	245,294	-27,856	4,34679	3,26036	6,17332	9,7863
6650	6643	244,970	-28,180	4,31667	3,23777	6,13866	9,7862
6700	6693	244,646	-28,504	4,28672	3,21530	6,10415	9,7860
6750	6743	244,322	-28,828	4,25693	3,19296	6,06978	9,7859
6800	6793	243,997	-29,153	4,22732	3,17075	6,03557	9,7857
6850	6843	243,673	-29,477	4,19787	3,14866	6,00150	9,7855
6900	6893	243,349	-29,801	4,16859	3,12670	5,96758	9,7854
6950	6942	243,024	-30,126	4,13947	3,10486	5,93381	9,7852

Figure 59 – Excerpt from ISO 2533, used to estimate temperature and pressure at an altitude of 6 km (Standardization 1975).

In the Initial Condition menu, in the intake option (Figure 60), the first step was to modify the intake air composition. Based on the analysis presented, in chapter 4.1, the oxygen concentrations considered in the simulations were 21 %, 25 %, 30 % and 35 %. The intake air temperature and pressure were adjusted according to the values highlighted in Figure 58.

It should be noted that at an altitude of 6000 m, the pressure is around 0.47 bar, but considering that the engine has turbochargers, which increase the intake pressure by around 1.5 bar, the pressure considered for the simulations was the sum of these two values, obtaining a pressure of 1.97 bar.

intake

[Initial Conditions](#)

Composition Constant

Composition Air21O2

Temperature Constant

Temperature 249.2 K

Pressure Constant

Pressure 1.97 bar

Figure 60 - Initial Conditions - intake setup menu.

Subsequent simulations were conducted at 4000 rpm, and the results are presented below. The analysis followed the same procedures described in Sections 4.1 and 4.2. For that for better understanding of the effect of altitude on the engine, a comparison between the values obtained in section 4.1 at 313.0 K ($\approx 40^\circ\text{C}$) and 2.54 bar, and values obtained in this section at 249.2 K ($\approx -24^\circ\text{C}$) and 1.97 bar was made.

4.3.1 Effect on Pressure and Temperature

The first study conducted to understand the effect of altitude on engine performance and efficiency consisted of evaluating how pressure and temperature evolve with variations in intake pressure and temperature and air composition.

Pressure Comparison

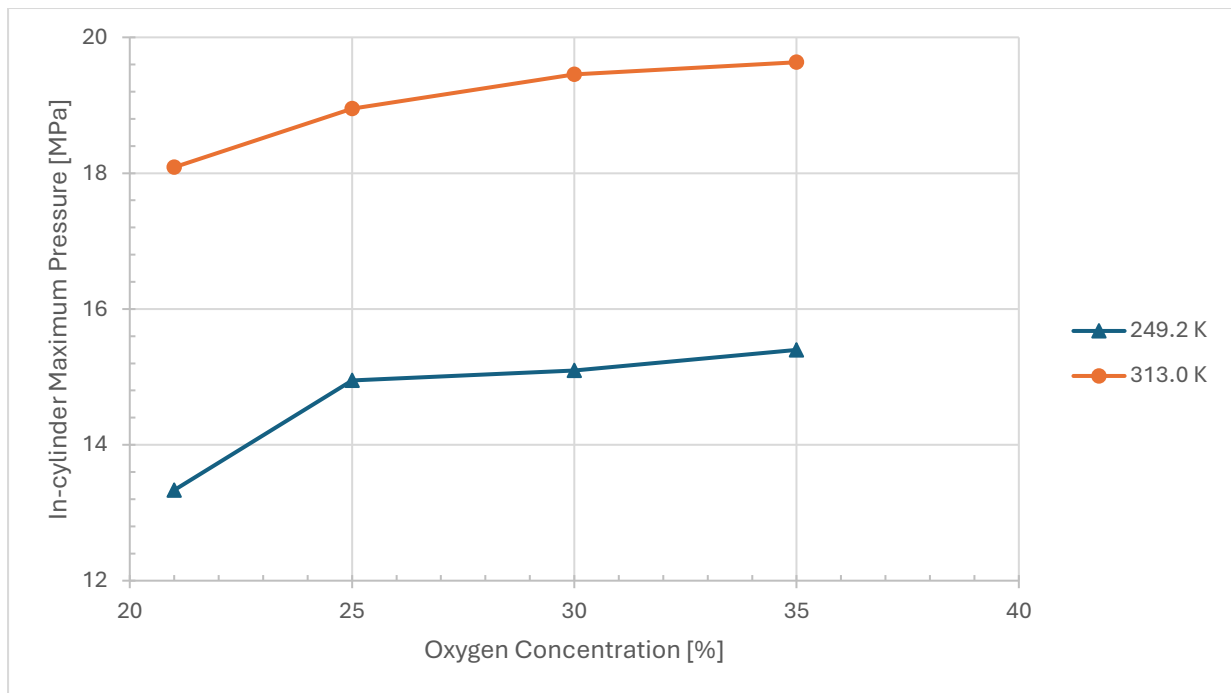


Figure 61 - In-cylinder maximum pressures at 313.0 K and 249.2 K for 21 to 35 % O₂.

Observing Figure 61 is it possible to observe that the pressure presents two distinct dynamics. Firstly, the increase in O₂ concentration from 21 to 35 % accelerates combustion, leading to an increase in peak pressure for both intake conditions. Secondly, it is observed that the operating condition at 313.0 K reaches substantially higher maximum pressures ($\approx + 4.5$ MPa) compared to the condition at 249.2 K. This phenomenon is associated with the intake pressure. The higher intake pressure establishes a significantly higher value at the beginning of the compression stroke, which leads to the high peak pressures observed, regardless of oxygen concentration.

Temperature Comparison

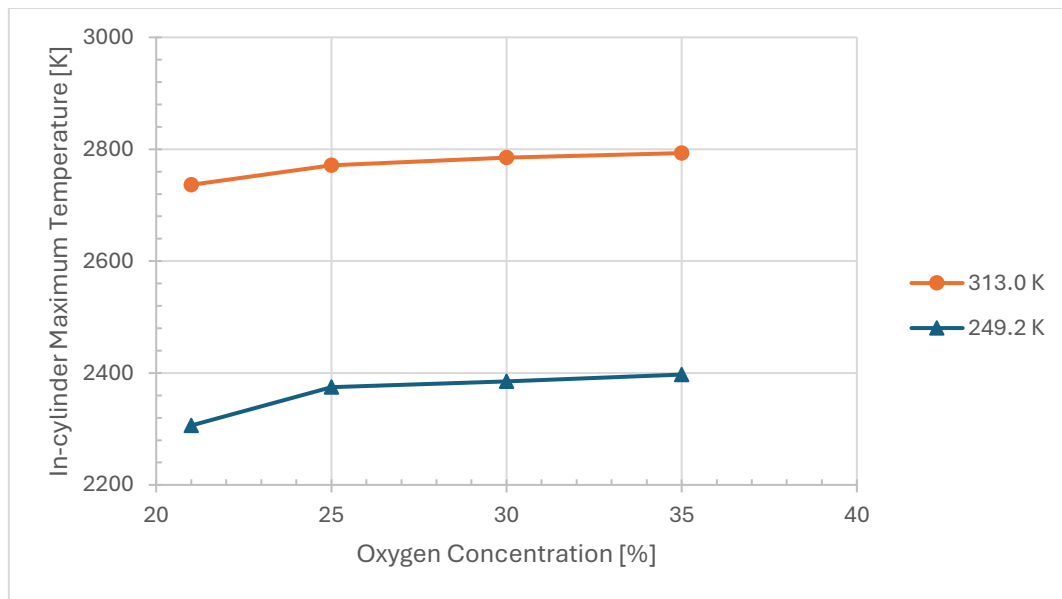


Figure 62 – In-cylinder maximum temperatures at 313.0 K and 249.2 K for 21 to 35 % O₂.

In Figure 62, the trend of the maximum temperature closely follows that of the peak pressure. In this case, reducing the concentration of N₂ in the intake air, which naturally limits the peak temperatures, the enrichment in O₂ increases the flame temperature. Moreover, operating with an intake condition of 313.0 K and 2.54 bar raises the peak temperature beyond 2700 K (approximately 400 K above the baseline).

4.3.2 Effect on pollutant emissions

A similar studied to that previously conducted was performed to understand and evaluate the effect on pollutant emissions, such as CO, CO₂, NO, NO₂, UHCs, and VOCs.

For a better understanding of the evolution, only the values before 650° were considered, due to the fact that they are approximately zero from 328° to 650°.

Figure 63 presents the evolution of CO emissions with the crank angle.

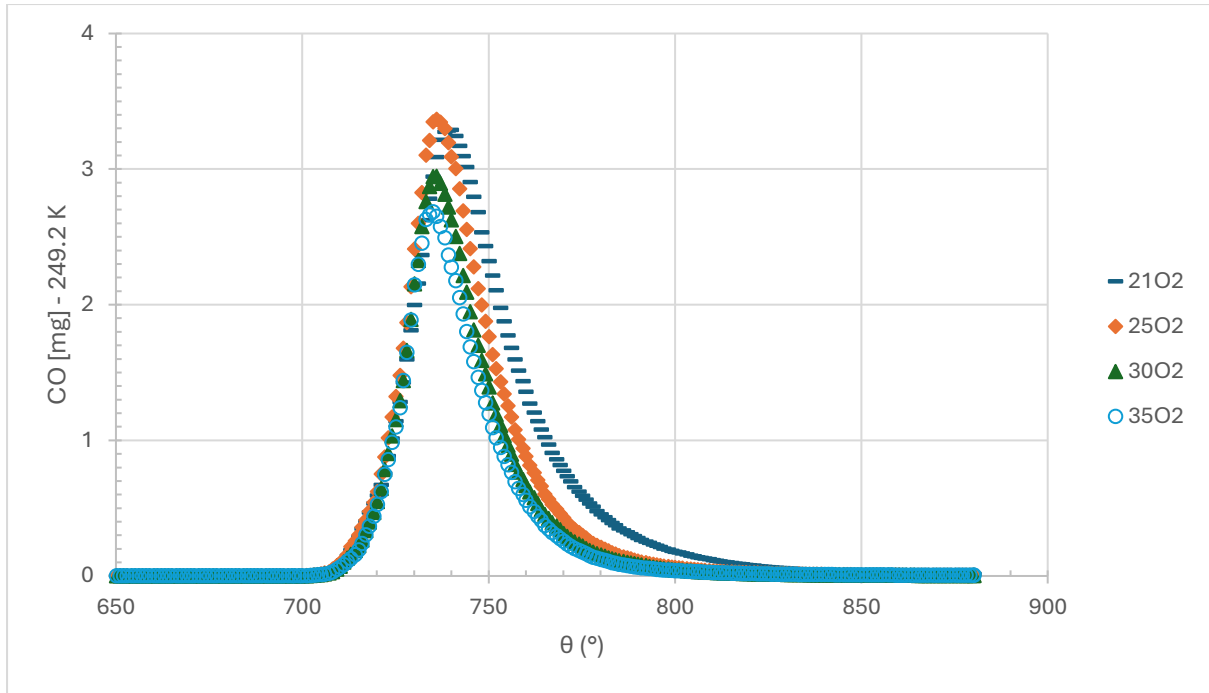


Figure 63 - Variation of carbon monoxide (CO) emissions with crank angle for different oxygen concentrations at 249.2 K.

According to Figure 63, it is possible to observe that between 21 and 25 % oxygen, the concentration of CO increased, but if the oxygen concentration increases, the CO concentration decreases. The increase is due to the fact that, between 21 and 25 %, the oxygen concentration enhances the formation of CO as an intermediate combustion product. Above these concentrations, the thermal effect and the oxygen enrichment enhance complete oxidation and, consequently, the decrease in CO concentration.

Figure 64 shows the CO concentration evolution at 313.0 K.

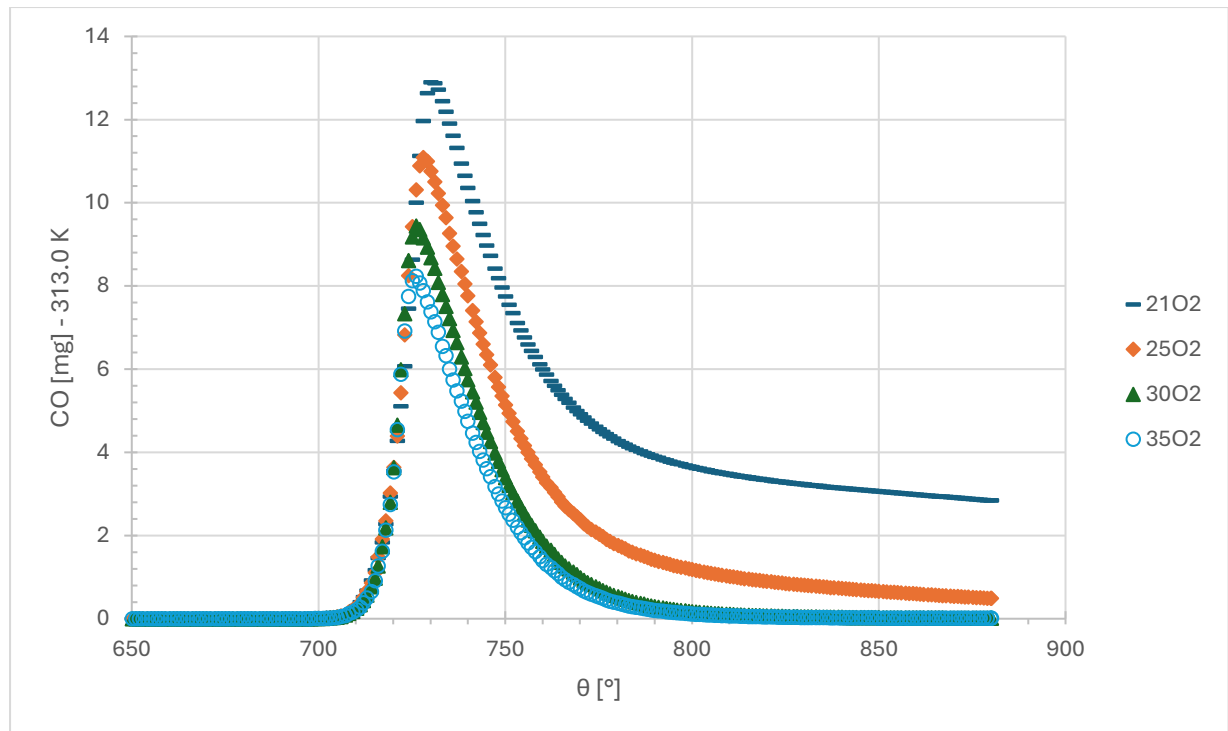


Figure 64 - Variation of carbon monoxide (CO) emissions with crank angle for different oxygen concentrations at 313.0 K.

With Figures 63 and 64 it is possible to compare the CO concentration evolution for 249.2 K and 313.0 K, respectively. Observing both figures, the decrease in intake temperature from 313.0 K to 249.2 K impacts CO formation, with peak decreasing from approximately 13 mg to 3.5 mg. At 313.0 K, CO profile exhibit higher peaks and more pronounced persistence after 750° crank angle, particularly for lower oxygen concentration of 21 %.

To understand the effects on the atmosphere, it is important to observe the CO concentration values when the exhaust valves open, at 249.2 K and compare them with conventional simulations taken at 313.0 K, where only the variation oxygen concentration was studied (Figure 65).

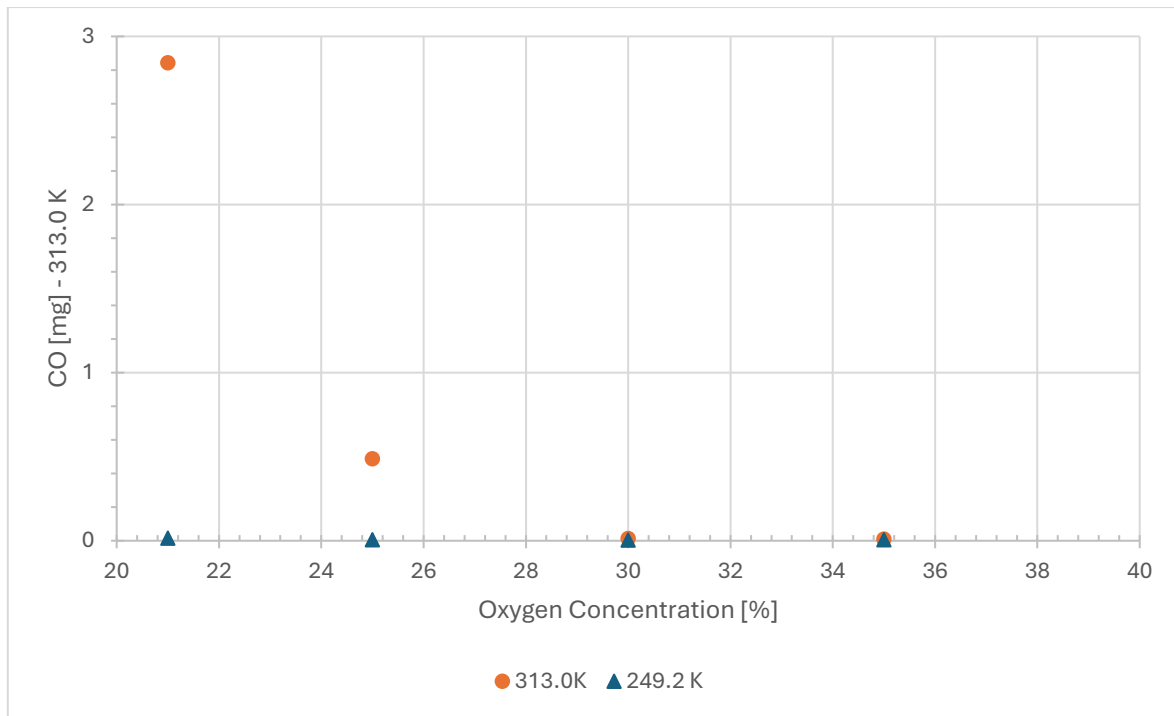


Figure 65 - CO concentrations when the exhaust valve opens at 249.2 K and 313.0 K.

Figure 65 shows that enriching the mixture from 21 to 35 % O₂ results in a drastic reduction of CO emissions. As previously explained, the greater availability of oxygen radicals and the higher combustion temperatures accelerate the oxidation of CO to CO₂. Furthermore, the difference in CO mass between 313.0 K and 249.2 K, is approximately two hundred times greater for 21 % O₂, and this difference is determined by the difference in intake pressure.

Figure 66 presents the evolution of CO₂ emissions, and it is possible to observe that the emissions increase as the combustion cycle progresses and then stabilize. As expected, CO₂ concentrations increase with higher oxygen concentrations, due to chemical dissociation.

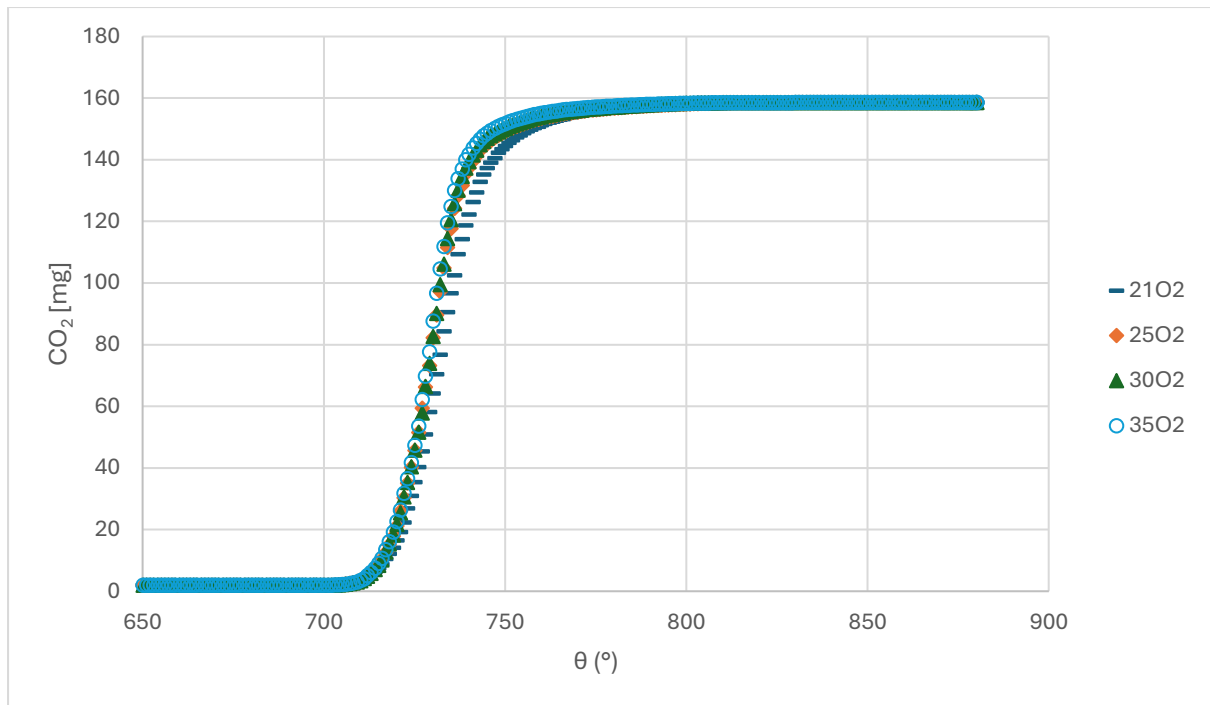


Figure 66 - Variation of carbon dioxide (CO_2) emissions with crank angle for different oxygen concentrations at 249.2 K.

Figure 67 shows the CO_2 concentration evolution at 313.0 K.

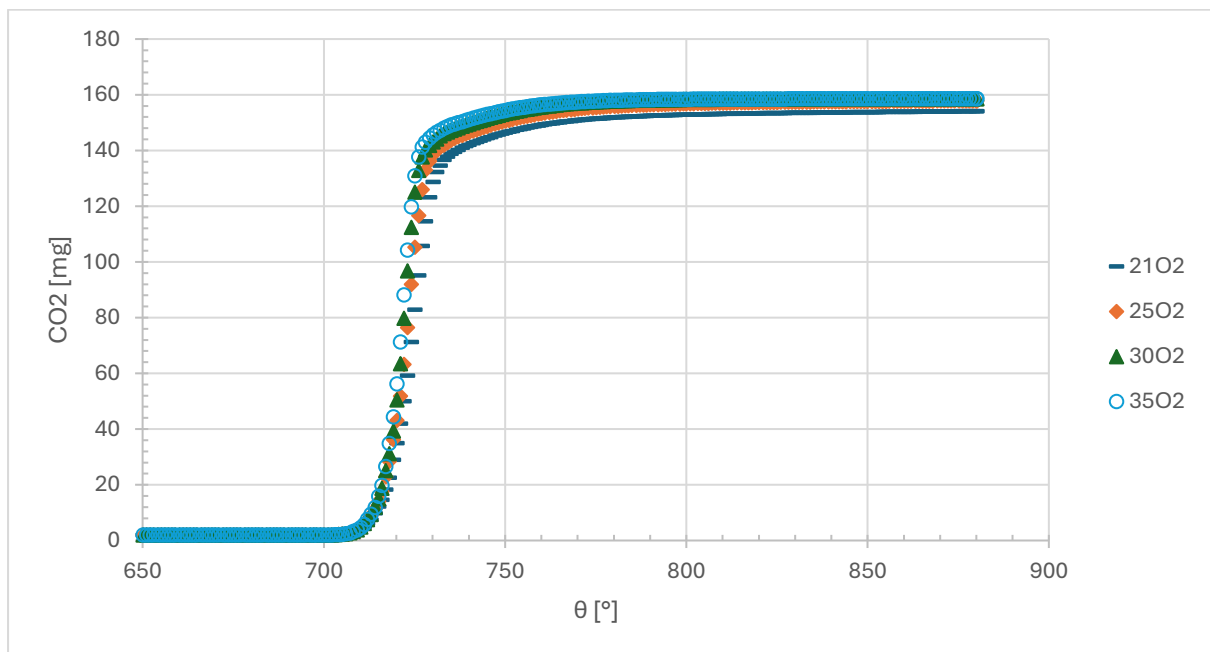


Figure 67 - Variation of CO_2 emissions with crank angle for different oxygen concentrations at 313.0 K.

