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Numerical study of an Homogeneous Compression Charge Ignition engine under oxygen enrichment in a power-to-gas system

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Abstract

In the midst of an energy and environmental crisis, the search for efficient and sustainable technologies is in full swing. Renewable energies appear to be a solution, but their intermittent nature makes them challenging to use. Therefore, the focus is on finding a way to store this energy. Various systems exist, including power-to-fuel, which aims to convert excess electricity into fuel through different processes. When electricity demand increases again, the stored fuel can be used to meet energy needs.

Among the different technologies, the HCCI (Homogeneous Charge Compression Ignition) engine seems to be well-suited for the power-to-fuel-to-power context. However, its limited operating range and resulting low power density pose significant challenges to its implementation. Numerous strategies exist to enhance its power density, and this study investigates the impact of oxygen enrichment.

Conducting experimental tests involves certain risks, which makes the numerical study of oxygen enrichment highly valuable for predicting its effect on engine performance. Therefore, this work develops a numerical 0D model of the HCCI engine to predict the influence of oxygen enrichment on engine performance. An uncertainty analysis of the model is then performed to assess its reliability, and finally, a comparison with other technologies situates this improved engine.

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Contents

Introduction	1
1 General Context	2
1.1 Transition to Renewable Energy	2
1.2 Energy Storage in the Energy Transition	2
1.3 Fuel Production	6
1.3.1 Getting Electricity	7
1.3.2 Electrolysis	8
1.3.3 Hydrogenation of Carbon Dioxide to Methane	10
1.4 From Gas to Power Technologies	13
2 Theoretical overview	15
2.1 Principle of the HCCI	15
2.1.1 Combustion Phenomenon	15
2.1.2 Limited Operating Range	19
2.1.3 Efficiencies and MEP	20
2.1.4 Emissions	24
2.2 HCCI Amelioration : Oxygen Enrichment	26
2.2.1 Equivalence Ratio	26
2.2.2 Intake Temperature	27
2.2.3 Power to Fuel Context	28
2.2.4 Oxygen-Enriched Combustion Emissions	30
3 HCCI Modeling : 0D Model	31
3.1 Mathematical and Thermodynamic Relations Necessary for the Model	32
3.1.1 Geometric Principles	32
3.1.2 Thermodynamic Principles	34
3.2 0D Model	37
3.2.1 Model Representation	37
3.2.2 Model Explanation	39
3.3 Model Limitations	40
3.4 Experimental Data	42
3.4.1 Experiment Specification	42
3.4.2 Experimental Results Analysis/Correction	43
3.5 Model Calibration and Validation	46
3.5.1 Bottom Dead Center State Calibration	47
3.5.2 Ignition Timing Calibration : Scaling Factor Alpha	49
3.5.3 Pressure Calibration	51

4	Results and Discussions	52
4.1	Data Choices Justification	52
4.2	MPRR/CA05-FuelMEP Correlation	53
4.3	Methane-Air Combustion	55
4.3.1	Ignition Timing	55
4.3.2	Power Output	57
4.4	Oxygen Enrichment	59
4.4.1	Alpha and MPRR Limit Choices	59
4.4.2	Method	60
4.4.3	Results	62
4.4.4	Discussion	67
4.4.5	Power output	69
4.5	Uncertainty Analysis	70
4.5.1	Uncertainty of the Inlet Conditions of the Model	70
4.5.2	Uncertainty Analysis on Cantera Integration	73
4.6	Technologies Comparison	74
	Conclusion	76
	References	78
	Appendix	80

Nomenclature

Abbreviations

IMEP _g	Indicated gross mean effective pressure
IMEP _n	Net indicated Mean effective Pressure
AEM	Anion exchange membrane
BDC	Bottom dead center
BMEP	Brake mean effective pressure
CA10	Crank angle at 10 % of the combustion
CA50	Crank angle at 50 % of the combustion
CA90	Crank angle at 90 % of the combustion
CAD	Crank angle degree
CAES	Compressed Air Energy Storage
CCS	Carbon capture systems
CHP	Combined heat and power
CHR	Cumulative Heat Release
CI	compression ignition
COV	Coefficient of Variation
DOC	Duration of combustion
EGR	Exhaust gas recirculation
ES	Energy storage
EVC	Exhaust valve closing
EVO	Exhaust valve opening
FMEP	Friction mean effective pressure
FuelMEP	Fuel mean effective pressure
HCCI	Homogeneous Charge Compression Ignition
HER	Hydrogen evolution reaction
HRR	Heat release rate