Observing Figures 66 and 67, it is possible to compare the CO₂ concentration evolution for 249.2 K and 313.0 K, respectively. Comparing both figures, it is possible to observe that between 710° and 750°, the CO₂ mass sharply increases, eventually reaching a stable plateau of approximately 160 mg.

Figure 68 presents a comparison of final CO₂ emissions for two of the cases studied.

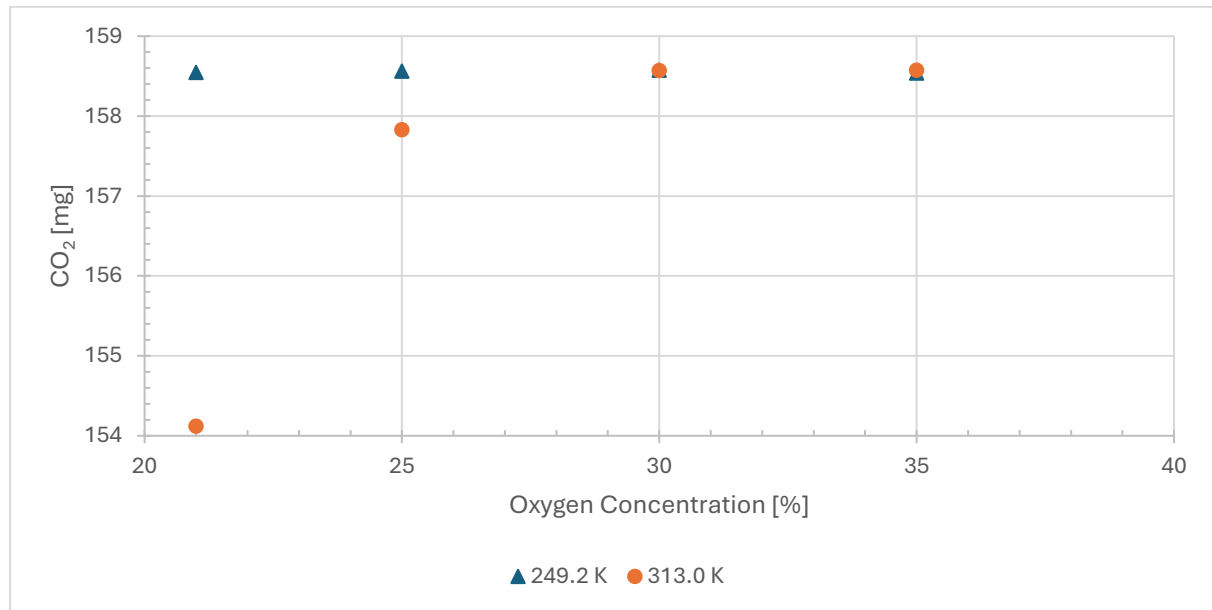


Figure 68 - CO₂ concentrations when the exhaust valve opens at 249.2 K and 313.0 K.

Figure 68 confirms the previous analysis of carbon monoxide emissions. Both intake conditions converge to a maximum value of approximately 158.5 mg for oxygen concentrations above 30 %. The lower CO₂ levels observed at for 21 % O₂ are related to a possible incomplete combustion, which is consistent with the higher CO peak reported previously. Gradual oxygen enrichment mitigates this deficit. The flat trend for 249.2 K curve across all O₂ concentrations demonstrates that, under those thermodynamic conditions, the intake mixture with 21 % O₂ ensured a nearly complete carbon oxidation. When intake air pressure and temperature are changed, the CO₂ mass remains almost constant, around 158.5 mg.

Figures 69 and 70 present NO and NO₂ emissions, which present a similar trend to that observed in previous studies.

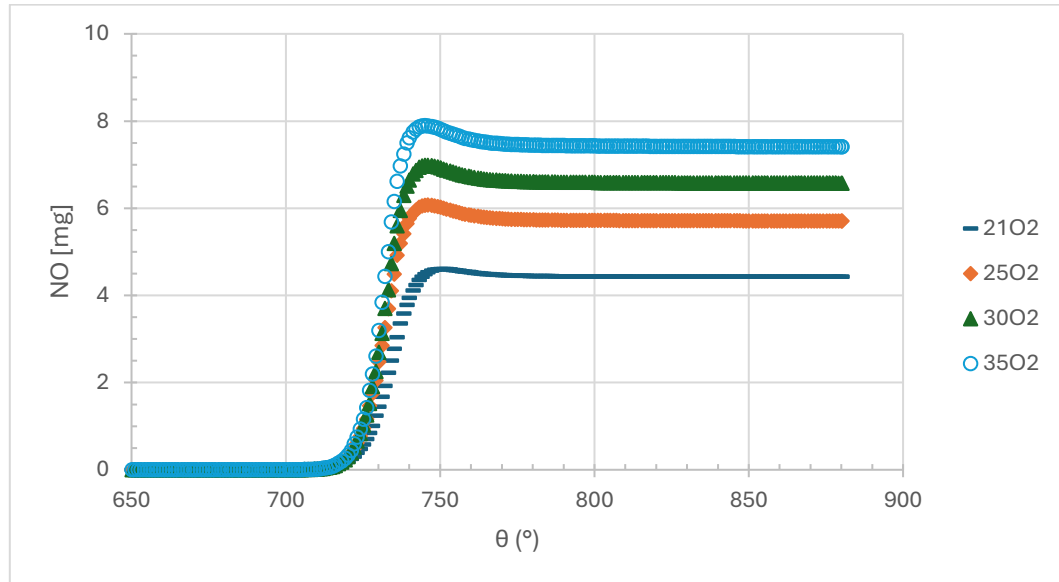


Figure 69 - Variation of nitrogen monoxide (NO) emissions with crank angle for different oxygen concentrations, at 249.2 K.

In NO evolution with the crank angle (Figure 69), it is possible to observe that the concentration of NO increases with the concentration of oxygen.

Figure 70 presents the NO evolution for 313.0 K.

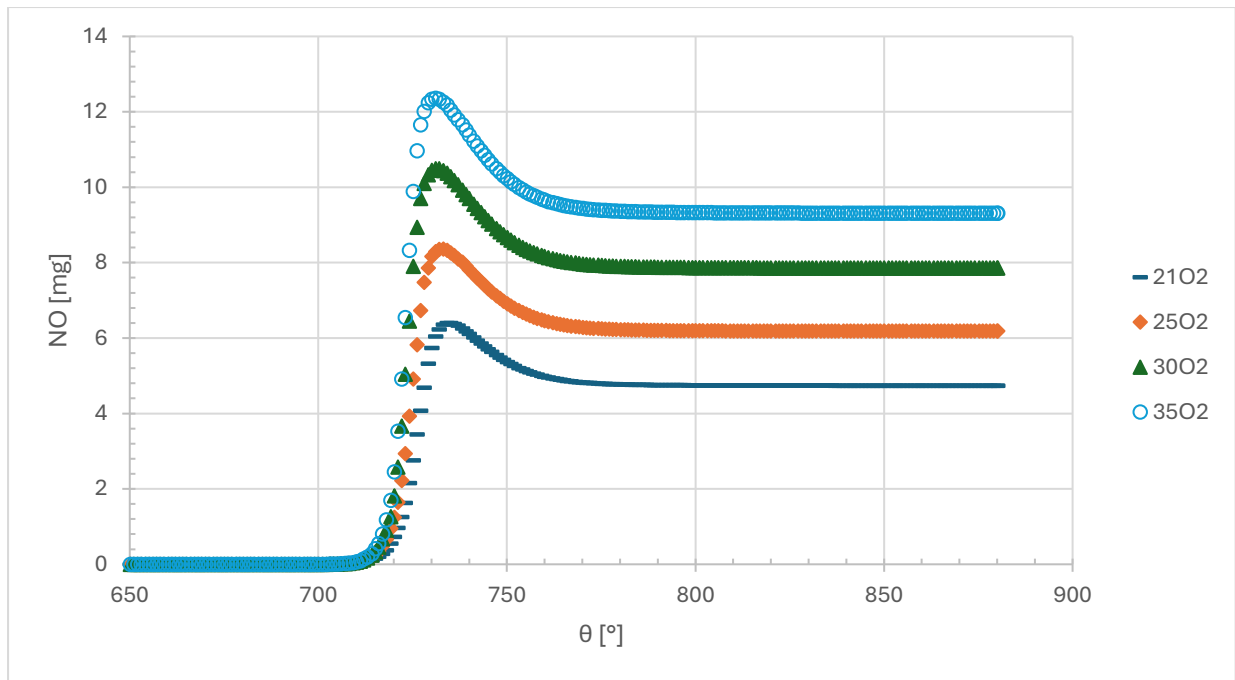


Figure 70 - Variation of NO emissions with crank angle for different oxygen concentrations, at 313.0 K.

Comparing NO concentration evolution, from Figures 68 and 69, it is possible to observe that at 249.2 K, NO mass follows a steady growth trend, stabilizing at a maximum of approximately 7.5 mg for 35 % O₂ concentration. However, for 313.0 K, the emission magnitude shifts upward, with 35 % O₂ curve reaching a peak of approximately 12.5 mg. This traduces in a 66 % increase from 249.2 K to 313.0 K.

However, the environmental effects are studied based on the values registered when the exhaust valves open (Figure 71).

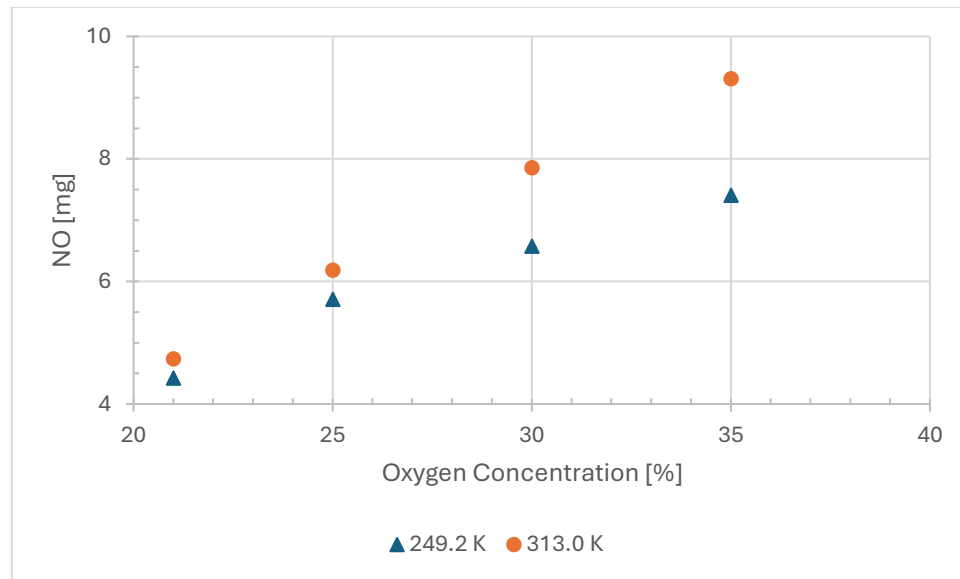


Figure 71 - NO concentrations when the exhaust valve opens at 249.2 K and 313.0 K.

The evolution of NO shown in Figure 72 demonstrates a strong dependence on oxygen concentration, temperature, and pressure. An increasing trend was observed for both operating conditions as the mixture is enriched with O_2 . This behaviour is explained by the formation of NO with the temperature increase. Furthermore, the operating condition at 313.0 K and 2.54 bar records higher NO emission values than the condition at 249.2 K. This difference can be explained by the higher maximum in-cylinder temperatures achieved at 313.0 K, influenced by the initial intake conditions.

Observing NO_2 emissions, there is an increasing trend, which was expected since the combustion reaches high temperature values.

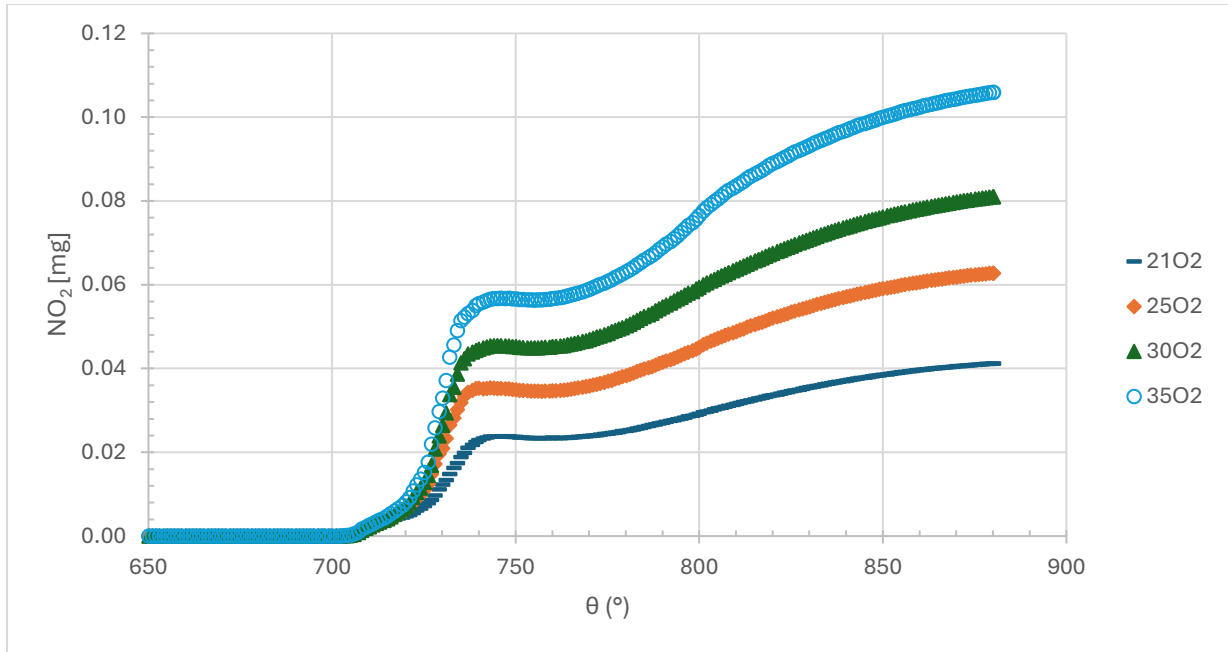


Figure 72 - Variation of NO_2 emissions with crank angle for different oxygen concentrations, at 249.2 K.

Figure 73 represents NO_2 concentrations with the crank angle at 313.0 K.

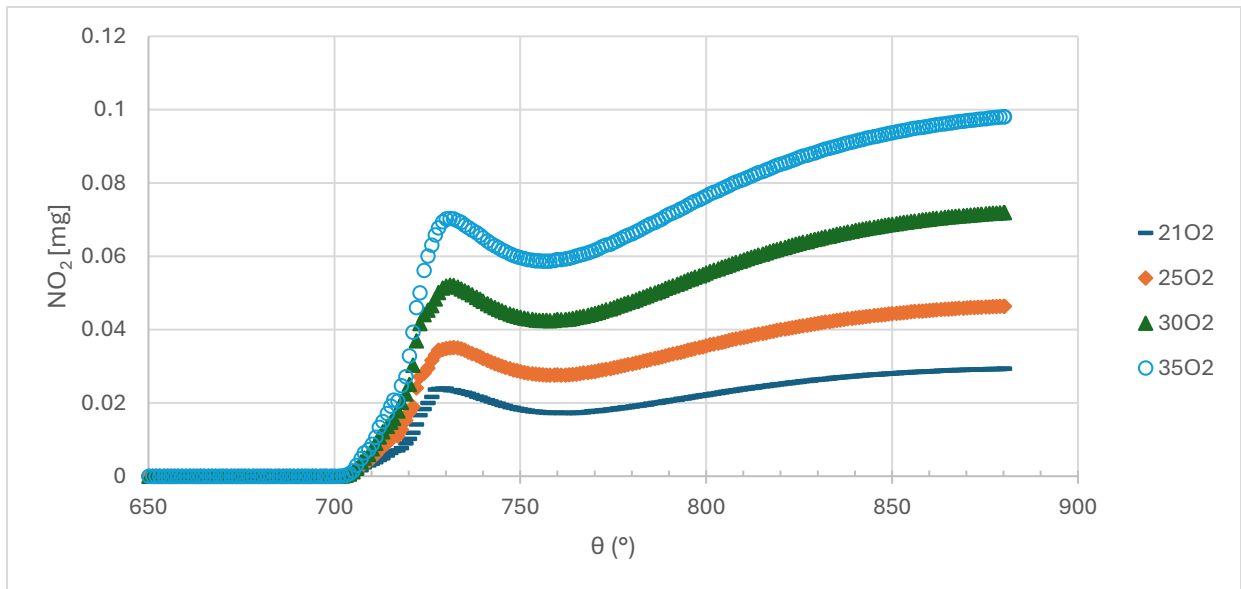


Figure 73 - Variation of nitrogen dioxide (NO_2) emissions with crank angle for different oxygen concentrations, at 313.0 K.

Comparing both Figures 72 and 73, reveals that NO_2 mass is significantly lower than NO mass, for 249.2 K and 313.0 K for all oxygen concentrations.

The values registered for the variation in intake temperature and pressure were very similar to the values registered for the variation in oxygen concentration, and the increase is approximately 0.01 mg for each 5 % increase in oxygen (Figure 74).

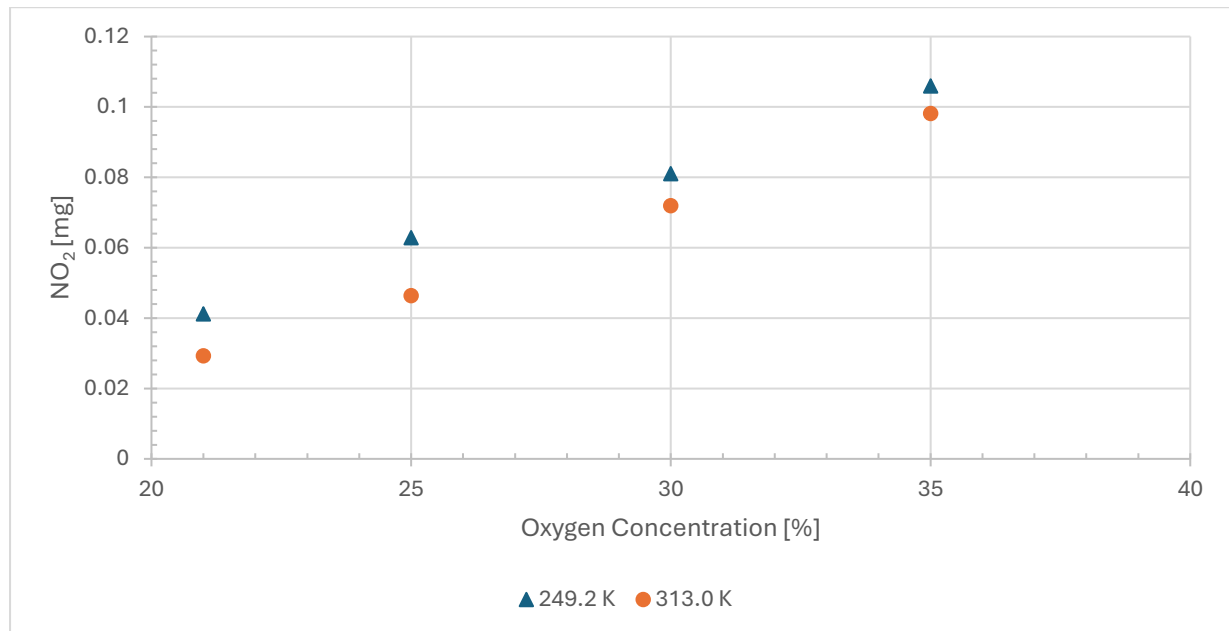


Figure 74 - NO₂ concentrations when the exhaust valve opens at 249.2 K and 313.0 K.

Figure 74 shows that NO₂ represents a minor fraction of total NO_x, with NO being the dominant species. NO₂ presents an increasing trend with oxygen enrichment, observed for both conditions, driven by the availability of O₂ radicals to oxidize the previously formed NO. However, an inversion is observed: the 249.2 K condition emits more NO₂ than the 313.0 K condition. This behaviour is attributed to the higher thermal levels reached under the 313.0 K condition, which promote thermal dissociation of NO₂ back to NO.

Finally, Figures 75 and 76 show the evolution of UHCs and VOCs. As it was observed before, these emissions exhibit a plateau, corresponding to the fuel injection, in this case, 50.85 mg of fuel. For both pollutants, concentrations approach zero by the end of combustion.