IMEP	Indicated mean effective pressure
IVC	Intake valve closing
IVO	Intake valve opening
LAES	Liquid air energy storage
LHV	Lower Heating Value
MEP	Mean effective pressure
MPRR	Maximum Pressure Rise Rate
ODE	Ordinary differential equation
OER	Oxygen evolution reaction
PCE	Polynomial Chaos Expansion
PCP	Peak cylinder pressure
PEM	Proton exchange membrane
PHS	Pumped Hydro Storage
PRR	Pressure rise rate
PtG	Power-to-Gas
RES	Renewable energy sources
RoHR	Rate of heat release
RPM	Rotations per minute
SI	Spark ignition
SMES	Superconducting Magnetic Energy Storage
SOC	Start of combustion
SOEC	Solid oxide water electrolysis cell
TDC	Top dead center
TDI	Turbocharged direct injection
VRES	Variable renewable energy sources
Chemicals	
CH ₄	Methane

CO₂ Carbon dioxide

H₂O Water

H₂ Hydrogen

NO_x Nitrogen oxides

O₂ Oxygen

CO Carbon monoxide

HC Hydrocarbons

Ru Ruthenium

Symbols

α Scaling factor

χ Percentage of oxygen

ϵ_{ex} Exhaust loss coefficient

ϵ_{ht} Parietal loss coefficients

η_b Break efficiency

η_c Combustion efficiency

$\eta_{ind,g}$ Gross indicated efficiency

$\eta_{ind,n}$ Net indicated efficiency

η_{mec} Mechanical efficiency

η_{ti} Thermodynamic efficiency

γ Specific heat ratio

n_f Number of moles of fuel

P_{in} Mean in-cylinder pressures during the intake stroke

p_{IVC} In-cylinder pressure at inlet valve closing

P_{out} Mean in-cylinder pressures during the exhaust stroke

Q_{exhMEP} Exhaust heat losses

Q_{gross} Gross heat release

Q_{htMEP} Parietal heat losses

Q_{loss}	Heat loss
Q_{net}	Heat release net
T_{IVC}	In-cylinder temperature at inlet valve closing
T_{wall}	Temperature of the walls of the cylinder
V_d	Displacement volume
ϕ	Fuel-air ratio
ρ	Density
τ	Compression ratio
c_p	Constant pressure specific heat capacity
c_v	Constant volume specific heat capacity
m_f	Fuel mass
m_{air}	Air mass
R	Gas constant
h	Convection coefficient
L	Conrod's length
n	Numbre of moles
p	Pressure
r	Crankshaft's radius
S	Stroke
T	Temperature
U	Internal energy
V	Volume

Introduction

The increasing demand for decarbonization solutions in the energy sector has become more prominent over the years. Society is urgently seeking rapid solutions to drastically reduce CO₂ emissions in pursuit of a net-zero emission future. One of the key steps in these solutions lies in energy storage, which remains one of the most discussed topics in the energy sector. Among various existing storage solutions, Power to Gas technology holds long-term promise. This technology involves converting surplus electricity into hydrogen through water electrolysis and subsequently transforming the hydrogen into methane by absorbing CO₂ from the air. The ultimate goal is to achieve a global-scale CO₂ emission of zero throughout the entire cycle.

In terms of energy conversion back to electricity, Homogeneous Charge Compression Ignition (HCCI) engines can play a significant role due to their high overall efficiency of compression ignition engines with low emission characteristics. It is in this direction that this research work will focus.

This work is based on both the experimental data from the UCLouvain research HCCI engine and the extensive research and theses available on the subject. The objective is to develop a 0D modeling approach using the Cantera software to simulate an HCCI engine running on methane under varying oxygen and power density conditions. The precise modeling of the combustion initiation is crucial to observe the engine's ability to vary its power density. This can be achieved by analyzing the cases where the engine's limit conditions are reached. The aim is to investigate the potential benefits that this variation can bring forth.