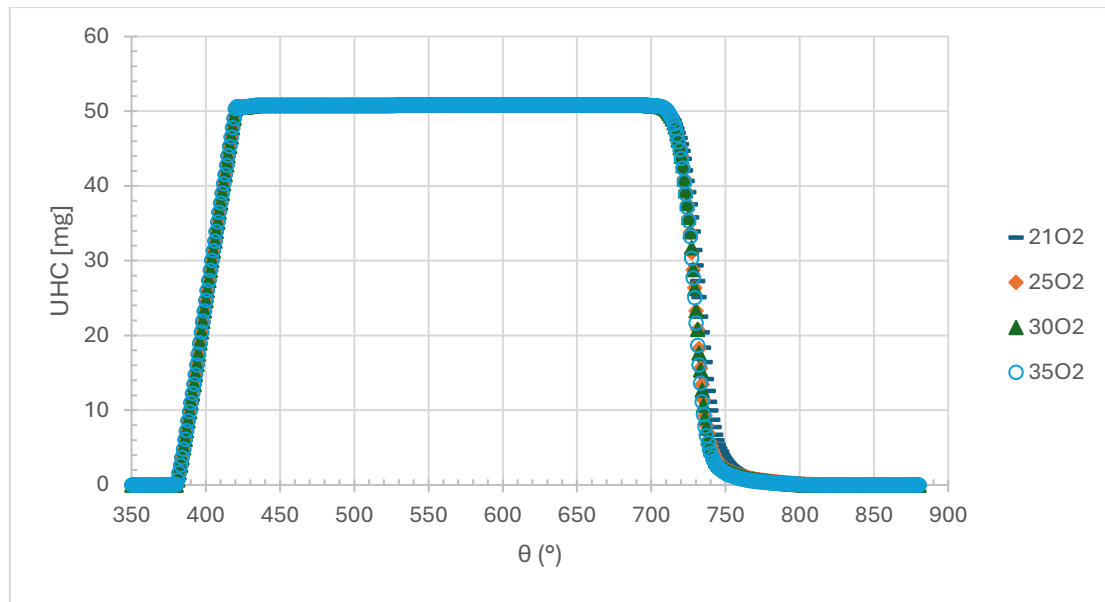


Figure 75 - Variation of unburnt hydrocarbons (UHCs) emissions with crank angle for different oxygen concentrations at 249.2 K

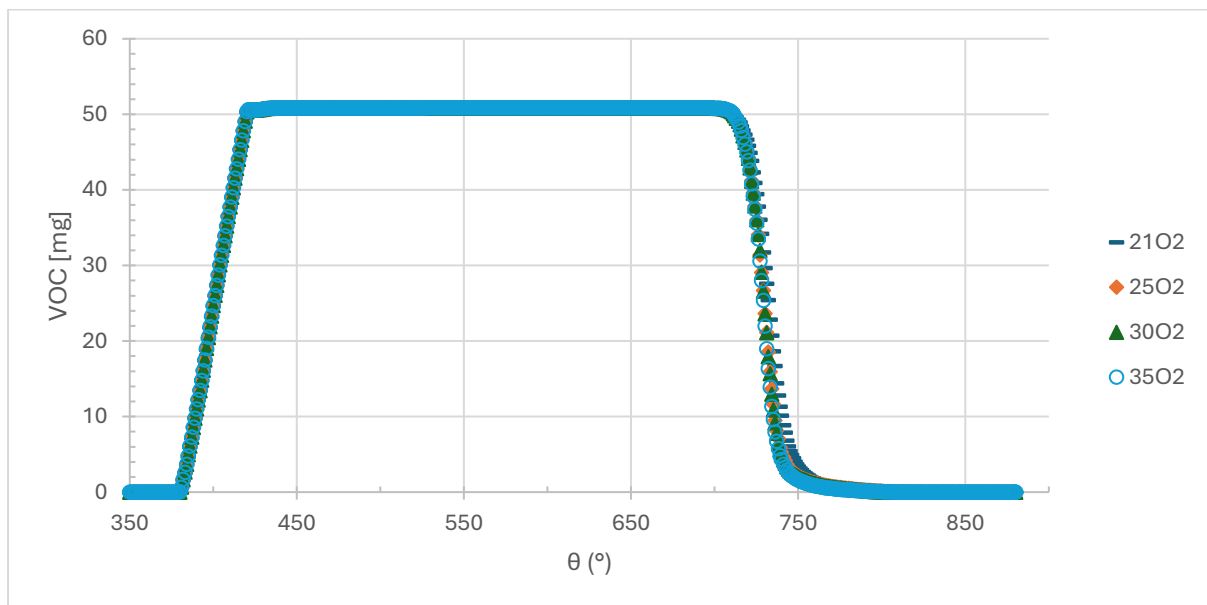


Figure 76 - Variation of volatile organic compounds (VOCs) emissions with crank angle for different oxygen concentrations at 249.2 K.

4.3.3 Effect on Power, Combustion Efficiency and Thermal Efficiency

Finally, a study of some engine performance parameters was developed. Table 27 presents the values obtained for engine power, combustion, and thermal efficiency.

Table 27 - Power, combustion and thermal efficiency for all simulated oxygen concentrations.

O₂ (%)	N₂ (%)	Power (kW)	Combustion Efficiency (%)	Thermal Efficiency (%)
21 %	79 %	33.1	100	44.4
25 %	75 %	33.5	100	45.0
30 %	70 %	33.5	100	45.0
35 %	65 %	33.6	100	45.1

Observing the performance parameters in Table 27, as the oxygen concentration increases, the power also increases, but with small differences; the same occurs with thermal efficiency. For combustion efficiency, the combustion is always successful (=100%), although it is relevant to observe if all the oxygen and fuel were completely consumed in the combustion process (Table 28). The values of the fuel species are not presented in Table 28 since they are approximately zero for all simulated oxygen concentrations.

Table 28 - Remaining oxygen concentration at the end of combustion.

O₂ [%]	O₂ [mg]
21	35.09
25	42.76
30	53.06
35	63.49

The remaining amounts of oxygen increase by around 10 mg, for each 5 % of oxygen added to the intake air composition. As previously concluded, to overcome this problem, it is necessary to increase the fuel mass, to guarantee that all reactants are consumed and consequently, achieve higher performance values.

Although the main purpose of this section was to understand the effects of altitude on an engine, as could be observed, altitude does not affect engine performance, and in some cases, for example, in power, there is a slight increase in the values.

4.4 Fuel Mass Variation

The previous analysis (Sections 4.1 and 4.2) revealed that a significant amount of unburned oxygen remained at the end of the combustion cycle. To overcome this excess oxygen, the 30 % O₂ concentration scenario from Section 4.2 was selected to investigate the effects of an increase in injected fuel mass. The baseline parameters for this study are detailed in Table 29.

Table 29 - Baseline condition.

O₂ concentration	30 %
Angular Speed	4000 rpm
Intake Temperature	313.0 K
Intake Pressure	2.54 bar
Fuel Mass	50.85 mg

Based on this reference condition, subsequent simulations were performed by incrementally increasing the baseline fuel mass (50.85 mg) in 5 % steps, up to a maximum of 20 %. The fuel mass associated with each of these increments is detailed in Table 30.

Table 30 - Fuel masses used for previous simulations.

Fuel Increment (%)	0	5	10	15	20
Fuel mass (mg)	50.85	53.39	55.94	58.48	61.02

4.4.1 Effect on Temperature, Pressure and power

To evaluate the impact of fuel mass variation on engine performance, its effect on temperature, pressure, and power was investigated. Throughout this study, the baseline condition (50.85 mg) served as the standard reference for comparison.

Temperature

Figure 77 shows the evolution of the maximum in-cylinder temperature with fuel mass increment.

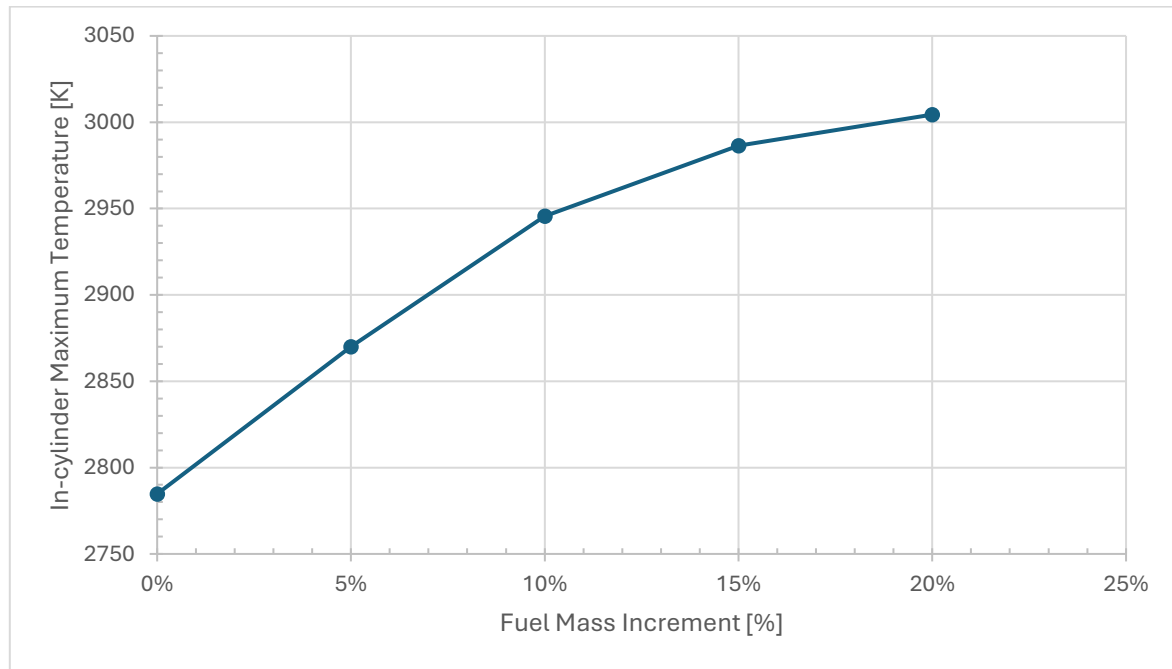


Figure 77 - In-cylinder maximum temperature with fuel mass increment.

Using an O_2 concentration of 30 % as baseline (0 % fuel mass increment), an upward trend was observed, with the maximum temperature rising from approximately 2785 K in the baseline setup to over 3000 K with a 20 % fuel mass increment. This thermal effect reflects the conversion of chemical energy into heat: by injecting more fuel into an oxygen-enriched environment, the unburned O_2 is effectively used, maximizing the heat release from combustion. However, the rate of temperature increase gradually decelerates as the increment approaches 20 %. This indicates that the mixture is closer to the stoichiometric ratio.

Pressure

Figure 78 shows the maximum in-cylinder pressure with the increase in fuel mass.

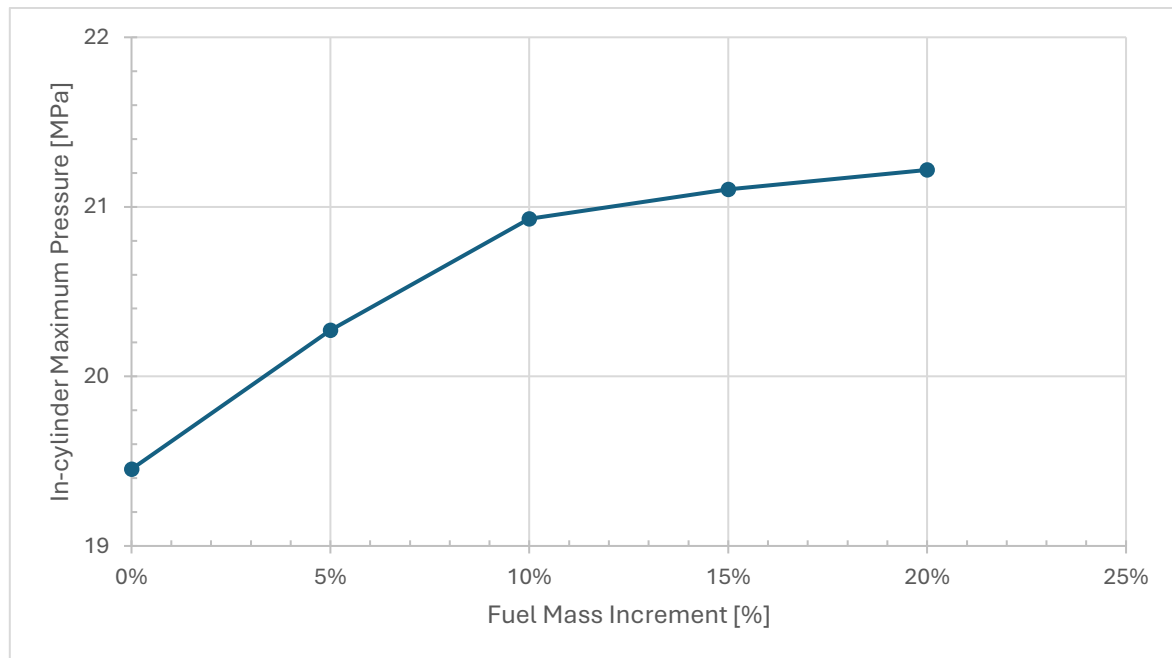


Figure 78 - In-cylinder maximum temperature with fuel mass increment.

Observing the evolution of maximum pressure, a similar behaviour was seen when compared to the evolution of temperature. A significant increase in maximum pressure is evident during the initial stages of fuel addition (0 % to 10 %), rising from approximately 19.4 MPa to 20.9 MPa. This increase is a direct consequence of the Ideal Gas Law: increasing the energy released from burning extra fuel mass for a confined volume generates a proportional increase in pressure. However, for increases above 10 %, the curve tends to stabilize. This flattening confirms the reduction of available oxygen, driving the mixture toward stoichiometric limits.

Power, Combustion Efficiency and Thermal Efficiency

Table 31 summarizes the engine performance parameters, such as power, combustion, and thermal efficiency.

Table 31 - Engine's performance parameters with fuel mass increment.

Fuel mass increment (%)	Fuel Mass (mg)	Power (kW)	Combustion Efficiency (%)	Thermal Efficiency (%)
0	50.85	32.6	100	43.8
5	53.39	33.6	100	43.0
10	55.94	34.2	99.6	41.8
15	58.48	34.5	96.0	40.3
20	61.02	34.0	89.5	38.0

Table 31 shows that the power increases progressively to a maximum of 34.5 kW with a 15 % increase, but suffers a penalty (dropping to 34.0 kW) with a 20 % increase. This inflection point is explained by examining the combustion efficiency. Up to a 5 % increase, the ample availability of oxygen ensures complete oxidation (100 %). However, at 20 %, the combustion efficiency drops drastically to 89.5 %, indicating that there is no excess of oxygen and that the mixture has become overly rich (fuel excess). At the same time, a continuous degradation in thermal efficiency was observed across all increments. This decline reflects substantial heat losses through the cylinder walls, driven by extreme temperatures. It can be concluded that the optimal increment lies at 10 %, a point that delivers a substantial power gain while maintaining a near-perfect combustion efficiency. Note that for this point the fuel mass used (55.94 mg) is very similar to the one used in angular velocity simulations, at 2000 rpm, and the maximum torque and power were achieved. Although adding more fuel is not enough to improve performance, it is necessary to modify engine parameters to reach a combustion efficiency near 100 % and a thermal efficiency near 44 %.

4.4.2 Effect on Pollutant Emissions

In this Section, the study will focus exclusively on the evaluation of emissions at the end of the combustion cycle. As observed in previous sections, emission formation trends remain consistent throughout the entire cycle. Therefore, the subsequent analysis will specifically cover the final concentrations of CO, CO₂, NO_x, UHC, and VOC.

Figures 79 and 80, respectively, represent the final concentration of CO and CO₂ emissions.

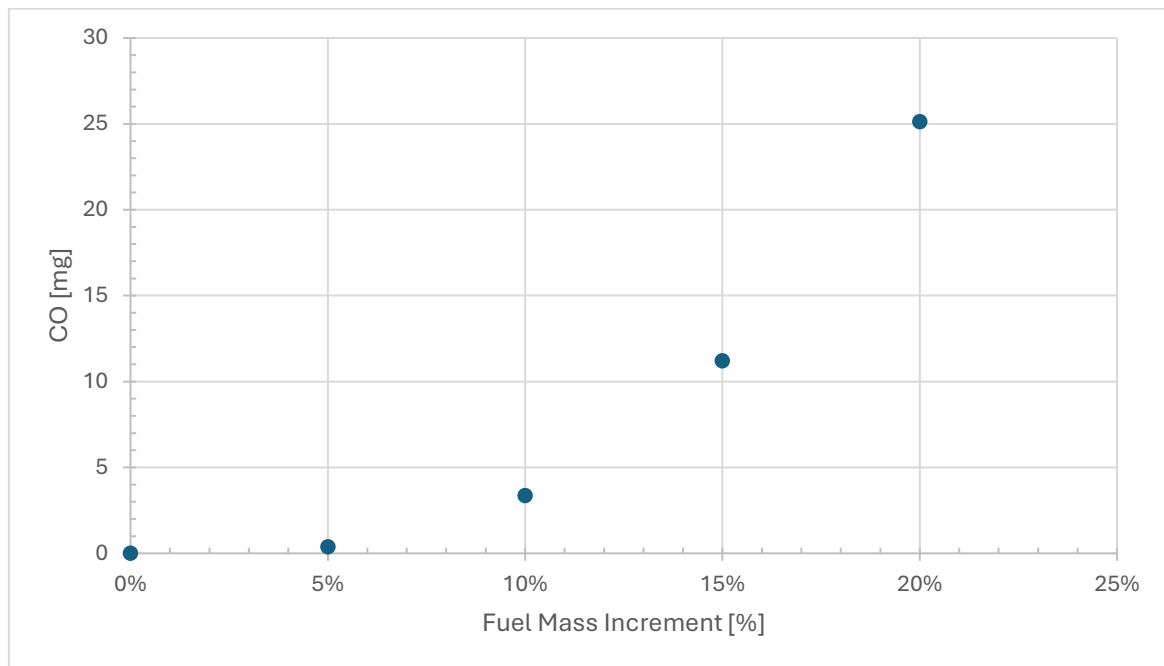


Figure 79 - CO emissions when exhaust valve opens, for all fuel mass increments.

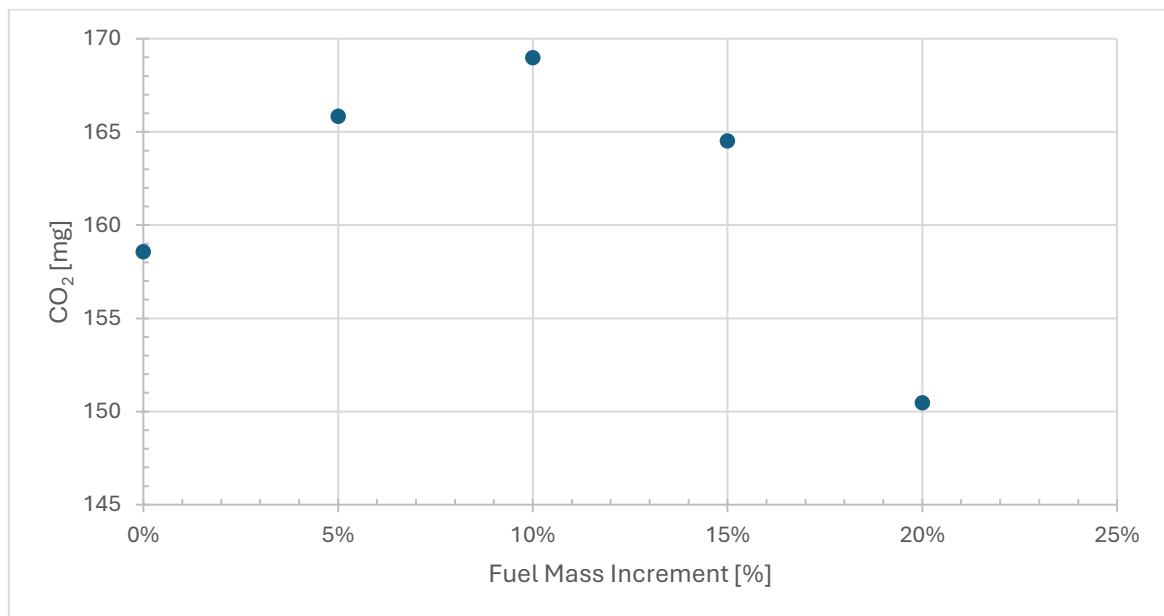


Figure 80 – CO₂ emissions when the exhaust valve opens, for all fuel mass increments.

The simultaneous analysis of CO and CO₂ emissions provides a clear illustration of the chemical kinetics of the combustion process. For fuel mass increments between 0 % and

10 %, the ideal behaviour is observed: CO₂ production increases progressively, reaching a peak of approximately 169 mg, while CO emissions remain negligible. This dynamic ensures that the abundant oxygen in the mixture promotes the complete oxidation of all injected carbon.

However, beyond the 10 % increment threshold, an inversion in this balance occurs. The CO₂ mass decreases, dropping to roughly 150 mg at the 20 % increment. This transition validates the previously documented degradation of combustion efficiency: the mixture reaches its stoichiometric limit and becomes excessively rich.

Figures 81 and 82 show NO_x emissions: NO and NO₂, respectively.

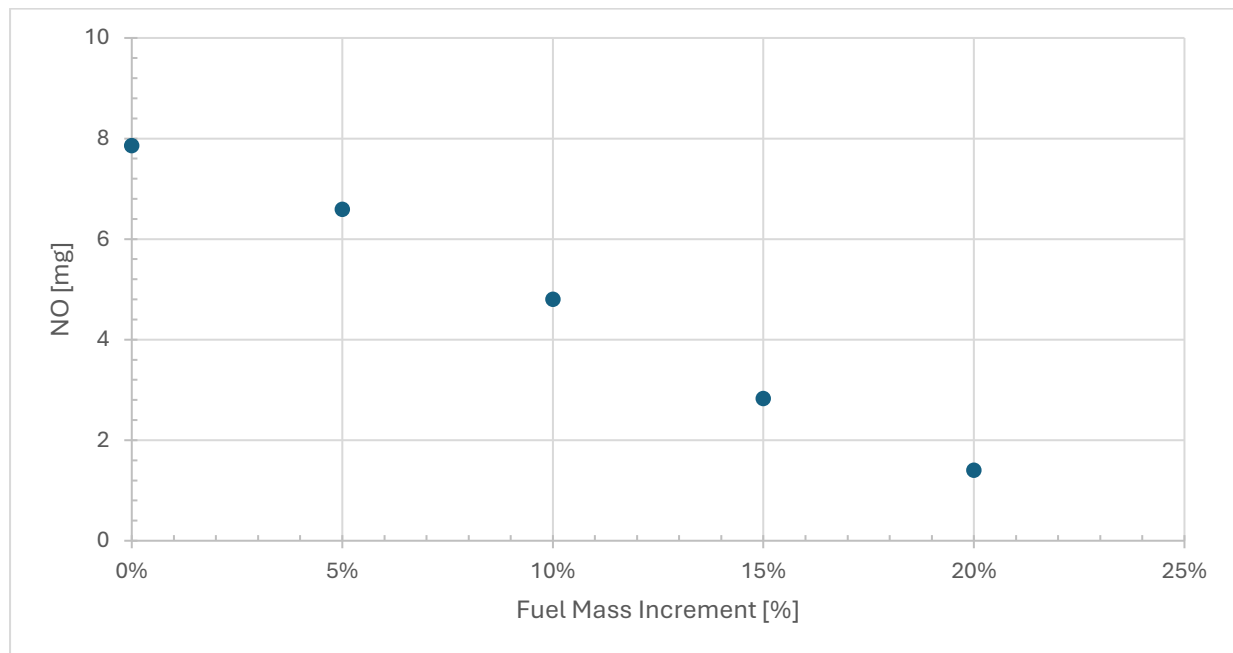


Figure 81 – NO emissions when exhaust valve opens, for all fuel mass increments.

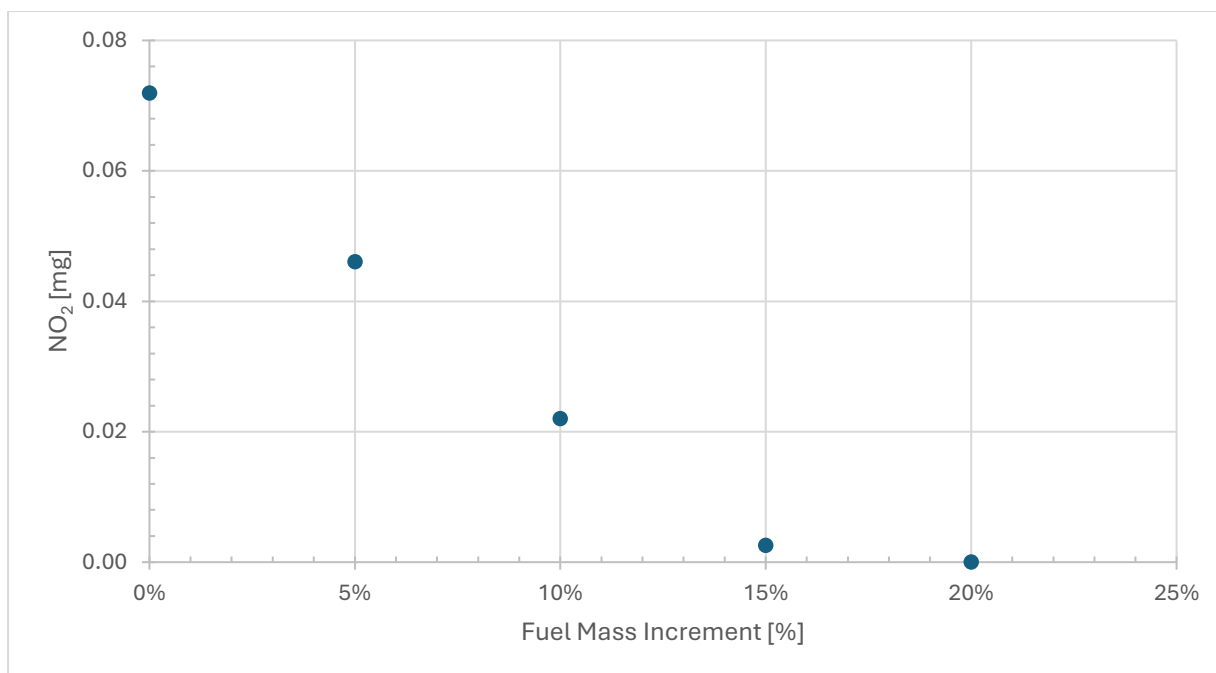


Figure 82 - NO₂ emissions when the exhaust valve opens, for all fuel mass increments.

The evolution of NO and NO₂ emissions, presented in Figures 81 and 82, illustrates a phenomenon driven by oxygen starvation. A drastic and continuous reduction of both pollutants was observed as the fuel mass increment increased, with NO decreasing from approximately 8 mg (at 0 %) to residual values near 1 mg (at 20 %).

This behaviour may seem contradictory, given that the maximum temperature increased with fuel enrichment. However, one of the mechanisms of NO_x formation requires not only elevated temperatures but also high availability of free oxygen. As the fuel mass increases, the initial excess oxygen is quickly consumed by the primary combustion process (carbon oxidation). Approaching to 15 % and 20 % increments, the mixture reaches its stoichiometric limit, becoming rich and reducing the available oxygen. Without the necessary oxygen to oxidize nitrogen, NO_x formation does not occur, despite the high temperatures reached during the combustion. The parallel drop in NO₂ emissions corroborates this dynamic, resulting from the scarcity of its precursor (NO).

Regarding UHC and VOC emissions, as observed in previous sections, these compounds, at the end of the combustion cycle, present residual values near zero milligrams.

4.4.3 Engine Calibration

Given that the fuel mass increases of 15 % and 20 % resulted in low combustion and thermal efficiencies, further simulations were conducted to improve these parameters. The objective was to investigate whether adjusting specific engine calibration parameters could mitigate the efficiency losses and provide performance.

So, some changes were made to the injection and ignition times and durations to improve engine performance for 15 % and 20 % increases. The previous and new injection and ignition values changed in the simulation are summarized in Table 32.

Table 32 – Comparison of calibration parameters between baseline (Condition I) and modified setup (Condition II) for 15 % and 20 % fuel increments.

	Baseline Simulations (Condition I)	New Simulations (Condition II)
Ignition Starting Angle	698°	698°
Ignition Duration	18°	22°
Injection Starting Angle	380°	440°
Injection Duration	40°	60°

The values for injection starting angle and duration, 440 ° and 60°, respectively, are provided by the manufacturer, based on data obtained through the engine control unit (ECU).

With these modifications implemented, the engine's performance parameters were analysed to assess whether the new calibration strategy effectively enhances overall performance.

Temperature

The effect of this new setup (Condition II) on the maximum cycle temperature, compared to the initial baseline (Condition I), is illustrated in Figure 83 for the 15% and 20% increments.

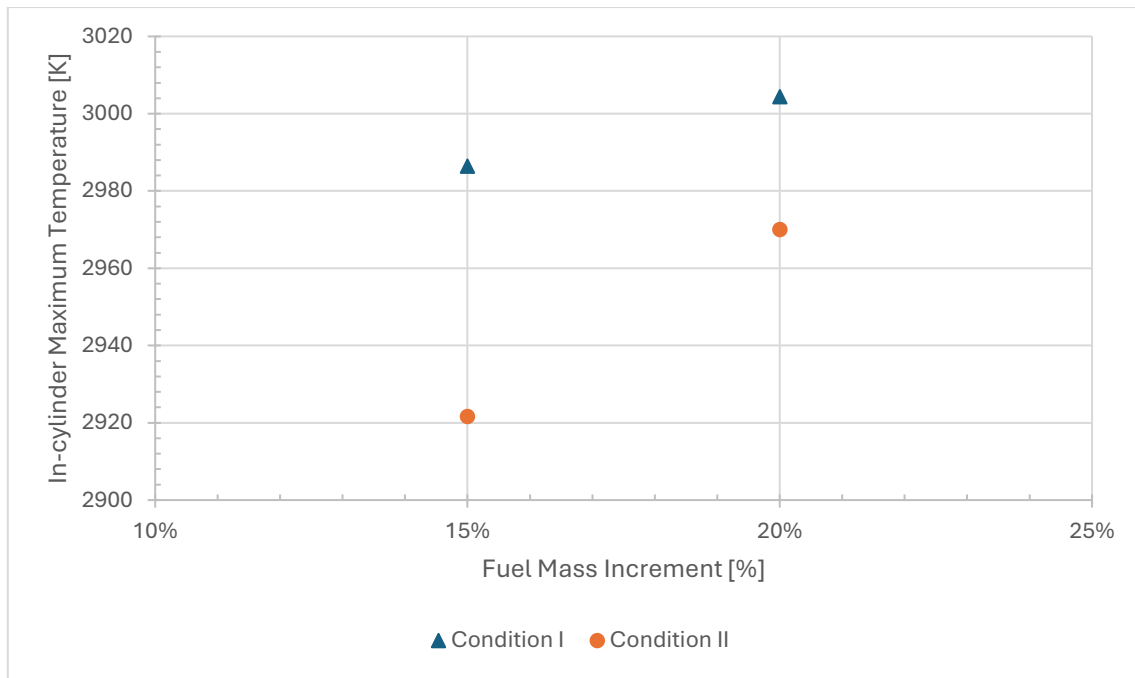


Figure 83 – In-cylinder maximum temperature for Condition 1 and 2 and fuel increments of 15 % and 20 %.

The analysis of Figure 83 reveals a consistent decrease in the maximum temperature when applying a new calibration strategy (Condition II) compared to the reference parameters (Condition I). For the 15 % fuel increment, a significant reduction is observed, dropping from approximately 2985 K to 2922 K, with a similar thermal mitigation trend seen in the 20 % scenario.

This cooling thermal peak is a direct consequence of the adjustments made to the injection profile. By extending the injection duration from 40° to 60° and delaying its start, the same mass of fuel is introduced much more gradually. This calibration prevents excessively explosive combustion. By distributing the release of thermal energy further into the expansion stroke, extreme temperature spikes are attenuated. This effect strongly aligned with the proposed optimization goal.

Pressure

The effect of the new calibration strategy on pressure is represented in Figure 84.

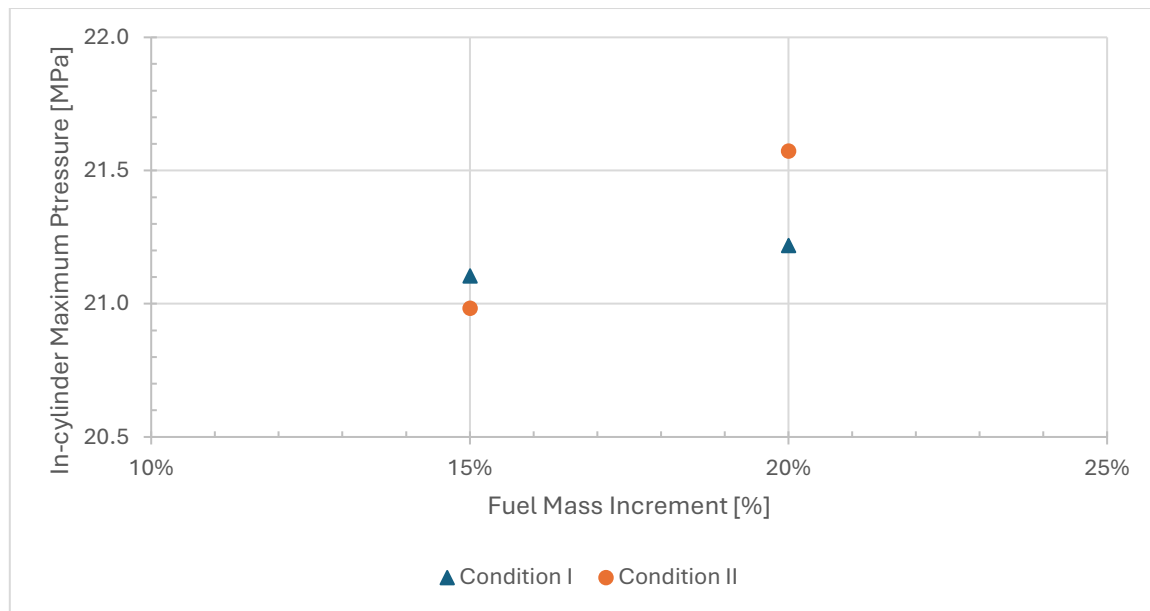


Figure 84 - In-cylinder maximum pressure for Conditions I and II and fuel increments of 15 % and 20 %.

The evolution of the maximum pressure, represented in Figure 84, reveals a non-linear behaviour and a trend inversion between the two calibration strategies. At a fuel mass increase of 15 %, Condition II exhibits a lower peak pressure than Condition I. This outcome is aligned with the previously analysed temperature behaviour.

However, at a 20 % fuel mass increase of 20 %, a clear inversion occurs, with Condition II generating a substantially higher-pressure peak (reaching approximately 21.6 MPa).

Power, Combustion Efficiency and Thermal Efficiency

Table 33 summarizes the engine performance parameters, such as power, combustion, and thermal efficiency, for both Conditions I and II.

Table 33 - Engine's performance parameters for both Condition I and II, and 15 % and 20 % fuel mass increment.

	15 %		20 %	
	I	II	I	II
Power (kW)	34.5	35.6	34.0	35.5
Combustion Efficiency (%)	96.0	98.2	89.5	93.9
Thermal Efficiency (%)	40.3	41.5	38.0	39.7

Table 33 shows the effectiveness of the new calibration strategy (Condition II) compared to the baseline setup (Condition I) through the overall engine performance parameters. The results demonstrate comprehensive improvements across critical fuel mass increments (15 % and 20 %).

The most decisive factor is the recovery of combustion efficiency, which jumps from 89.5 % to 93.9 % at the 20 % increment. Physically, the extended injection duration prevented the local oxygen starvation that occurred during the rapid injection phase of Condition 1. The new calibration ensured the oxidation of a significantly larger fraction of the injected mass. This optimized combustion directly translates into a substantial gain, effectively reversing the previously observed penalty. At the 20 % increment, power rises from 34.0 kW to 35.5 kW, proving that the additional fuel is now generating useful work rather than being wasted. An improvement in thermal efficiency was recorded (reaching 39.7 % in the scenario of 20 % increase). This increase is a direct consequence of the smoother heat release profile induced by the prolonged injection.

With this improvement in engine performance parameters (Condition II), it is possible to say that by implementing new calibration strategies, 30 % oxygen (at 313.0 K and 2.54 bar) can be used in intake air composition, and the increase in fuel mass by 15 % results in an 9.2 % improvement in the engine power.

Pollutant Emissions

Regarding CO and CO₂, Figures 85 and 86 represent the emissions at the exhaust valve at the end of the combustion cycle.

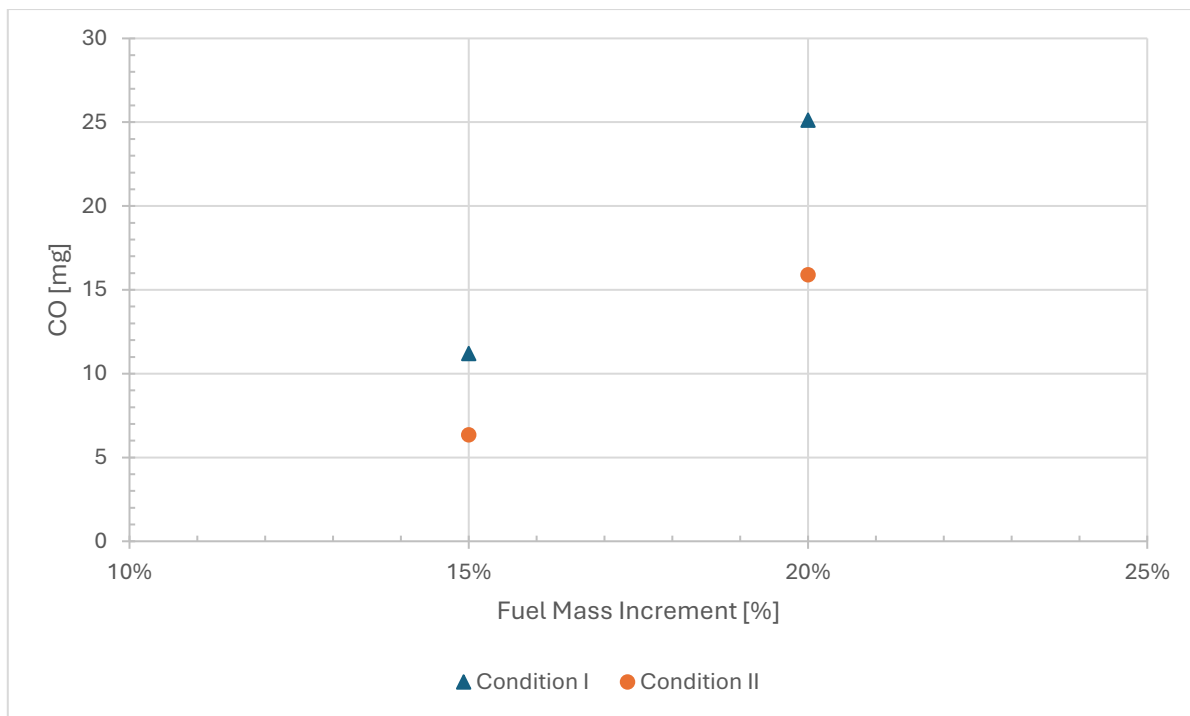


Figure 85 - CO emissions when the exhaust valve opens, for Conditions I and II.

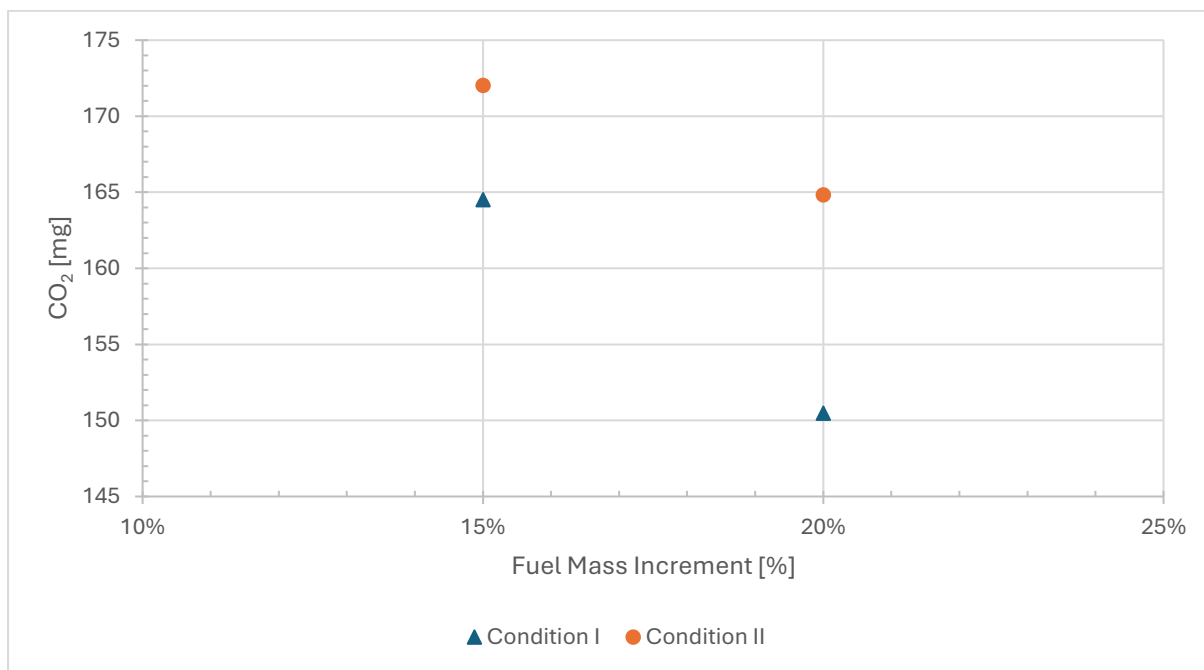


Figure 86 – CO₂ emissions when the exhaust valve opens, for Conditions I and II.

Figures 85 and 86 allow the validation of the recovery of combustion efficiency achieved by the new calibration strategy (Condition II).

A drastic reduction in CO emissions is observed with the adoption of Condition II for both fuel increments. This is particularly notable in the 20 % scenario, where the values drop from approximately 25 mg to 16 mg. Simultaneously, CO₂ emissions increase significantly, rising from 150 mg to 165 mg at the same operating point.

This phenomenon proves that the performance drop recorded under Condition I was driven by poor air-fuel mixing, caused by an excessively rapid fuel delivery that generated carbon oxidation at an intermediate stage (CO). By extending the injection event, Condition II optimized residence time and mixture homogenization. Consequently, a much larger fraction of the carbon was able to access the remaining oxygen, completing oxidation into CO₂.

Figures 87 and 88 represent, respectively, the final emissions of NO and NO₂ in the final stage of the combustion cycle.

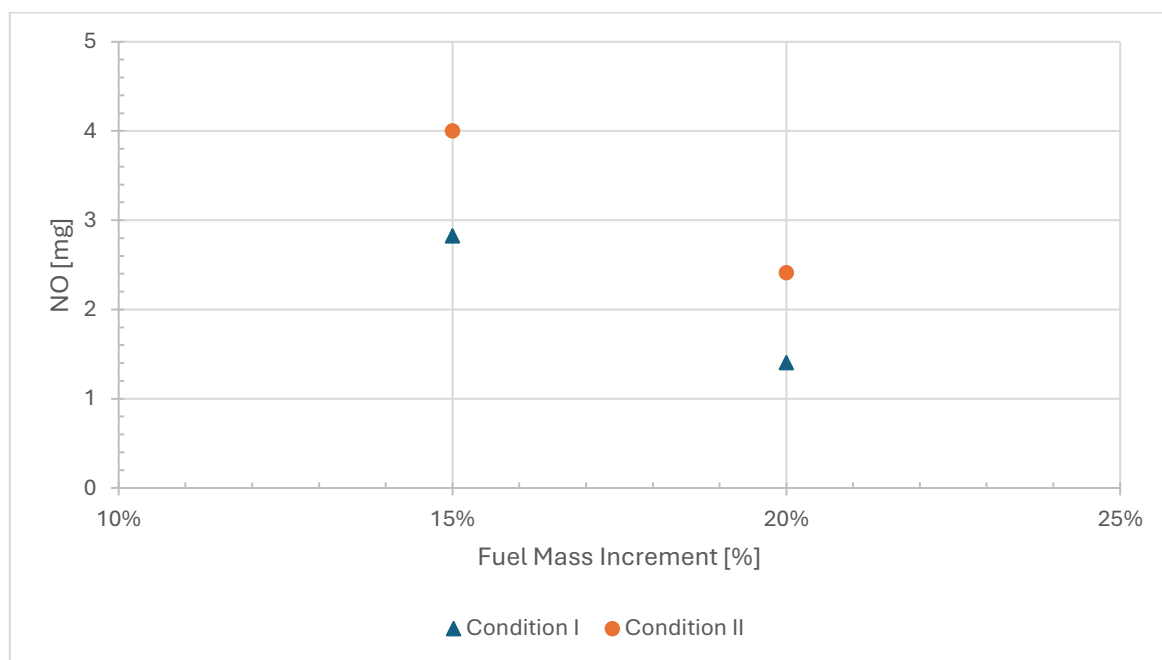


Figure 87 - NO emissions when the exhaust valve opens, for Conditions I and II.

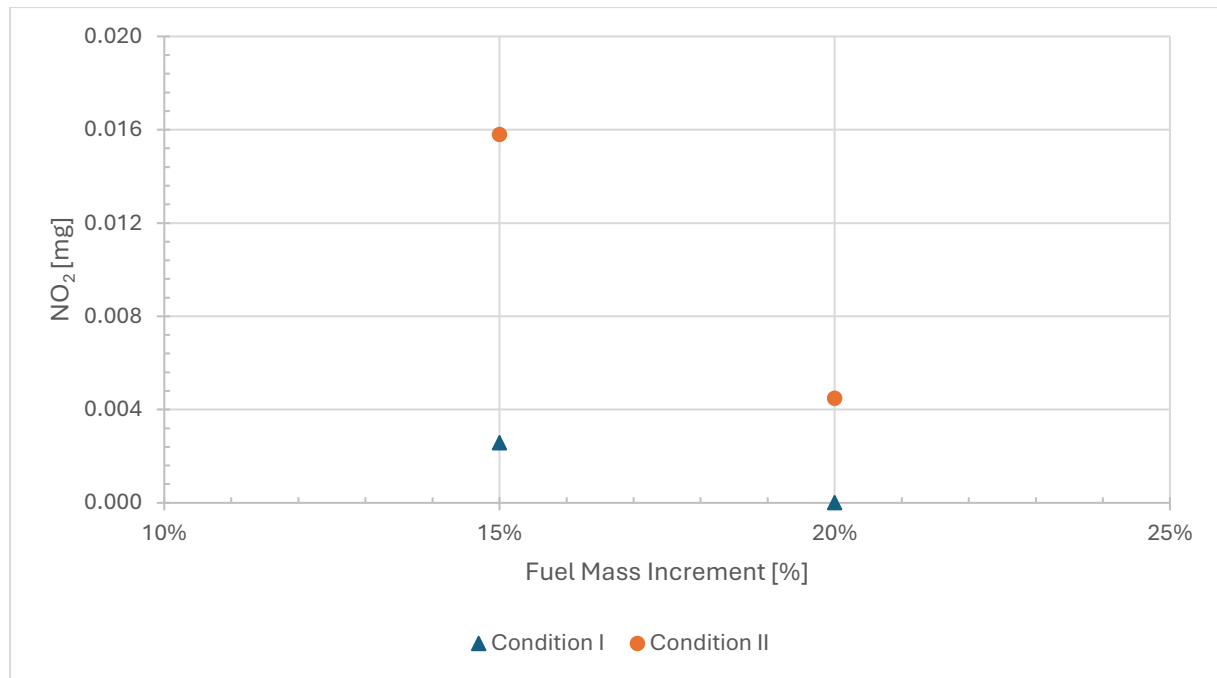


Figure 88 - NO₂ emissions when the exhaust valve opens, for Conditions I and II.