The structure of this work can be divided into four main parts. The first and second parts are based on the literature and are considered the state of the art in our document. They respectively cover the general context, focusing on the power-to-gas-to-power system, and the theory of HCCI engines, which is essential for the rest of the thesis.

The third part begins by explaining the general model and its capabilities and limitations. It further delves into the management of result data, outlining how the values obtained from our model were calibrated based on the provided experimental data.

Finally, the last part presents our results and discussions, culminating in a comprehensive analysis of the findings.

By combining experimental data, existing research, and advanced modeling techniques, this research aims to provide valuable insights into the performance and potential advantages of utilizing methane in an HCCI engine under varying oxygen and power density conditions. The results obtained from this study can contribute to the optimization and further development of HCCI engines for efficient and clean energy conversion, aligning with the global goals of decarbonization and sustainable energy utilization.

1 General Context

The beginning of this section entails providing a brief overview of the current environmental situation. Subsequently, the significance of energy storage technologies and the various types will be elucidated, ultimately unveiling the power-to-gas concept utilized throughout the rest of this work.

Following this, the process of electricity production and its transformation into the desired final gas form will be explained, encompassing the stages of electrolysis and methanation. Lastly, a concise explanation of the different technologies comparable to our study subject will be provided.

1.1 Transition to Renewable Energy

For many years now, climate change has been one of the biggest threats to global health. The warming of the Earth's surface is primarily caused by greenhouse gas emissions, which trap heat from the sun and envelop the Earth. The emission of these gases is mainly due to the extraction, transformation, and combustion of fossil fuels (such as oil, natural gas, and coal) required for energy consumption. In response to this, the European Union aims to achieve carbon neutrality by 2050 through the implementation of three key measures: reducing the current use of fossil fuels within the EU by 95%, recycling carbon through the promotion of technologies that capture it from the atmosphere, and finding long-term storage solutions [1].

Renewable energy sources appear to be the solution for this energy transition to achieve the desired reduction in greenhouse gas emissions. However, the intermittency of some renewable energy sources, such as solar and wind energy, due to weather conditions, can make it challenging to rely solely on these sources for a consistent and stable energy supply. In fact, renewable energy sources operate at maximum power for only about 2000 hours per year, compared to fossil fuel power plants that can operate on average up to 7500 hours per year at their installed capacity [2]. Therefore, it is necessary to ensure the availability of sufficient alternative energy reserves when renewable energy is not available. This makes energy storage one of the biggest challenges in this energy transition.

1.2 Energy Storage in the Energy Transition

The energy systems need to be more flexible as we move towards a more sustainable future. And there are a variety of options available for this, including energy storage, which is crucial given the variability of various renewable energy sources (RES). The most significant RES, such as the ones working with wind and solar energy, are the main ones when discussing variability since they are less predictable and more variable than RES like biomass or geothermal, which tend to operate more like a constant power supplier.

Energy input	Energy output	Conversion process	Storage classification
Electricity	Electricity		Electricity Mechanical Energy Storage Energy Electrochemical Energy Storage Storage Electrical Energy Storage
Electricity	Thermal Energy	Power-to-Thermal	
Thermal Energy	Thermal Energy	N/A	Thermal Energy Storage
Electricity	Gaseous Fuels	Power-to-Gas	
Electricity	Liquid Fuels	Power-to-Liquids	Chemical Energy Storage
Solar Thermal Energy	Gaseous/Liquid Fuels	Solar-to-Fuels	

Table 1.1: ES technologies classification [6]

As a result, those RES are referred to as variable renewable energy sources (VRES) [3].

So, sure, there are additional potential ways to combat this VRES and boost this flexibility, such as expanding or upgrading the grid, increasing the amount of dispatchable backup power, and refining the VRES forecast. However, these solutions frequently face significant challenges. For instance, enhancing the grid faces significant public opposition [4], dispatchable backup power typically produces high levels of greenhouse gas emissions, and enhancing VRES predictions reduces uncertainty but not variability. As a result, we understand that energy storage has a greater potential than the others and must be taken into account.

Energy storage (ES) can improve not only VRES-related applications but also other stages of the value chain for electricity. By lowering the cycle of base load generation and raising its average generating power, ES boosts chain efficiency overall while decreasing the operation of expensive and polluting peaking power plants. Grid reliability and security are assured by ES, which can ease frequency and voltage variations and relieve grid congestion.