Figures 87 and 88 show the evolution of NO and NO₂ emissions for the two calibration strategies (Conditions I and II). Condition II presents higher NO_x values than Condition I for both fuel increments.

First, this increase might appear contradictory, given the previously documented reduction in maximum temperature. However, this phenomenon is justified by the improvement in air-fuel mixture homogeneity, and it means that more oxygen is available and actively participating in high temperature reactions.

Second, although the absolute thermal peak was attenuated, extending the injection duration (from 40° to 60°) promotes NO_x formation. The formation of nitrogen oxides is a consequence of the reduction in CO emissions and the successful recovery of combustion efficiency.

Chapter 5

Conclusions, Limitations and Future Works

5.1 Conclusions

The aim of this study was to investigate the feasibility of implementing oxy-combustion in drone engines. The main results and conclusions are summarized below.

Regarding the oxygen separation method, the analysis indicated that membrane separation is the most suitable technology under the considered conditions. However, technological options are limited. Commercially available membranes can achieve oxygen purities of approximately 40 %. Although research continues to develop membranes capable of higher purities, such technologies are currently scarce and expensive. Consequently, for the practical implementation of oxy-combustion in drones, the most viable solution will be to use a pressurized oxygen cylinder to supply the required oxygen stream or to develop a new membrane capable of achieving high oxygen purities.

In terms of oxy-combustion application, simulations were conducted to study the effect of varying oxygen concentration. In the first set of simulations, only the oxygen concentration was modified. It was possible to observe that the maximum in-cylinder temperature increased until approximately 70 % O_2 , then decreased between 70 and 80 % O_2 , and finally stabilized between 80 and 95 % O_2 . A very similar behaviour occurs with pressure, but pressure stabilizes between 70 and 95 % O_2 . This occurred due to chemical dissociation and the fact that the combustion process occurs near the top dead centre (720°). Regarding the pollutant emissions, the CO concentration decreased at all simulated O_2 concentrations, while CO_2 concentrations increased, confirming that O_2 reduces the formation of CO and improves CO_2 formation, due to the carbon monoxide formation mechanism. NO_x concentrations increased due to the high temperatures reached during the combustion cycle, being the main promoter of the nitrogen oxides formation mechanism. Finally, regarding performance parameters, it was observed that

there is an optimal value for oxygen concentration (25 %), where the highest power, combustion and thermal efficiency were achieved, although it was concluded that, at the end of the combustion process, a considerable amount of oxygen remained, leading to the conclusion that the mass of the fuel used in this combustion simulation should be increased to achieve higher performance values.

In the second set of simulations, an appropriate oxygen concentration (30 %) was selected, and the angular speed was varied from 1500 rpm to 4500 rpm, with the aim of achieving the performance values corresponding to 21 % oxygen. In these simulations, the fuel mass was also adjusted to the values provided by the manufacturer. A temperature and pressure peak was registered at 2000 rpm, related to the increasing of wall heat transfer as well as the increase in fuel mass. The pressure peak can be explained by the combustion velocity. Regarding pollutant emissions, both for 21 % and 30 % O₂, the study was developed only at 2000 rpm, since this was the value with the highest power and torque due to the fuel mass used. For CO and CO₂, a decrease and an increase were observed, respectively. This behaviour, as mentioned above, is due to the CO formation mechanism and dissociation. A considerable increase was observed for NO₂, due to the high temperature reached. The performance parameters presented a decreasing trend of 21 to 30 % for all angular velocities, due to combustion and thermal efficiency, and, consequently, to the excess of oxygen at the end of combustion. It was concluded that the fuel mass should be adjusted to improve these parameters.

In the third set of simulations, the effect of altitude was studied, and it was possible to observe that both temperature and pressure decreased due to the low temperature and pressure values used in the intake air setup. As presented before, the same study was conducted for pollutant emissions, and the same trends were observed. Regarding performance parameters, a slight increase in power was observed compared to the reference simulation (21 % at 313.0 K), but it was observed that, at the end of combustion, considerable amounts of oxygen remained, leading to the conclusion that the fuel mass should be increased, as well as some engine calibration parameters, such as, the intake pressure.

Finally, in the fourth set of simulations, an increase in fuel mass was applied in the simulation with 30 % O₂, in the engine's initial configuration. An improvement was

observed in all parameters, although after a 15 % increase in fuel mass, combustion and thermal efficiency were penalized. The evolution of pollutant emissions observed was very similar to the ones previously observed. To overcome the low performance values obtained with 15 % and 20 % fuel mass increases, a new calibration strategy was applied, changing the injection and ignition times and durations. It was then possible to observe that engine performance improved.

Globally, it is possible to affirm that oxy-combustion is an emerging technology with high potential. However, to apply this technology in engines, it is important to consider that the combustion reaches very high temperatures when compared to conventional combustion, so the materials should be adjusted to this use. It is also important to implement different calibration strategies in the engine to achieve its maximum performance.

5.2 Limitations

One of the main limitations of this work was the development and modelling of the two-stroke engine. Once the model was completed in SolidWorks, additional preparations and adjustments were required to make it suitable for simulations in ANSYS Forte. The transition from SolidWorks to ANSYS Forte presumed refinement and some changes applied in SpaceClaim, a 3D modelling tool developed by ANSYS. After this step, when the model was implemented in ANSYS Forte, some mesh issues appeared and, even with ANSYS support, were not surpassed until the end of this work. For this reason, it was decided to change to a four-stroke engine and develop the simulation with that model.

5.3 Future Work

There is a wide range of potential future work that can be pursued following this project. The main topics are presented below:

Development of an oxygen cylinder suitable for integration into drones. The cylinder must be designed to avoid compromising the drone's payload. Although membrane technology can achieve relatively high oxygen purities, if the main objective is to achieve higher power output and efficiency, it is necessary to use high concentrations of oxygen. In this context, an oxygen cylinder represents a practical solution, although it is heavy and occupies significant space.

Development and implementation of an oxygen separation membrane suitable for drone integration. Development of a membrane capable of reaching purities higher than those currently available on the market and implementation in the drone engine with the necessary modifications, without compromising payload or drone size.

Development and study of post-combustion technology. In oxy-combustion, the main products are CO_2 and water vapor, with CO_2 being the main pollutant. Some post-combustion technologies, such as membranes, are capable of capturing and storing the CO_2 produced. Developing a membrane system integrated into the engine exhaust could be an effective approach to reduce emissions in internal combustion engines.

Additional simulations for validation and practical assessment. The results obtained in this study could be further validated through additional simulations. Different engine calibrations should also be studied to obtain better performance. Furthermore, if feasible, testing oxy-combustion in a real engine would allow the results to be analysed under real-world operating conditions.

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Appendices

Appendix A

This appendix provides detailed information on the equations and methods used in CFD modelling, particularly in ANSYS Forte.

A.1 Governing Equations for combustion flows

To proceed to CFD modelling of a combustion system, it is important to know and understand the governing equations implemented in CFD software.

Continuity

The continuity equation is represented by

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial t}(\rho u_i) = 0 \quad (A.1)$$

It should be noted that density in combustions flows is a variable and depends on pressure, temperature, and species concentration (Versteeg 2007).

Momentum Equations

As in other flows, the velocity field is governed by momentum equations:

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_i}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_i} + F_i \quad (A.2)$$

Where τ_{ij} is the viscous stress tensor and F_i is the body force (which includes gravity) (Versteeg 2007).

$$\tau_{ij} = \mu \left(\frac{\partial u}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) \quad (A.3)$$

Transport Equations for species (k)

$$\frac{\partial}{\partial t}(\rho Y_k) + \frac{\partial}{\partial x_i}(\rho u_i Y_k) = \frac{\partial}{\partial x_i} \left(\rho D_k \frac{\partial Y_k}{\partial x_i} \right) + \dot{\omega}_k \quad (A.4)$$

Where,

D_k - species diffusion coefficient ($\frac{m^2}{s}$)

$\dot{\omega}_k$ - volumetric rate of generation (or destruction) of a species due to chemical reactions

To simplify Equation 4, it is common to assume a single D. This assumption is not always accurate but enables a far-reaching simplification of combustion calculations (Versteeg 2007).

$$\frac{\partial}{\partial t}(\rho Y_k) + \frac{\partial}{\partial x_i}(\rho u_i Y_k) = \frac{\partial}{\partial x_i} \left(\rho D \frac{\partial Y_k}{\partial x_i} \right) + \dot{\omega}_k \quad (A.5)$$

Energy Equation

In combustion flows, the temperature depends on the thermodynamic state and the composition of the mixture. There are some combustion models that do not require a transport equation for enthalpy, for example, in the laminar flamelet model is obtained from flamelet library curves. Other combustion sub models, require the solution from the transport equation for enthalpy

During combustion process, chemical energy is released as heat, and the resulting enthalpy is obtained by solving its transport equation:

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x_i}(\rho u_i h) = \frac{\partial}{\partial x_i} \left[\frac{\mu}{\sigma_h} \frac{\partial h}{\partial x_i} + \mu \left(\frac{1}{S_{C_k}} - \frac{1}{\sigma_h} \right) \sum_{k=1}^N h_k \frac{\partial Y_k}{\partial x_i} \right] + \frac{\partial p}{\partial t} + S_{rad} \quad (A.6)$$

Where S_{rad} is the radiation loss or gain and the viscous energy dissipation neglectable in low Mach number combustion flows. Here h is the mixture enthalpy per unit mass and h_k is the specific enthalpy of species, and summation is carried out over all N species considered in the chosen reaction mechanism. σ_h is the mixture Prandtl number, and S_{C_k} is the species Schmidt number (Equations A.7 and A.8).

$$S_{C_k} = \frac{\mu}{\rho D_k} \quad (A.7)$$

$$\sigma_h = \frac{c_p \mu}{k} = \frac{\text{Rate of momentum transport}}{\text{Rate of energy transport}} \quad (A.8)$$

The Lewis number is defined as:

$$Le_k = \frac{k}{\rho c_p D_k} = \frac{\text{Rate of energy transport}}{\text{Rate of mass transport}} \quad (A.9)$$

The Schmidt number is defined as:

$$S_{C_k} = \frac{\mu}{\rho D_k} = \frac{\text{Rate of momentum transport}}{\text{Rate of mass transport}} = Le \sigma_h \quad (A.10)$$

Assuming a single diffusion coefficient D is used for $k = 1, 2, \dots, N$, equation A.6 can be written as:

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x_i}(\rho u_i h) = \frac{\partial}{\partial x_i} \left[\frac{\mu}{\sigma_h} \frac{\partial h}{\partial x_i} + \frac{\mu}{\sigma_h} \left(\frac{\sigma_h}{S_c} - 1 \right) \sum_{k=1}^N h_k \frac{\partial Y_k}{\partial x_i} \right] + \frac{\partial p}{\partial t} + S_{rad} \quad (A.11)$$

And can be rewritten as:

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x_i}(\rho u_i h) = \frac{\partial}{\partial x_i} \left[\frac{\mu}{\sigma_h} \frac{\partial h}{\partial x_i} + \frac{\mu}{\sigma_h} \left(\frac{1}{Le} - 1 \right) \sum_{k=1}^N h_k \frac{\partial Y_k}{\partial x_i} \right] + \frac{\partial p}{\partial t} + S_{rad} \quad (A.12)$$

Therefore, in the case where the Lewis number is equal to one, the enthalpy equation simplifies to:

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x_i}(\rho u_i h) = \frac{\partial}{\partial x_i} \left[\frac{\mu}{\sigma_h} \frac{\partial h}{\partial x_i} \right] + \frac{\partial p}{\partial t} + S_{rad} \quad (A.13)$$

For low-speed models $\frac{\partial p}{\partial t}$ can be neglected (Versteeg 2007).

Other relations

The total mass fraction of fuel, oxidant and inert species is equal to 1, therefore:

$$\sum_k^{all\ species} Y_k = 1 \quad (A.14)$$

Where k represent the species.

The temperature can be calculated from the enthalpy by means of:

$$T = \frac{h - \sum_k^{fuel\ species} Y_k \Delta h_{fk}}{\bar{c}_p} \quad (A.15)$$

Where Δh_{fk} is the enthalpy of combustion.

The average value of the specific heat $\bar{c}_p$ is defined as follows:

$$\bar{c}_p = \frac{1}{(T - T_{ref})} \int_{T_0}^T c_p dT \quad (A.16)$$

$$c_p \equiv \sum_k^{all\ species} Y_k c_{p,k} \quad (A.17)$$

And $c_{p,k}$ is the specific heat of species.

The local density of the mixture depends on the pressure, reactants and products concentrations and the temperature of the mixture. Its value can be calculated from the following equation of state:

$$\rho = \frac{p}{R_u T \sum_k^{all\ species} \frac{Y_k}{(MW)_k}} \quad (A.18)$$

Where:

$(MW)_k$ - molecular weight of species

R_u - universal gas constant ($8.314 \frac{kJ}{kmol \cdot K}$)

The flow field is affected by changes in temperature and density, so in addition to the species and enthalpy equations, all flow equations must solve. The resulting set of transport equations can be very large, and models that include numerous intermediate equations require vast computational resources. Therefore, simpler models incorporating only a few number of reactions are often preferred in CFD combustion modelling (Versteeg 2007).

A.2 Turbulence Models

Reynolds-Averaged Navier-Stokes (RANS) Approach

The RANS approach is focused on the mean flow and the effects of turbulence on mean flow properties. Before applying numerical methods, the Navier-Stokes equations are time averaged, and extra terms appear in time-averaged flow equations due to the interactions between various turbulent fluctuations. These extra terms are modelled with classical turbulence models, for example $k - \varepsilon$ model. To obtain a reasonably accurate flow computation, the computing resources required are modest, so this approach is a good option over the last three decades (Versteeg 2007).

Reynolds-Averaged Navier-Stokes Equations

The consequences of turbulent fluctuations will be examined for the mean flow equations for an incompressible flow with constant viscosity. This assumption simplifies the algebra involved.

For start, the rules which govern time averages of fluctuating properties will be summarized: $\varphi = \Phi + \varphi'$ and $\psi = \Psi + \psi'$ and their summation, derivatives and integrals:

$$\begin{aligned} \overline{\varphi'} = \overline{\psi'} = 0; \quad \overline{\Phi} = \Phi; \quad \frac{\partial \overline{\varphi}}{\partial s} = \frac{\partial \Phi}{\partial s}; \quad \overline{\int \varphi ds} = \int \Phi ds; \\ \overline{\varphi + \psi} = \Phi + \Psi; \quad \overline{\varphi\psi} = \Phi\Psi + \overline{\varphi'\psi'}; \quad \overline{\varphi\Psi} = \Phi\Psi; \quad \overline{\varphi'\Psi} = 0 \end{aligned} \quad (\text{A. 19})$$

The order of time averaging and summation, further integration, and /or differentiation can be swapped or commuted, and it is called the commutative property.

Since div and grad are both differentiations, the rules above can be extended to a fluctuating vector quantity $\mathbf{a} = \mathbf{A} + \mathbf{a}'$ and its combinations with a fluctuating scalar $\varphi = \Phi + \varphi'$:

$$\begin{aligned} \overline{\text{div } \mathbf{a}} = \text{div } \mathbf{A}; \quad \overline{\text{div}(\varphi \mathbf{a})} = \text{div}(\overline{\varphi \mathbf{a}}) = \text{div}(\Phi \mathbf{A}) + \text{div}(\overline{\varphi' \mathbf{a}'}); \\ \overline{\text{div grad } \varphi} = \text{div grad } \Phi \end{aligned} \quad (\text{A. 20})$$

Considering the instantaneous continuity and Navier-Stokes equations in a Cartesian coordinate system so that the velocity vector $\mathbf{u}$ has x -component u , y -component v , and z -component w .

$$\text{div } \mathbf{u} = 0 \quad (\text{A. 21})$$

$$\frac{\partial u}{\partial t} + \text{div}(u\mathbf{u}) = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \text{div}(\text{grad}(u)) \quad (\text{A. 22a})$$

$$\frac{\partial v}{\partial t} + \text{div}(v\mathbf{u}) = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \nu \text{div}(\text{grad}(v)) \quad (\text{A. 22b})$$

$$\frac{\partial w}{\partial t} + \text{div}(w\mathbf{u}) = -\frac{1}{\rho} \frac{\partial p}{\partial w} + \text{div}(\text{grad}(w)) \quad (\text{A.22c})$$

These equations govern every turbulent flow, but the aim is to investigate the effects of fluctuations on the mean flow using the Reynold decomposition on equations 21 and 22a-c and replace the flow variables $\mathbf{u}$, with its components u , v , and w , and p by the sum of a mean and fluctuating component, so

$$\mathbf{u} = \mathbf{U} + \mathbf{u}'; u = U + u'; v = V + v'; w = W + w'; p = P + p' \quad (\text{A.23})$$

Applying the rules written in Equation A.19, the time-average is taken. Considering the continuity equation (Equation A.21), and noting that $\overline{\text{div } \mathbf{u}} = \text{div } \mathbf{U}$, and then obtaining the continuity equation for the mean flow

$$\text{div } \mathbf{U} = 0 \quad (\text{A.24})$$

A similar process is made in x -momentum equation (Equation A.22a), to obtain the time averages of the individual terms. These terms are written as follows.

$$\begin{aligned} \overline{\frac{\partial u}{\partial t}} &= \frac{\partial U}{\partial t}; \overline{\text{div}(u\mathbf{u})} = \text{div}(U\mathbf{U}) + \text{div}(\overline{u'\mathbf{u}'}); \overline{-\frac{1}{\rho} \frac{\partial p}{\partial x}} = -\frac{1}{\rho} \frac{\partial P}{\partial x}; \\ \nu \text{div}(\text{grad}(u)) &= \nu \text{div}(\text{grad}(U)) \end{aligned} \quad (\text{A.25})$$

Then, substituting the previous results gives the time-average x -momentum equation:

$$\frac{\partial U}{\partial t} + \text{div}(U\mathbf{U}) + \text{div}(\overline{u'\mathbf{u}'}) = -\frac{1}{\rho} \frac{\partial P}{\partial x} + \nu \text{div}(\text{grad}(U)) \quad (\text{A.26a})$$

The process is also repeated to obtain the time-average y - and z -momentum equation:

$$\frac{\partial V}{\partial t} + \operatorname{div}(V\mathbf{U}) + \operatorname{div}(\overline{v'\mathbf{u}'}) = -\frac{1}{\rho}\frac{\partial P}{\partial y} + \nu \operatorname{div}(\operatorname{grad}(V)) \quad (\text{A.26b})$$

$$\frac{\partial W}{\partial t} + \operatorname{div}(W\mathbf{U}) + \operatorname{div}(\overline{w'\mathbf{u}'}) = -\frac{1}{\rho}\frac{\partial P}{\partial z} + \nu \operatorname{div}(\operatorname{grad}(W)) \quad (\text{A.26c})$$

It is important to note that the first and second terms of the left side of the equation and the terms of the right side also appear in the instantaneous equations A.22a-c, but the process of time averaging introduces new terms, such as the third one on the left side of the equation. The terms involve products of fluctuating velocities and are associated with convective momentum transfer due to turbulent eddies, and it is usual to place those terms on the right-hand side of the equations A.27a-c, to reflect their role as additional turbulent stresses on the mean velocity components U , V and W .

$$\frac{\partial U}{\partial t} + \operatorname{div}(U\mathbf{U}) = -\frac{1}{\rho}\frac{\partial P}{\partial x} + \nu \operatorname{div}(\operatorname{grad}(U)) + \frac{1}{\rho} \left[\frac{\partial(-\rho\overline{u'^2})}{\partial x} + \frac{\partial(-\rho\overline{u'v'})}{\partial y} + \frac{\partial(-\rho\overline{u'w'})}{\partial z} \right] \quad (\text{A.27a})$$

$$\frac{\partial V}{\partial t} + \operatorname{div}(V\mathbf{U}) = -\frac{1}{\rho}\frac{\partial P}{\partial y} + \nu \operatorname{div}(\operatorname{grad}(V)) + \frac{1}{\rho} \left[\frac{\partial(-\rho\overline{u'v'})}{\partial x} + \frac{\partial(-\rho\overline{v'^2})}{\partial y} + \frac{\partial(-\rho\overline{v'w'})}{\partial z} \right] \quad (\text{A.27b})$$

$$\frac{\partial W}{\partial t} + \operatorname{div}(W\mathbf{U}) = -\frac{1}{\rho}\frac{\partial P}{\partial z} + \nu \operatorname{div}(\operatorname{grad}(W)) + \frac{1}{\rho} \left[\frac{\partial(-\rho\overline{u'w'})}{\partial x} + \frac{\partial(-\rho\overline{v'w'})}{\partial y} + \frac{\partial(-\rho\overline{w'^2})}{\partial z} \right] \quad (\text{A.27c})$$

The new extra terms are three normal stresses:

$$\tau_{xx} = -\rho\overline{u'^2}; \tau_{yy} = -\rho\overline{v'^2}; \tau_{zz} = -\rho\overline{w'^2} \quad (\text{A.28})$$

And three shear stresses:

$$\tau_{xy} = \tau_{yx} = -\rho\overline{u'v'}; \tau_{yz} = \tau_{zy} = -\rho\overline{v'w'}; \tau_{xz} = \tau_{zx} = -\rho\overline{u'w'} \quad (\text{A.29})$$

These extra stresses are called the Reynold stresses. The normal stresses involve the respective variances of the x -, y -, and z -velocity fluctuations, and they are always non-zero because they contain squared velocity fluctuations. The shear stresses contain second moments associated with correlation between different velocity components. If two fluctuating velocity components, for example u' and v' , were independent random fluctuations the time average $\overline{u'v'}$ would be zero. But the correlations between pairs of different velocity components due to the structure of the vortical eddies ensure that the turbulent shear stresses are non-zero.

The group of Equations A.26 and A.27 is called the Reynolds-averaged Navier-Stokes equations.

All the equations deduced above can also be applied to an arbitrary scalar quantity, for example, temperature. The time-average equation for an arbitrary scalar φ is:

$$\frac{\partial \Phi}{\partial t} + \text{div}(\Phi \mathbf{U}) = \frac{1}{\rho} \text{div}(\Gamma_{\Phi} \text{grad} \Phi) + \left[-\frac{\partial \overline{u'\varphi'}}{\partial x} - \frac{\partial \overline{v'\varphi'}}{\partial y} - \frac{\partial \overline{w'\varphi'}}{\partial z} \right] + S_{\Phi} \quad (\text{A.30})$$

Until now, it was assumed that the fluid density was constant, but in practical flows, the mean density may vary, and the instantaneous density always shows turbulent fluctuations.

So, in some cases it is important to consider the density-weighted averaged or Favre-averaged form of the mean flow equations for compressible, where effects of density fluctuations are neglectable, but mean density variations are not. In CFD simulations, these equations are widely used, and they are summarized in the following table. Note, that the overbar indicates a time-averaged variable and the tilde indicates a density-weighted or Favre-averaged variable (Versteeg 2007).

Table A 1 – Turbulent flow equation for compressible flows.

Continuity	
$\frac{\partial \bar{\rho}}{\partial t} + \text{div}(\bar{\rho} \tilde{\mathbf{U}}) = 0$	(A. 31)
Reynolds equations	
$\begin{aligned} \frac{\partial(\bar{\rho} \tilde{U})}{\partial t} + \text{div}(\bar{\rho} \tilde{U} \tilde{\mathbf{U}}) = & -\frac{\partial \bar{P}}{\partial x} + \text{div}(\mu \text{grad } \tilde{U}) + \\ & \left[-\frac{\partial(\bar{\rho} u'^2)}{\partial x} - \frac{\partial(\bar{\rho} u' v')}{\partial y} - \frac{\partial(\bar{\rho} u' w')}{\partial z} \right] + S_{Mx} \end{aligned}$	(A. 32a)
$\begin{aligned} \frac{\partial(\bar{\rho} \tilde{V})}{\partial t} + \text{div}(\bar{\rho} \tilde{V} \tilde{\mathbf{U}}) = & -\frac{\partial \bar{P}}{\partial y} + \text{div}(\mu \text{grad } \tilde{V}) + \\ & \left[-\frac{\partial(\bar{\rho} u' v')}{\partial x} - \frac{\partial(\bar{\rho} v'^2)}{\partial y} - \frac{\partial(\bar{\rho} v' w')}{\partial z} \right] + S_{My} \end{aligned}$	(A. 32b)
$\begin{aligned} \frac{\partial(\bar{\rho} \tilde{W})}{\partial t} + \text{div}(\bar{\rho} \tilde{W} \tilde{\mathbf{U}}) = & -\frac{\partial \bar{P}}{\partial z} + \text{div}(\mu \text{grad } \tilde{W}) + \\ & \left[-\frac{\partial(\bar{\rho} u' w')}{\partial x} - \frac{\partial(\bar{\rho} v' w')}{\partial y} - \frac{\partial(\bar{\rho} w'^2)}{\partial z} \right] + S_{Mz} \end{aligned}$	(A. 32c)
Scalar transport equation	
$\begin{aligned} \frac{\partial(\bar{\rho} \tilde{\Phi})}{\partial t} + \text{div}(\bar{\rho} \tilde{\Phi} \tilde{\mathbf{U}}) = & \text{div}(\Gamma_{\Phi} \text{grad } \tilde{\Phi}) + \\ & \left[-\frac{\partial(\bar{\rho} u' \phi')}{\partial x} - \frac{\partial(\bar{\rho} v' \phi')}{\partial y} - \frac{\partial(\bar{\rho} w' \phi')}{\partial z} \right] + S_{\Phi} \end{aligned}$	(A. 33)

Eddy viscosity and eddy diffusivity

This approach models the turbulent transport processes with gradient-diffusion assumptions. For the momentum equation, Boussinesq proposed that the components of the Reynolds stress are assumed to be proportional to the mean rates of deformation. Using suffix notation:

$$\tau_{ij} = -\overline{\rho u'_i u'_j} = \mu_t \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \rho k \delta_{ij} \quad (\text{A. 34})$$

Where $k = \frac{1}{2} (\overline{u'^2} + \overline{v'^2} + \overline{w'^2})$ is the turbulent kinetic energy per unit mass.

In the first term on the right-hand side appears the turbulent viscosity, μ_t and it is related to the turbulent kinematic viscosity denoted by $\nu_t = \frac{\mu_t}{\rho}$ with dimensions $\frac{m^2}{s}$. The second term on the right-hand side evolves δ_{ij} , the Kronecker delta ($\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$). This contribution ensures that the formula gives the correct Reynolds stress.

Turbulent transport of heat, mass, and other scalar properties can be modelled similarly. Equation A.35 shows that turbulent momentum transport is assumed to be proportional to mean gradients of velocity. By analogy, turbulent transport of a scalar is taken to be proportional to the gradient of the mean value of the transported quantity. Then we get

$$-\overline{\rho u_i \phi'} = \Gamma_t \frac{\partial \Phi}{\partial x_i} \quad (A. 35)$$

Where Γ_t is the turbulent diffusivity.

Since turbulent transport of momentum and heat or mass is due to the same mechanism, it is expected that the value of turbulent diffusivity, Γ_t , is close to the turbulent viscosity μ_t . This assumption is better known as the Reynolds analogy and introduces the Prandtl/Schmidt number, represented as follows (Versteeg 2007).

$$\sigma_t = \frac{\mu_t}{\Gamma_t} \quad (A. 36)$$

The $k - \varepsilon$ model

The $k - \varepsilon$ model focus on the mechanisms that affect the turbulent kinetic energy. To understand the model, some preliminary definitions are required: The instantaneous kinetic energy $k(t)$ of a turbulent flow is the sum of the mean kinetic energy $K = \frac{1}{2}(U^2 + V^2 + W^2)$ and the turbulent kinetic energy $k = \frac{1}{2}(\overline{u'^2} + \overline{v'^2} + \overline{w'^2})$:

$$k(t) = k + K \quad (A. 37)$$

In the next developments it is necessary to use extensively the rate of deformation and the turbulent stresses. To make the process easier, it is common to write the components of the rate of deformation s_{ij} and the stresses τ_{ij} in matrix form.

$$s_{ij} = \begin{bmatrix} s_{xx} & s_{xy} & s_{xz} \\ s_{yx} & s_{yy} & s_{yz} \\ s_{zx} & s_{zy} & s_{zz} \end{bmatrix} \text{ and } \tau_{ij} = \begin{bmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{bmatrix}$$

Decomposition of the rate of deformation of a fluid element in a turbulent flow into a mean and a fluctuating component, $s_{ij} = S_{ij} + s'_{ij}$ gives the following matrix elements (Versteeg 2007):

$$s_{xx}(t) = S_{xx} + s'_{xx} = \frac{\partial U}{\partial x} + \frac{\partial u'}{\partial x} \quad (\text{A. 38a})$$

$$s_{yy}(t) = S_{yy} + s'_{yy} = \frac{\partial V}{\partial y} + \frac{\partial v'}{\partial y} \quad (\text{A. 38b})$$

$$s_{zz}(t) = S_{zz} + s'_{zz} = \frac{\partial W}{\partial z} + \frac{\partial w'}{\partial z} \quad (\text{A. 38c})$$

$$s_{xy}(t) = S_{xy} + s'_{xy} = s_{yx} = S_{yx} + s'_{yx} = \frac{1}{2} \left[\frac{\partial U}{\partial y} + \frac{\partial V}{\partial x} \right] + \frac{1}{2} \left[\frac{\partial u'}{\partial y} + \frac{\partial v'}{\partial x} \right] \quad (\text{A. 38d})$$

$$s_{xz}(t) = S_{xz} + s'_{xz} = s_{zx} = S_{zx} + s'_{zx} = \frac{1}{2} \left[\frac{\partial U}{\partial z} + \frac{\partial W}{\partial x} \right] + \frac{1}{2} \left[\frac{\partial u'}{\partial z} + \frac{\partial w'}{\partial x} \right] \quad (\text{A. 38e})$$

$$s_{yz}(t) = S_{yz} + s'_{yz} = s_{zy} = S_{zy} + s'_{zy} = \frac{1}{2} \left[\frac{\partial V}{\partial z} + \frac{\partial W}{\partial y} \right] + \frac{1}{2} \left[\frac{\partial v'}{\partial z} + \frac{\partial w'}{\partial y} \right] \quad (\text{A. 38f})$$

Governing equation for mean flow kinetic energy K

Multiplying x -component Reynolds equation by U , y -component by V and z -component by W , and after adding all equations and do some arrangements, the equation for mean kinetic energy K is obtained (Versteeg 2007).

$$\frac{\partial(\rho K)}{\partial t} + \text{div}(\rho K \mathbf{U}) = \text{div}(-P\mathbf{U} + 2\mu\mathbf{U}S_{ij} - \rho U\overline{u'_i u'_j}) - 2\mu S_{ij} \cdot S_{ij} - \rho\overline{u'_i u'_j} \cdot S_{ij} \quad (\text{A.39})$$

Governing equation for turbulent kinetic energy k

The equation for turbulent kinetic energy is obtained from the multiplication of each of the instantaneous Navier-Stokes equations (Equation A.26a-c) by the correct fluctuating velocity components, for example x -component multiplied by u' , repeating the process for y - and z -components, and after that repeat the process for the Reynolds equations (Equations A.33a-c). Then subtract both, instantaneous Navier-Stokes and Reynolds equations, and proceed into a rearrangement, it's possible to obtain equation A.41 for turbulent kinetic energy, k

$$\frac{\partial(\rho k)}{\partial t} + \text{div}(\rho k \mathbf{U}) = \text{div}\left(-\overline{p'\mathbf{u}'} + 2\mu\overline{\mathbf{u}'s'_{ij}} - \rho\frac{1}{2}\overline{u'_i \cdot u'_i u'_j}\right) - 2\mu\overline{s'_{ij} \cdot s'_{ij}} - \rho\overline{u'_i u'_j} \cdot S_{ij} \quad (\text{A.40})$$

Equations A.39 and A.40 look similar, however the appearance of the quantities on the right side of the k -equation (Equation A.40) shows that the changes to the turbulent kinetic energy are due to turbulent interactions.

The rate of dissipation per unit volume is a product of density ρ and the rate of dissipation of turbulent kinetic energy per unit mass, ε ($\frac{m^2}{s}$):

$$\varepsilon = 2\nu\overline{s'_{ij} \cdot s'_{ij}} \quad (\text{A.41})$$

ε is a really important quantity in the turbulence dynamics studies, this is the destruction term in the turbulent kinetic energy equation, and has a similar magnitude as the production term, and is never neglectable. In a case where the Reynolds number is high, the viscous transport term (second term on the right side of equation A.40), is always

small when compared with the turbulent transport term (third term on the right side of equation A.40) and the dissipation term (fourth term on the right side of equation A.40) (Versteeg 2007).

The $k - \varepsilon$ model equations

For all turbulence quantities, including the rate of viscous dissipation, ε , it is possible to develop transport equations. But the exact solution for ε -equation, contains many unknown and unmeasurable terms, so to simply the problem it was developed the standard $k - \varepsilon$ model, resumed in two equations, one for ε and the other for k , based on relevant processes causing changes in these variables.

k and ε can be used to define velocity scale ϑ , and length scale ℓ , two value representative of the large-scale turbulence.

$$\vartheta = k^{\frac{1}{2}} \quad (A.42)$$

$$\ell = \frac{k^{\frac{3}{2}}}{\varepsilon} \quad (A.43)$$

The use of a ‘small eddy’ variable ε , to define a large eddy scale, ℓ , may seem questionable. However, this is a reasonable choice at high Reynolds numbers. In these flows, as long as conditions do not change rapidly, the energy taken from the mean flow by large eddies is balanced by the energy passed down through the turbulence spectrum to the smaller, dissipative eddies. Without this balance, energy at certain scales would grow or decay without limit. Since this does not happen in practice, it is possible to use ε to define the large eddy scale.

From a dimensional analysis, it is possible to specify eddy viscosity as presented in the following equation:

$$\mu_t = C\rho\vartheta\ell = \rho C_\mu \frac{k^2}{\varepsilon} \quad (A.44)$$

Where C_μ is a dimensionless constant.

The following equations for k and ε are used for the standard $k - \varepsilon$ model:

$$\frac{\partial(\rho k)}{\partial t} + \text{div}(\rho k \mathbf{U}) = \text{div} \left[\frac{\mu_t}{\sigma_k} \text{grad } k \right] + 2\mu_t S_{ij} \cdot S_{ij} - \rho \varepsilon \quad (\text{A.45})$$

$$\frac{\partial(\rho \varepsilon)}{\partial t} + \text{div}(\rho \varepsilon \mathbf{U}) = \text{div} \left[\frac{\mu_t}{\sigma_\varepsilon} \text{grad } \varepsilon \right] + C_{1\varepsilon} \frac{\varepsilon}{k} 2\mu_t S_{ij} \cdot S_{ij} - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} \quad (\text{A.46})$$

There are five adjustable constants in the equations: C_μ , σ_k , σ_ε , $C_{1\varepsilon}$ and $C_{2\varepsilon}$. The values for these constants are summarized in the following table and can be used in a wide range of turbulent flows. (Versteeg 2007). The values presented on table A2 are the same used in Ansys Forte Software.

Table A 2 -Constants for standard $k-\varepsilon$ model

C_μ	σ_k	σ_ε	$C_{1\varepsilon}$	$C_{2\varepsilon}$
0.09	1.00	1.30	1.44	1.92

RNG $k - \varepsilon$ model

At low Reynolds numbers, $k - \varepsilon$ need to be modified, and wall damping needs to be applied.

$$C_{1\varepsilon}^* = C_{1\varepsilon} - \frac{\eta \left(1 - \frac{\eta}{\eta_0}\right)}{1 + \beta \eta^3}; \quad \eta = \frac{k}{\varepsilon} \sqrt{2S_{ij} \cdot S_{ij}}; \quad \eta_0 = 4.377; \quad \beta = 0.012 \quad (\text{A.47})$$

The only adjustable parameter is β and all the other parameters are explicitly computed as part of RNG process.

In ANSYS Forte Theory manual there was implemented another variable $C_{3\varepsilon}$ (Equation A.48), that considers the compressibility effects. The equation was adapted with the nomenclature used.

$$C_{3\varepsilon} = \frac{-1 + 2C_{2\varepsilon} - 3m(n-1) + (-1)^\delta \sqrt{6} C_\mu C_{1\varepsilon}^* \eta}{3} \quad (\text{A. 48})$$

Where $m = 0.5$ and $n = 1.4$ for an ideal gas and δ was defined previously as being the Kronecker delta ($\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$).

In the following table are summarized the values of the RNG parameters used in Ansys Forte Software. (Versteeg 2007)

Table A 3 -Values of the RNG parameters used in ANSYS Forte. (ANSYS 2024)

C_μ	$C_{1\varepsilon}$	$C_{2\varepsilon}$	$C_{3\varepsilon}$	$\frac{1}{\sigma_k}$	$\frac{1}{\sigma_\varepsilon}$	η_0	β
0.0845	1.42	1.68	Equation A.48	1.39	1.39	4.38	0.012

A.3 Chemical Kinetics Formulation

As mentioned above, chemical kinetics helps to understand how long it takes for a system to reach equilibrium, briefly it is the study of reaction mechanisms and reaction rates.

Below are described some chemical kinetics mechanisms used in combustion modelling.

Reaction Rate

In combustion modelling, it is important to determine rates of reactant consumption and product formation.

During combustion, many intermediate processes occur, in other words, one species may be formed and consumed in different reactions, and some of those reactions can be reversible. For a better understanding of this behaviour, a scheme of reaction is represented on stoichiometric equation below.

$$\sum_{k=1}^N v'_{kj} M_k \rightarrow \sum_{k=1}^N v''_{kj} M_k \text{ for } j = 1, 2, \dots, m \quad (\text{A. 49})$$

Where v'_{kj} and v''_{kj} are the stoichiometric coefficients of reactants and products species M_k , respectively, in the reaction j . N is the total number of species involved and m is the total number of reactions.

Using mass conservation:

$$\sum_{k=1}^N v'_{kj} (MW)_k \rightarrow \sum_{k=1}^N v''_{kj} (MW)_k \text{ for } j = 1, 2, \dots, m \quad (\text{A. 50})$$

Production Rate

In complex chemical processes, the production rate $\dot{\omega}_k$ of the k species is written as being the summation of the rate of progress variables for all involving k th species.

$$\dot{\omega}_k = \sum_{j=1}^N v_{kj} q_j \quad (j = 1, \dots, m) \quad (\text{A. 51})$$

Where,

$$v_{kj} = v''_{kj} - v'_{kj} \quad (\text{A. 52})$$

The rate of progress variable q_i for the i reaction is given by the difference between forward and reverse rates, using the following equation

$$q_i = k_{fj} \prod_{k=1}^N [X_k]^{v'_{kj}} - k_{rj} \prod_{k=1}^N [X_k]^{v''_{kj}} \quad (\text{A. 53})$$

Where X_k is the molar concentration of the k species and k_{fi} and k_{ri} are the forward and reverse rate constants for the i reaction (Design 2015).

A.4 Boundary Conditions

In all CFD studies it is necessary to define boundary conditions. The user must specify correctly and understand their role in the numerical algorithm.

Inlet and Outlet Boundary Condition

In CFD simulations, and in Ansys Forte particularly, a proper specification of inflow and outflow boundaries is important to ensure accurate and stable results. These boundaries are considered open boundaries, because they allow mass, energy, and momentum exchange between the computational domain and the external environment, requiring information about the fluid state outside the domain to properly solve the transport equations.

ANSYS Forte uses ghost cells adjacent to the boundaries, whose values directly influence the flow variables within the domain. There are four types of boundary conditions specified in the manual: velocity or mass flow inlet, pressure inlet, pressure outlet, and continuous outflow. Each type has its specific characteristics and has a different way to specify fluid properties such as density, velocity, internal energy, and species composition for the mixtures.

At inlet boundaries, physical quantities like velocity or mass flow can be directly imposed, or a pressure condition can be applied, leaving velocity as a variable determined by the solver.

At outlet boundaries, flow can either continue as without additional constraints or pressure can be specified, which differently affects the internal flow field.

Inlet and outlet boundary conditions have to be properly defined, as it governs mass and energy balance within the domain, affect numerical stability, and determine how external

physical information, such as inflow rates and outflow pressures, is incorporated into the numerical solution.

Wall Boundary Condition

Heat transfer between the working fluid and the cylinder wall in an engine can significantly affect engine performance, efficiency, and emissions. The heat flux in the chamber wall is due to gas-phase convection, fuel-film conduction, and radiation. Gas-phase convective heat is the dominant factor in typical engine operating conditions. In the case of rigid-walls, boundary conditions must be specified or assumed for each governing equation, and often velocity and temperature wall functions are employed to solve near-wall shear stress and heat transfer.

Firstly, a flux balance is required for each gas-phase species in the system. The equation for the surface boundary condition for the gas-phase is:

$$\dot{m}_k = \rho Y_k u + \rho Y_k V_k \quad (k = 1, \dots, K_g) \quad (A.56)$$

Where,

K_g – number of gas-phased species in the system

u – convective velocity normal to the surface

V_k – diffuse velocity of the species

Y_k – mass fraction of the species

$\dot{m}_k$ – sum of any external flu imposed at the boundary

For a non-slip condition, the net flux, including diffusive and convective flux of each species to the wall, must be zero, and the sum of all species fluxes to the surface must also be zero.

A fluid momentum boundary condition on rigid walls is introduced by imposing a value for the velocity or calculating the shear stress at the wall. On non-slip walls, the gas velocity is equal to the wall velocity (Equation A.57). In this case, the wall shear stress is calculated by resorting to Equation A.3.

$$\mathbf{u} = \mathbf{u}_w \quad (\text{A.57})$$

On free-slip and turbulent law-of-the-wall boundaries, the normal gas velocity is set equal to the normal wall velocity (Equation A.58)

$$\mathbf{u} \cdot \mathbf{n} = \mathbf{u}_w \cdot \mathbf{n} \quad (\text{A.58})$$

The tangential components of the wall shear stress are explicitly specified. For free-slip walls, the tangential components of the wall shear stress are zero. For turbulent flow, the wall shear stress is determined by the law-of-the-wall, explicated below:

$$\frac{v}{u^*} = \begin{cases} \frac{1}{\kappa} \ln y^+ + B & Re \geq R_c \\ Re^{\frac{1}{2}} & Re < R_c \end{cases} \quad (\text{A.59})$$

Where u^* is the shear speed or friction velocity, and is related to the wall shear stress through the following relation:

$$\tau_w = \rho(u^*)^2 \frac{\mathbf{v}}{|\mathbf{v}|} \quad (\text{A.60})$$

$\mathbf{v}$ is the tangential velocity and is defined by $\mathbf{v} = \mathbf{u} - \mathbf{u}_w - [(\mathbf{u} - \mathbf{u}_w) \cdot \mathbf{n}]\mathbf{n}$. The Reynolds number is related to the gas velocity relative to the wall and is by defined by $Re = \frac{\rho y |\mathbf{v}|}{\mu_{air}(T)}$, which y represents the distance from the wall, considered to be the wall adjacent cell size. R_c is the Reynolds number that defines the transition from the logarithmic regime ($Re \geq R_c$) to the viscous sublayer regime ($Re < R_c$). In viscous sublayer regime, the laminar formula is used for shear stress. In logarithmic regime, the wall unit $y^+ = \frac{\rho y u^*}{\mu_{air}(T)}$ is replaced for the following solution to decompose the solution for u^*

$$y^+ = c_{lw}(Re)^{\frac{7}{8}} \quad (A.61)$$

For equations 59 and 60, it is assumed that the wall-adjacent cell size y is small enough to be in the logarithmic regime or in the laminar sublayer of the turbulent boundary layer. The constants mentioned above, κ , c_{lw} , R_C and B are related with $k - \varepsilon$ model and their values can be found in the KIVA-II documentation (Appendix I).

From equations A.59 and A.60, the shear stress is calculated. The total change in fluid momentum occurring in a time step due to the wall fraction can be calculated in the cell. This change is distributed to the vertices in the cell that are on the wall surface and affects the momentum on those vertices.

The logarithmic formulation assumes a smooth wall, if is to assume wall roughness, it is used the following equation:

$$\frac{\nu}{u^*} = \min\left(Re^{\frac{1}{2}}, \frac{1}{\kappa} \ln y^+ + B + \Delta B\right) \quad (A.62)$$

Where ΔB are roughness effects and is modeled as

$$\Delta B = \begin{cases} 0 & (if K_S^+ \leq 2.25) \\ \frac{1}{\kappa} \ln \left[\frac{K_S^+}{87.75} + C_S K_S^+ \right] \times \sin[0.4258(\ln K_S^+ - 0.811)] & (if 2.25 < K_S^+ \leq 90) \\ \frac{1}{\kappa} \ln[1 + C_S K_S^+] & (if K_S^+ > 90) \end{cases} \quad (A.63)$$

And $K_S^+ = \frac{y^+ K_S}{y}$ where K_S is the roughness height, C_S is a constant depending on the type of surface roughness.

To calculate the wall heat transfer flux for turbulent flows, it is used the wall temperature and the properties of the near wall fluid. There are two different models of heat transfer implemented in ANSYS Forte, but for this study only one is used: Han-Reitz Model, developed by Han-Reitz and Rakopoulos.

In Han-Reitz Model, the energy conservation equation (Equation A.6) and some assumptions are applied:

1. Gradients normal to the wall are bigger than the ones parallel to the wall.
2. The flow velocity is parallel to the flat wall.
3. Spatial gradients of pressure, viscous dissipation, enthalpy diffusion effects on energy flux, and radiation heat transfer are neglected.
4. Turbulent dissipation is small when compared with internal energy, due to low Mach number.
5. No spray source term.
6. Ideal gas law and constant specific heat.

With these assumptions, the energy conservation equation is resumed to a one-dimensional equation near the wall region, written as follows:

$$c_p \rho \frac{\partial T}{\partial t} + c_p \rho v \frac{\partial T}{\partial y} = -\frac{\partial J}{\partial y} + \frac{\partial p}{\partial t} + \dot{Q}_c \quad (\text{A. 64})$$

With

$$J = -(k + k_t) \frac{\partial T}{\partial y} \quad (\text{A. 65})$$

Where T is the temperature, J is the heat flux, y is the normal distance to the wall, v is the velocity in the normal-to-wall direction, ρ is the gas density, c_p is the specific heat of the gas mixture, p is the pressure and $\dot{Q}_c$ is the volumetric heat release rate.

k and k_t are laminar and turbulent conductivity associated with laminar and turbulent viscosity by Prandtl numbers, with the following relations

$$k = \frac{\mu}{\sigma} \text{ and } k_t = \frac{\mu_t}{\sigma_t} \quad (\text{A. 66})$$

According to Rakopoulos, the left side of the equation 64 is negligible, thus zero.

Integrating the equation A.64 over the distance y from the wall ($y = 0$), taking into consideration the variation of gas density, turbulent viscosity, and turbulent Prandtl number in the turbulent boundary layer, it is possible to obtain a temperature wall function formulated as:

$$T^+ = 2.1 \ln y^+ + 1.24 - 2.1(G^+ + P^+)y^+ - 17.2(G^+ + P^+) \quad (A.67)$$

Where T^+ , y^+ , G^+ and P^+ are define as:

$$T^+ = \int_{T_w}^T \frac{\rho c_p u^*}{J_w} dT = \frac{\rho c_p u^* \ln\left(\frac{T}{T_w}\right)}{J_w} \quad (A.68)$$

And

$$y^+ = \frac{u^* y}{\nu}; \quad G^+ = \frac{\dot{Q}_c \nu}{J_w u^*}; \quad P^+ = \frac{\overline{\partial p}}{\partial t} \frac{\nu}{J_w u^*} \quad (A.69)$$

Here u^* is the friction velocity defined in terms of the turbulence kinetic energy, $k = k^{\frac{1}{2}} c_\mu^{\frac{1}{4}}$, y is the distance to the wall, J_w is the heat flow through the wall and it is positive if the heat goes to the wall and negative if it comes from the wall). $\overline{Q_c}$ is the averaged volumetric chemical heat release rate, $\frac{\overline{\partial p}}{\partial t}$ is the average pressure fluctuation rate and ν is the laminar kinematic viscosity. The equation for the heat flux is:

$$J_w = \frac{\rho c_p u^* \ln\left(\frac{T}{T_w}\right) + \frac{(2.1y^+ + 17.2) \left(\overline{Q_c} + \frac{\overline{\partial p}}{\partial t}\right) \nu}{u^*}}{2.1 \ln y^+ + 1.24} \quad (A.70)$$

Where T and T_w is the gas temperature and the wall temperature, respectively. Following Han-Reitz implementation, $\overline{Q_c}$ term is neglected, obtained:

$$J_w = \frac{\rho c_p u^* \ln\left(\frac{T}{T_w}\right) + \frac{(2.1y^+ + 17.2) \frac{\overline{\partial p}}{\partial t} \nu}{u^*}}{2.1 \ln y^+ + 1.24} \quad (A.71)$$

And if the pressure fluctuation term is also neglected, because its effects can be considered secondary, the following equation is the one used in ANSYS Forte Han-Reitz modelling.

$$J_w = \frac{\rho c_p u^* \ln\left(\frac{T}{T_w}\right)}{2.1 \ln y^+ + 1.24} \quad (\text{A.72})$$

For turbulent flow, boundary conditions for turbulent kinetic energy k and its dissipation rate ε are also needed (ANSYS 2024a).

$$\nabla k \cdot \mathbf{n} = 0 \quad (\text{A.73})$$

$$\varepsilon = c_{\mu\varepsilon} \frac{k^{\frac{3}{2}}}{y} \text{ and } c_{\mu\varepsilon} = \left[\frac{c_\mu}{\sigma_\varepsilon (C_{2\varepsilon} - C_{1\varepsilon})} \right] \quad (\text{A.74})$$

Symmetry Boundary Condition

The symmetry boundary condition is created by applying lines or surfaces about which the flow is symmetric, allowing the use just a portion of the domain. At the axis, the velocity components normal to the boundary are zero, and gradients of scalar and vector variables are constrained according to the symmetry. This helps reduce computational costs (ANSYS 2024a).

A.5 Spray Models

ANSYS Forte has a comprehensive and advanced framework for modelling multi-component and fuel-spray and their interaction with component gases, covering subprocesses such as nozzle flow, spray atomization, droplet breakup, collision and coalescence, vaporization, and wall impingement. Different modelling strategies are applied for solid-cone and hollow-cone: solid-cone sprays rely on nozzle-exiting conditions defined by a discharged coefficient or detailed nozzle-flow models, coupled Kelvin-Helmholtz/Rayleigh-Taylor (KH/RT) model. Hollow-cone sprays employ the Linearized Atomization (LISA) model for both initialization and breakup. Common sub-models are shared across spray types, including advanced collision and vaporization

treatments. To reduce the mesh size sensitivity and time-step resolution, Forte integrates techniques such as unsteady gas-jet breakup, radius of influence collision modelling, and so improves computational efficiency.

Solid-Cone Spray Models

The nozzle-flow model describes the instantaneous flow condition inside the nozzle, with the main purpose of providing initial conditions for the spray model. Input parameters to the nozzle-flow are:

1. Mass flow rate
2. Physical properties of liquid fuel
3. Geometrical hole diameter
4. L/D ratio and R/D ratio, where R is the radius of curvature of the injector entrance region (Figure A

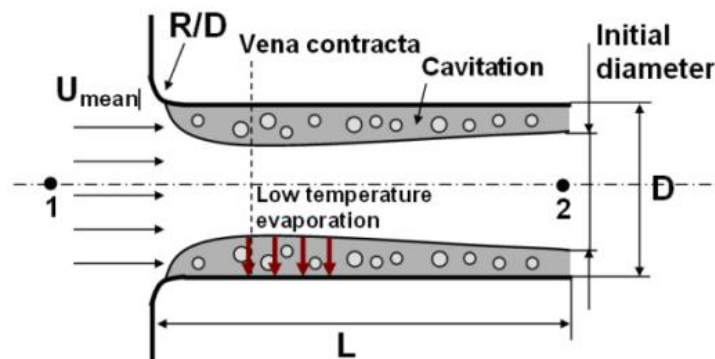


Figure A 1 - Flow through nozzle passage (ANSYS 2024).

With these inputs, the nozzle-flow model is capable to determine the instantaneous discharge coefficient C_d , spray angle, effective injection velocity, and effective flow exit area, this last one is used to determine the initial injected liquid droplet size.

The volumetric mean flow velocity of the liquid fuel at the inlet of the nozzle passage, U_{mean} , is calculated as

$$U_{mean} = \frac{\dot{m}}{\rho_l A} = \frac{4\dot{m}}{\rho_l \pi D^2} \quad (A.75)$$

Where $\dot{m}$ is fuel mass flow rate, ρ_l is liquid fuel density, A is nozzle cross-sectional area and D is the nozzle diameter.

Because of the losses caused by acceleration and formation of the velocity profile in the inlet, the expansion after the *vena contracta*, and the wall friction, the mean flowthrough the nozzle exit is always lower than predicted by the Bernoulli equation. To quantify the difference, the discharge coefficient, C_d is defined:

$$C_d = \frac{U_{mean}}{\sqrt{\frac{2(p_1 - p_2)}{\rho_1}}} \quad (A.76)$$

Using tabulated inlet loss coefficient (K_{inlet}) and Blasius or the laminar equation for wall friction, the discharge coefficient is given by the equation A.77 and in the equation A.78 Re_D is the Reynolds number based on the nozzle diameter.

$$C_d = \frac{1}{\sqrt{K_{inlet} + f \cdot \frac{L}{D} + 1}} \quad (A.77)$$

$$f = \max\left(0.316Re^{-0.25}, \frac{64}{Re_D}\right) \quad (A.78)$$

A first estimation of p_1 , the inlet pressure for a turbulent flow is made:

$$p_1 = p_2 + \frac{\rho_1}{2} \left(\frac{U_{mean}}{C_d} \right)^2 \quad (A.79)$$

Next, Forte checks the flow under this condition is cavitating, assumes a flat velocity profile and using Nurick's expression for the size of the contraction, continuity gives the velocity at the smallest flow area:

$$U_{vena} = \frac{U_{mean}}{C_C} \quad (A.80)$$

$$C_C = \left(2.6 - \frac{11.4R}{D} \right)^{-0.5} \quad (A.81)$$

In case of cavitation, it is possible to apply the Bernoulli equation:

$$p_{vena} = p_1 - \frac{\rho_1}{2} U_{vena}^2 \quad (A.82)$$

If p_{vena} is lower than vapor pressure p_{vapor} , it is assumed that the flow must be fully cavitating and a new inlet and discharge coefficient are calculated by:

$$p_1 = p_{vapor} + \frac{\rho_1}{2} U_{vena}^2 \quad (A.83)$$

$$C_d = C_c \sqrt{K} = C_c \sqrt{\frac{p_1 - p_{vapor}}{p_1 - p_2}} \quad (A.84)$$

In case of non-cavitating turbulent flows, the exit velocity of the droplets is equal to mean velocity, and the diameter of the jet at the nozzle is equal to the nozzle diameter. When the nozzle is cavitating, those values are calculated as:

$$U_{eff} = U_{vena} - \frac{p_2 - p_{vapor}}{p_1 \cdot U_{mean}} \quad (A.85)$$

$$A_{eff} = A \cdot \frac{U_{mean}}{U_{eff}} \quad (A.86)$$

$$D_{eff} = \sqrt{\frac{4 \cdot A_{eff}}{\pi}} \quad (A.87)$$

The spray angle (θ) in the nozzle is estimated using an aerodynamic model.

$$\tan\left(\frac{\theta}{2}\right) = \frac{4 \cdot \pi}{A} \sqrt{\frac{\rho_g}{\rho_l}} \cdot f(T) \quad (A.88)$$

Where $A = 3 + 0.28 \left(\frac{L}{D}\right)$ and $\frac{L}{D}$ is the length-to-diameter ratio of the nozzle. The function $f(T)$ is approximated by:

$$f(T) = \frac{\sqrt{3}}{6} (1 - \exp(-10T)) \quad (A.89)$$

$$T = \left(\frac{Re}{We} \right)^2 \cdot \frac{\rho_l}{\rho_g} \quad (A.90)$$

Instead of using the nozzle flow model, it is possible to specify empirical constant values for discharge coefficient and spray angle. Then the empirical discharge coefficient is used to calculate the effective injection velocity and initial drop size at the nozzle exit.

There are two options for specify the spray cone angle: one is user-specified constant value the other is using a correlation.

The correlation has the quadratic form and is:

$$\vartheta = -0.0025\eta^2 + 0.908\eta - 7.07 \quad (A.91)$$

$$\eta = (0.3R_p)^{0.5} \log_{10} \left(\frac{R_p^2 \theta^3}{m^2} \right) \quad (A.92)$$

R_p , θ and m represent the pressure ratio, dimensionless surface tension and fuel molecular weight:

$$R_p = \frac{P_{sat}(T_{inj})}{P_\infty} \quad (A.93)$$

$$\theta = \frac{a_0 \sigma}{k_b T_{inj}} \quad (A.94)$$

Where $P_{sat}(T_{inj})$, P_∞ , σ and k_b represent fuel saturation pressure at injection temperature T_{inj} , ambient gas pressure, surface tension and Boltzmann constant, respectively. a_0 is the molecular surface area defined by $a_0 = (36\pi)^{\frac{1}{3}}(V_l)^{\frac{2}{3}}$, and V_l is the liquid molecular volume. (ANSYS 2024a)

Appendix B

This appendix explains in detail all the processes made to achieve a valid model to implement in ANSYS Forte.

Figures B1 and B2 show the two models drawn.

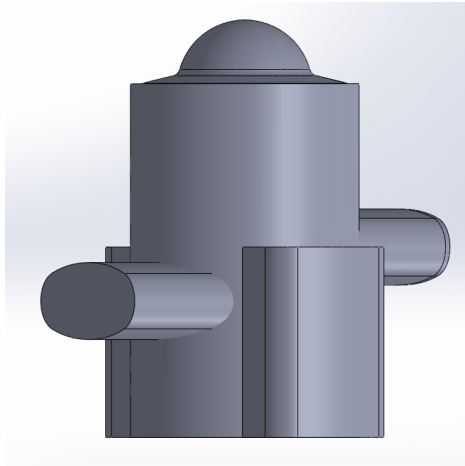


Figure B 1 – Two-stroke engine without crankshaft.

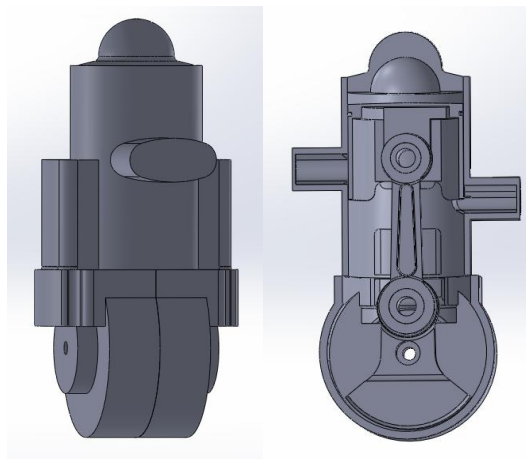
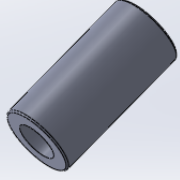
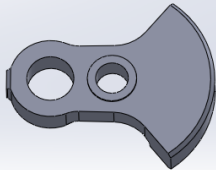
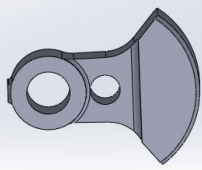
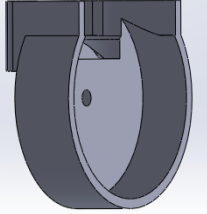
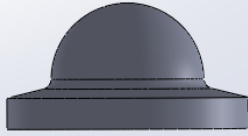
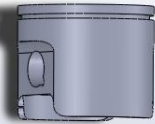
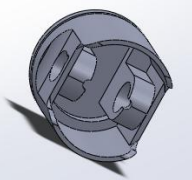
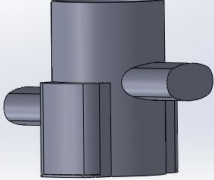
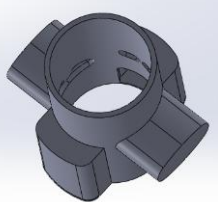


Figure B 2 – Two-stroke engine with the crankshaft.

On the table B1, there is a list of the engine parts drawn on SolidWorks.

Table B 1 - Drawings of engine parts.

Part name	Part Drawing	
Connecting Rod		
Connecting Rod Pin		
Crank		
Crankcase		
Dome		
Piston		
Piston Pin		
Piston Skirt		

The other model used was a four-stroke engine, provided by ANSYS Forte, and its parts are explicit in Figure B3.

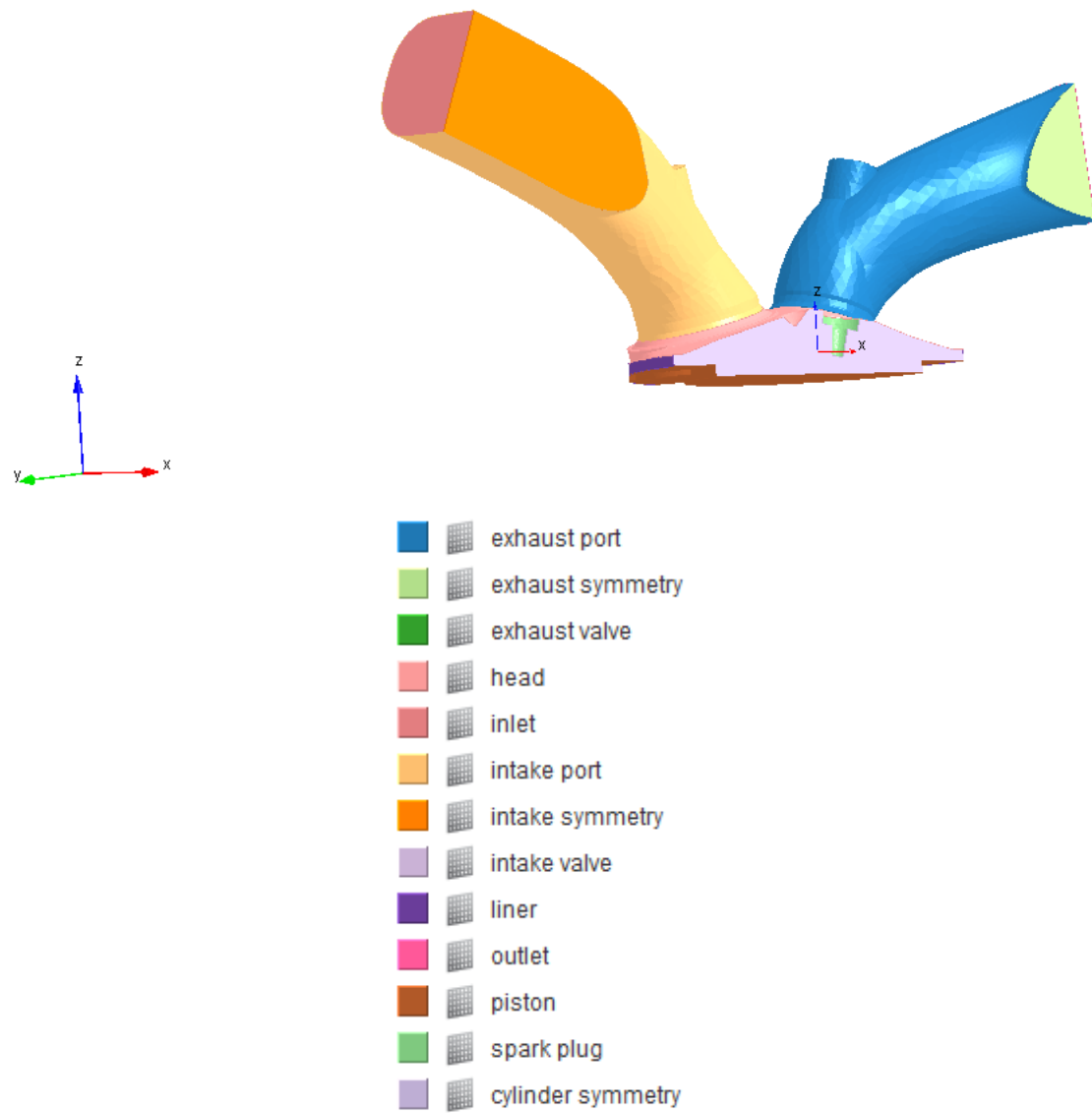


Figure B 3 – Four-stroke engine and its parts. (Images from ANSYS Forte)

Appendix C

Mesh update intervals are controlled by a combination of the following parameters and constraints.

Time interval

Mesh will be updated if the elapsed time since the previous mesh update exceeds this user-specified time interval.

Rotation/crank Angle Interval

The mesh update interval is controlled to be approximately equivalent to this angle interval. This angle is with respect to the rotation motion of the highest RPM in the simulation system, including both slider-crank motion (piston motion in ICs engine cases), simple rotation, and planetary motion (including both primary rotation and secondary rotation).

Flow Travel Distance

This distance threshold is used to limit the mesh update interval to be sufficiently small such that the distance the flow with the largest velocity magnitude can travel between two consecutive mesh updates will not exceed this threshold.

Spray Particle Travel Distance

This distance threshold is used to limit the mesh update interval to be sufficiently small such that the distance the fastest-traveling spray particle can travel between two consecutive mesh updates will not exceed this threshold.

Flame Propagation Distance

This distance threshold is used to limit the mesh update interval to be sufficiently small such that the distance the fastest-traveling flame can propagate between two consecutive mesh updates will not exceed this threshold.

The values used are resumed in Table C1 and they are the default values from the system.

Table C 1 - Parameters for Mesh Update Controls.

Mesh Update Controls	
Time Interval	0.0001 s
Rotation/Crank Angle Interval	0.75°
Flow Travel Distance	0.5 cm
Spray Particle Travel Distance	0.1 cm
Flame Propagation Distance	0.1 cm

Material Point

This point has to be inside the geometry, during the entire cycle, and it enables the automatic generation to stay within the boundaries. This should be set properly so the automatic meshing can work properly.

Global Mesh Size

This parameter affects meshing and refinement throughout the system. This is a specified dimension of a cell throughout the system to use as a standard for specifying other mesh sizes, usually as a fraction of this value.

Point Refinement Depth

A Point Refinement is a sphere of mesh-size influence, where you specify the minimum size for a cell edge within that sphere, relative to the Global Mesh Size, the location of the

point at the centre of the sphere, and the radius of the sphere in absolute physical units. These parameters are entered in the Point Refinement Editor panel after a new control is created.

Surface Refinement Depth

Surface refinement allows you to specify a mesh-size constraint at any surface defined in the geometry, such as an inlet or valve surface. The Editor panel includes specification of the minimum size relative to the Global Mesh Size, as well as selection of one or more boundaries at which the size constraint will apply.

Solution Adaptive Meshing

Solution adaptive meshing allows refining the mesh based on a solution field (or gradient) at the current time step. Both a solution field and selection criteria must be specified. Cells meeting the selected criteria will be refined one level per mesh update, up to the maximum depth specified in the control. Previously refined cells that no longer meet the criteria will be coarsened one level per mesh update, up to the default cell depth, unless influenced by another control. Two types of criteria were used in this simulation:

1. Statistical

This will target cells whose field value lies beyond a user-specified statistical significance of the bulk fluid value, given as a multiple of the standard deviation (sigma) of the field or gradient average:

$$\begin{aligned} low_{threshold} &= field_{average} + sigma_{threshold} \times sigma \\ high_{threshold} &= infinity \end{aligned}$$

Cells whose field or gradient value is greater than $low_{threshold}$ and less than $high_{threshold}$ will be targeted for refinement. This approach is especially useful when applied to gradients. A sigma threshold value between 0.5 and 1.0 is recommended. A lower value lowers the threshold used to target cells and therefore leads to more refinement, while a higher value raises the threshold and results in less refinement.

2. Absolute value

This allows expressing the range of values used to target cells directly. Cells whose field or gradient value is greater than the given lower bound and less than the given upper bound will be targeted for refinement (ANSYS 2024b).

In Figure C1 there is a representation of the mesh refinement window setup window in ANSYS Forte. The setup is similar for all different types of refinements, the parameters that change are described in Table C2.

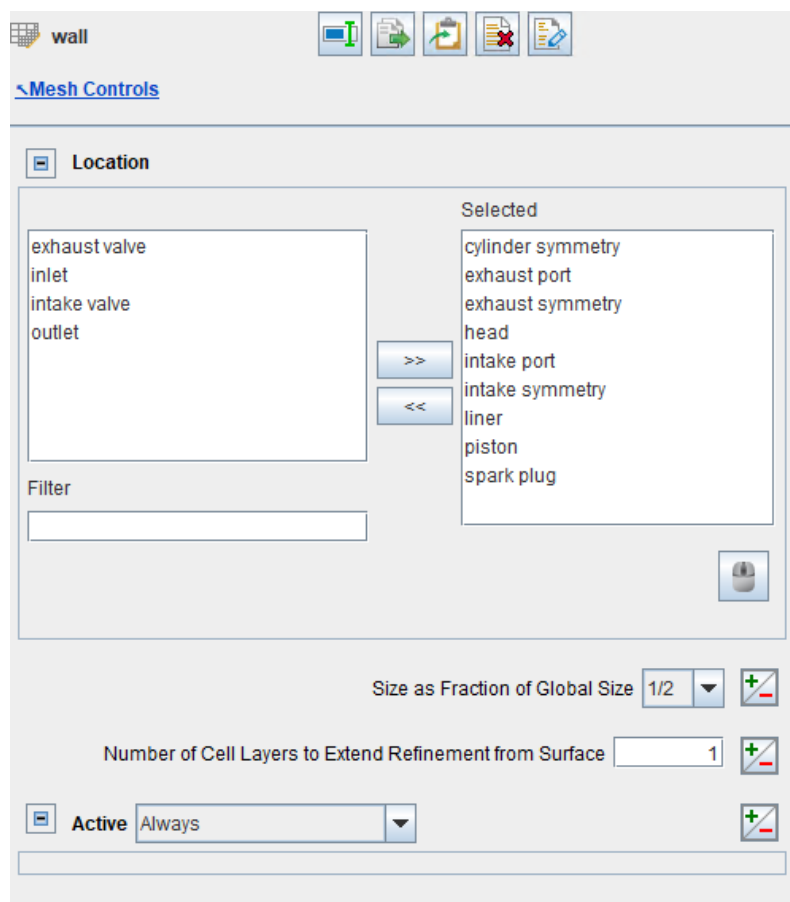


Figure C 1 – Mesh refinement setup window.

Table C 2 - Details of the refinement types and settings.

Name	Location	Refinement Type	Size Fraction
wall	cylinder symmetry; exhaust port; exhaust symmetry; head; intake port; intake symmetry; liner; piston	Surface	1/2
open	inlet; outlet	Surface	1/2
spark	$x = 0.47937 \text{ cm}$ $y = 0.082215 \text{ cm}$ $z = -0.14599 \text{ cm}$	Point radius = 0.5 cm	1/8
valves	exhaust valve; intake valve	Surface	1/4
tdc1	head; liner; piston	Surface	1/4
tdc2	head; liner; piston	Surface	1/4

Name	Cell Layers	Active
wall	1	Always
open	2	Always
spark	N/A	Always
valves	2	Always
tdc1	2	340-380 CA
tdc2	2	700-740 CA

Other mesh refinements were the Solution Adaptive Mesh Refinement, and they are described in Table C3.

Table C 3 – Solution Adaptive Mesh refinement parameters.

Name	Quantity Type	Solution Variables	Bounds
SAM-Temperature	Gradient of Solution Field	Temperature	Statistical; sigma threshold=0.5
SAM-Velocity	Gradient of Solution Field	VelocityMagnitude	Statistical; sigma threshold=0.5
SAM-G	Solution Field	G	Absolute Range Lower Bound = -0.3 Upper Bound = 0.3

Table C 4 - Solution Adaptive Mesh refinement parameters – Continuation.

Name	Size Fraction	Active	Location
SAM-Temperature	1/4	700-800CA	Sub-volumes = chamber
SAM-Velocity	1/2	Always	Entire Domain
SAM-G	1/4	700-760 CA	Sub-volume=chamber

Appendix D

In this Appendix, all the configurations used in the four-stroke engine are resumed, from ANSYS Forte User's Guide (ANSYS 2024b)

Transport

Next in the workflow is the definition of the fluid transport models using the Transport workflow item. The Editor panels for the two items under the Transport node, Turbulence and Fluid Properties, are described below. The Transport Editor panel provides settings for **Fluid Properties**. The parameters on this panel are reference properties used to calculate the turbulent fluid properties. These fluid property correlations are explained in the following paragraphs and also described in the tool tips. The Body Acceleration terms in the fluid transport model can be used to specify acceleration due to gravity. The equations that use these properties are defined in the Ansys Forte Theory Manual.

- **Prandtl Number:** Prandtl number of the laminar fluid flow, defined as

$$Pr_L = \frac{c_p \mu}{\lambda} \quad (D.1)$$

Where c_p is the specific heat at constant pressure, μ is dynamic viscosity of laminar flow, and λ is the thermal conductivity of laminar flow. Note that Pr_L is only used in the wall heat transfer model.

- **Reciprocals of Turbulent Prandtl Number and Reciprocal Turbulent Schmidt Number:** The reciprocals of turbulent Prandtl Number and turbulent Schmidt Number. These two parameters are used to convert dynamic viscosity into thermal diffusivity and mass diffusivity, respectively, for turbulent flow transport calculation. The turbulent Prandtl Number and turbulent Schmidt Number are defined as:

$$Pr_T = \frac{\nu_T}{\alpha_T} \quad (D.2)$$

$$Sc_T = \frac{\nu_T}{D_T} \quad (D.3)$$

Where α_T is turbulent thermal diffusivity, D_T is turbulent mass diffusivity, ν_T is turbulent kinematic viscosity. In Ansys Forte, the effective dynamic viscosity for turbulent flows, $\mu_T = \rho\nu_T$, is the sum of two terms, a laminar term and a turbulent term, that is,

$$\mu_T = \mu_L + \rho c_\mu \frac{k^2}{\varepsilon} \quad (D.4)$$

Where k and ε are turbulent kinetic energy and its dissipation rate, respectively, and c_μ is a constant in the turbulence model. In turbulent flow simulations, the laminar term μ_L is typically much smaller than the turbulent term, and hence the effective dynamic viscosity is simply noted as μ_T .

- **Air Mu Coefficient 1** ($C_{\mu1}$) and **Air Mu Coefficient 2** ($C_{\mu2}$): Coefficients in Sutherland's formula for calculating laminar viscosity of the fluid as a function of temperature:

$$\mu_L = \frac{C_{\mu1} T^{1.5}}{(T + C_{\mu2})} \quad (D.5)$$

- **Air Lambda Coefficient 1** ($C_{\lambda1}$) and **Air Lambda Coefficient 2** ($C_{\lambda2}$): Coefficients in the correlation for calculating laminar thermal conductivity of the flow as a function of temperature:

$$\lambda_L = \frac{C_{\lambda1} T^{1.5}}{(T + C_{\lambda2})} \quad (D.6)$$

Note that λ_L is only used in spray vaporization model for computing the thermal conductivity of air (ANSYS 2024b).

Solid Cone Injector

Table D 1 – Parameters for Solid Injector.

Solid Injector	
Composition (Mass Fraction)	Name: E5 iso-Octane (ic8h18) = 0.954 Ethanol (c2h5oh) = 0.045 Methanol (ch3oh) = 0.001
Injection Type	Pulsed Injection
Parcel Specification	Droplet Density Droplet Number Density = 1
Inflow Droplet Temperature	400 K
Spray Initialization	Discharge Coefficient and Angle Discharge Coefficient = 0.7
Cone Angle Specification	User-Specified Cone Angle = 14.0°
Droplet Size Distribution	Rosin-Rammler Distribution Shape Parameter = 3.5 Initial Sauter Mean Diameter = 120.0μm
KH Model Constants	Size Constant of KH Breakup = 0.5 Time Constant of KH Breakup = 10.0 Critical Mass Fraction for New Droplet Generation = 0.03 Impose SMR Conservation for KH Breakup = Activate
RT Model Constants	Size Constant of RT Breakup = 0.5 Time Constant of RT Breakup = 1.0 RT Distance Constant = 1.9
Use Gas Jet Model = Activate	Gas Entrainment Constant = 0.5

Injection

Table D 2 – Parameters for injection.

Injection	
Injection Type	Pulsed
Timing	Crank Angle
Crank Angle Option	Cyclic Start = 380.0° Duration = 40.0°
Velocity Profile	Figure X

Total Mass Injected	50.85 mg
---------------------	----------

Editor

injection_380_40

Column 1 Units: Angle degrees

Column 2 Units: None None

Profile Data

Column 1	Column 2
3.799E2	0
380	2.941176E-3
420	2.941176E-3
420.1	0

Insert Row Append Row Remove Selected Rows Load CSV

Name: injection_380_40

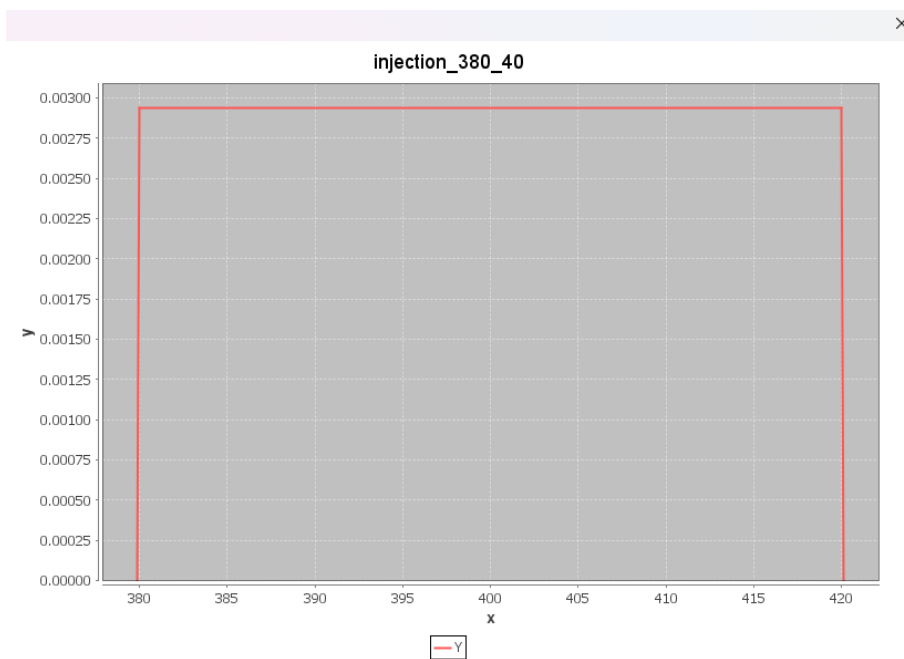


Figure D 1 – Injection velocity profile.

Nozzles

Table D 3 – Positions and diameters for nozzles.

nozzle1	
Location	$x = -4.60752 \text{ mm}$ $y = 0.55158 \text{ mm}$ $z = 5.62716 \text{ mm}$
Spray Direction	$x = 3.0415 \text{ mm}$ $y = 2.73735 \text{ mm}$ $z = -9.12449 \text{ mm}$
Nozzle Size	Nozzle Diameter = 90.0 μm
nozzle2	
Location	$x = -4.9155 \text{ mm}$ $y = 1.033995 \text{ mm}$ $z = 5.741271 \text{ mm}$
Spray Direction	$x = 1.49781 \text{ mm}$ $y = 5.08692 \text{ mm}$ $z = -8.4782 \text{ mm}$
Nozzle Size	Nozzle Diameter = 90.0 μm
nozzle3	
Location	$x = -5.88529 \text{ mm}$ $y = 0.630237 \text{ mm}$ $z = 5.363811 \text{ mm}$
Spray Direction	$x = -2.90254 \text{ mm}$ $y = 2.74977 \text{ mm}$ $z = -9.16592 \text{ mm}$
Nozzle Size	Nozzle Diameter = 90.0 μm

Spark Ignition

Table D 4 - Parameters for spark ignition.

Spark0	
Location	$x = 0.47937 \text{ cm}$ $y = 0.082215 \text{ cm}$ $z = -0.14599 \text{ cm}$
Timing	Crank Angle
Crank Angle Option	Cyclic Starting Angle = 717.5° Duration = 1.0°
Spark Energy	Energy Release Rate = 30.0 J/sec Energy Transfer Efficiency = 0.5 Initial Kernel Radius = 0.5 mm Number of Flame Particles = 3000

Appendix E

In this appendix are described the parameters of some Boundary Conditions.

Exhaust

Table E 1 - Parameters for the exhaust wall boundary condition.

exhaust_port	
Location	exhaust_port
Thermal Boundary Condition	Wall Temperature, Constant Temperature = 485 K

Liner

Table E 2 -Parameters for the wall boundary condition.

liner	
Location	liner
Thermal Boundary Condition	Wall Temperature, Constant Temperature = 500 K

Head

Table E 3 -Parameters for the head wall boundary condition.

head	
Location	head
Thermal Boundary Condition	Wall Temperature, Constant Temperature = 485 K

Spark Plug

Table E 4 - Parameters for the spark plug wall boundary condition.

spark-plug	
Location	Spark-plug
Thermal Boundary Condition	Wall Temperature, Constant Temperature = 485 K

Intake-valve

The intake lift profile is a document provided by ANSYS Forte.

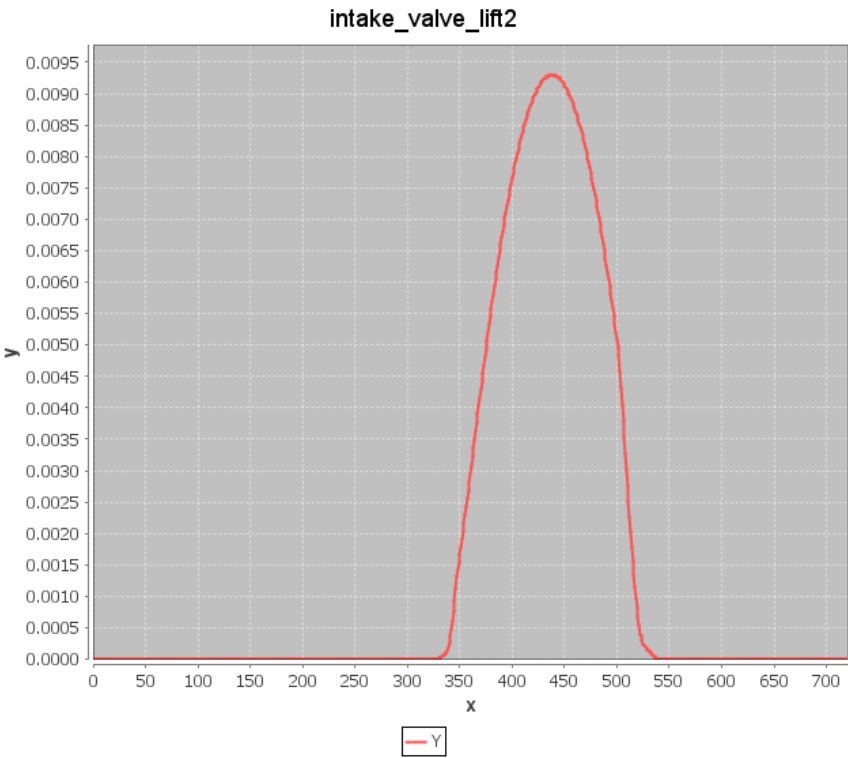
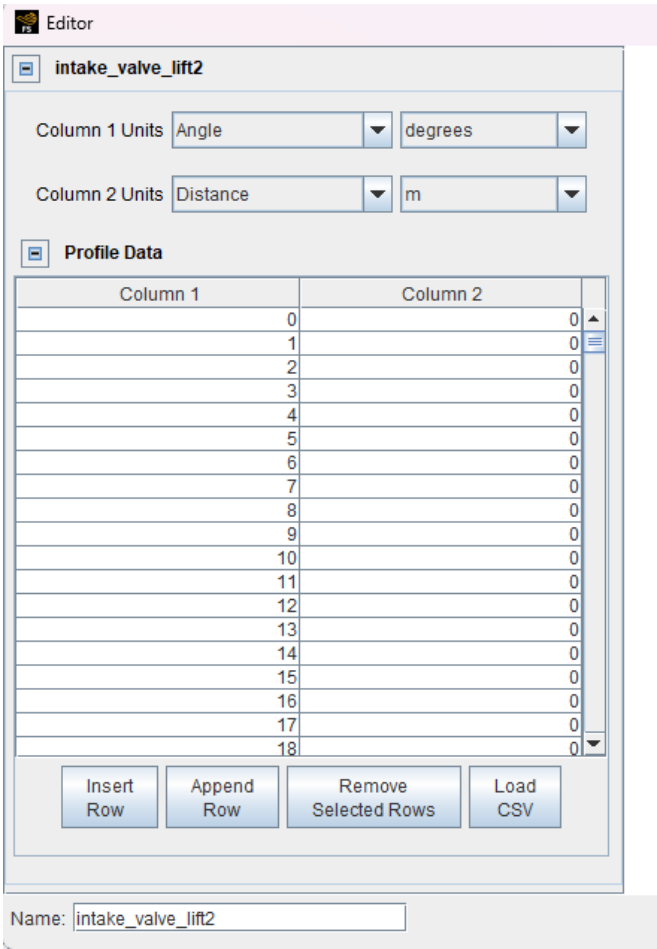


Figure E 1 – Intake valve lift profile.

Exhaust Valves

Table E 5 - Parameters for the exhaust valves wall boundary condition.

exhaust_valve	
Location	exhaust_valve
Thermal Boundary Condition	Wall Temperature, Constant Temperature = 777 K
Wall Motion – ON	Motion Type: Offset Table
Direction	$x = -0.327218 \text{ cm}$ $y = 0.0 \text{ cm}$ $z = -0.944949 \text{ cm}$
Time Option	Crank Angle Lift Profile – Figure X
Moment Type	Valve
Multi Select the Valve Seat and the Surface it Contacts	head exhaust-valve
Valve Motion Activation Threshold	0.02 cm
Approx. Cells in Gap At Min. Lift	1.5

The exhaust lift profile is a document provided by ANSYS Forte.

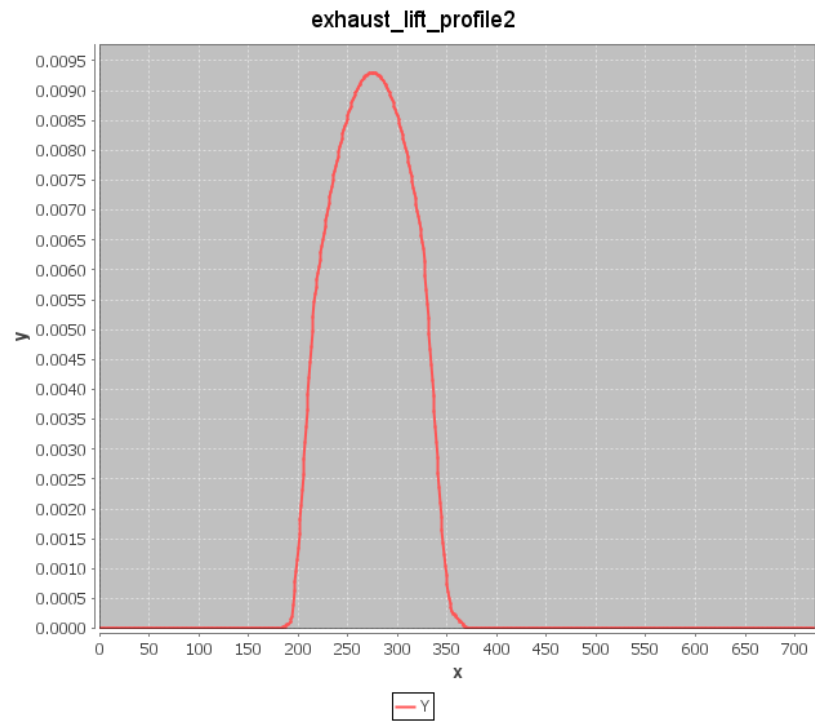
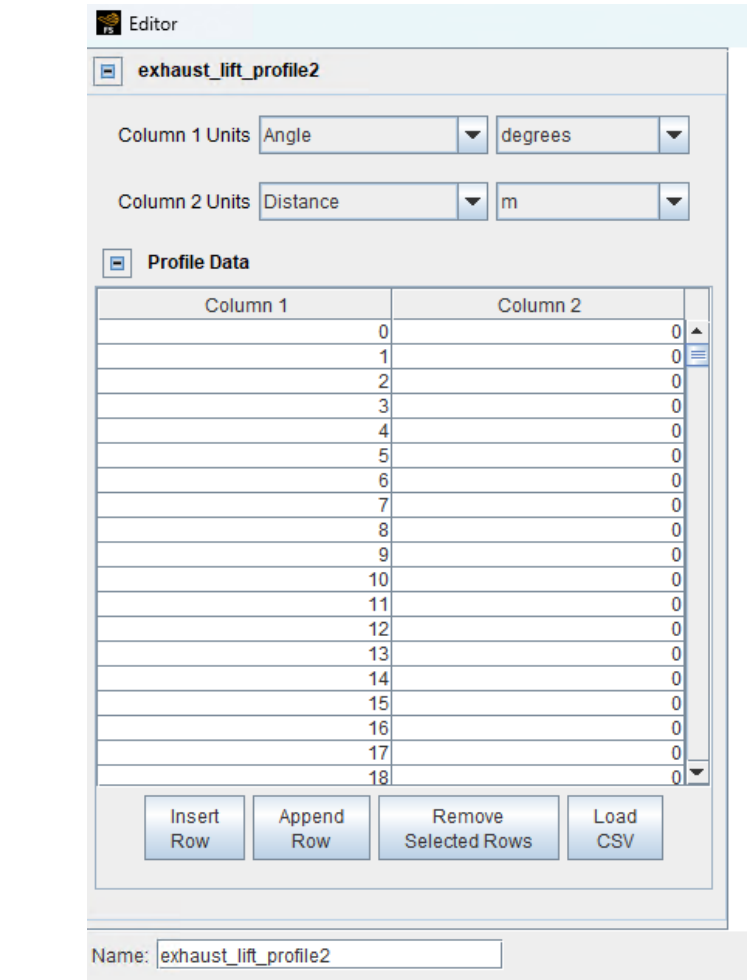


Figure E 2 - Exhaust lift profile.