Technologies for energy storage can be categorised based on their energy input and output. Although the input, which can be either thermal or electrical, is rather straightforward, the output has the option to be more varied. Table 1.1 clearly shows this categorisation based on their output.

Firstly, before delving into the description of these technologies, it's crucial to note that the quantification of these descriptions can be found in section 4.6, derived from the article [5], to prevent the text from being overwhelmed with numerical values.

Mechanical Energy Storage Technologies

First, there is mechanical energy storage [5], with Pumped Hydro Storage (PHS) being the most common technology. PHS involves two water reservoirs at different elevations, with energy stored by pumping water from the lower reservoir to the higher one. PHS can store large amounts of energy for months, but has a low energy density (0.5-1.5 Wh/l) and is limited by geographic location and environmental impact.

Another technology is Compressed Air Energy Storage (CAES), where air is compressed by an electrically-powered compressor and then preheated with fuel for expansion in a turbine to generate electricity. D-CAES has high power rating, large storage capacity, and moderate response time, but has low to moderate efficiency (40-60%) and emits carbon due to fossil fuel usage.

Flywheels store energy as rotational kinetic energy by spinning a flywheel with an electric motor, and have high power rating, high efficiency (75-85%), fast response time, and long lifetime, but have a high self-discharge rate.

Lastly, Liquid Air energy storage (LAES) stores thermal energy by air liquefaction and has a higher density than PHS or CAES, but has high costs associated with the liquefaction process and only shows high efficiencies if waste heat is recovered.

Electrochemical Energy Storage Technologies

Lead-acid or nickel-cadmium rechargeable batteries are examples of conventional batteries. They have a wide range of uses, including in power tools, automobiles, and laptops. Conventional batteries are inexpensive, have a moderate energy density, and are simple to use and charge. They are poisonous due to their chemical makeup, have a short lifespan, and need regular upkeep.

Redox batteries, commonly referred to as flow batteries, are built differently from standard batteries. They offer a higher energy storage capacity than ordinary batteries because they use two liquid reservoirs with different electrodes. Additionally, flow batteries are safer since a hazardous thermal discharge can be avoided by changing the liquid. However, they are more expensive than standard batteries and have a lower energy density. They also need a pumping mechanism to function.

Advanced batteries created to function at high temperatures of several hundred degrees Celsius include solid oxide and sodium-sulfur batteries. They have a lot of energy density, are durable, and are energy-efficient. However, they are more difficult to build, more expensive, and require cooling and thermal insulation to function.

Electrical Energy Storage Technologies

By accumulating positive and negative charges and creating a static electric field, supercapacitors are the most direct way to store electricity. They have a far longer cycle life than batteries and can execute several tens of thousands of cycles before needing to be recharged or discharged. In comparison to ordinary batteries, supercapacitors have a higher energy density (10–30 kWh/m³), improved efficiency (85–95%), but a way higher self-discharge rate (20–40%/day). Their high power density (500–10,000 W/kg), which is suggested for high power applications, is another important property. This technology is suitable for applications requiring quick response times because the storage capacity typically varies from milliseconds to seconds or a few minutes. To enhance power rating and storage capacity, supercapacitors can also be arrayed in modular systems by serialising or parallelizing [7].

In this type of energy storage we can also find Superconducting Magnetic Energy Storage (SMES). Instead of building up charges and creating a static electric field, the SMES sends current through a superconducting coil to create a dynamic electric field or magnetic field. Costly SMES and environmental problems brought on by potential effects of the powerful magnetic field, which are still unknown characteristics and effects, should be considered as major negatives for the moment.

Chemical Energy Storage Technologies

A Power-to-Gas (PtG) technology is a technology that converts surplus electricity into storable energy carriers such as hydrogen and methane, which can then be utilized as fuel for heating and transportation, as raw materials for the chemical industry, or transformed back into electricity. This technology is considered an important CO₂-free solution for the future energy landscape, particularly in the context of increasing renewable energy participation.

The PtG process consists of three main steps: input conversion to produce hydrogen from electricity, followed by a secondary conversion that produces methane from hydrogen and carbon dioxide, and finally utilization, which can encompass several usages. Alkaline electrolyzers are the most mature and commercially available technology for converting this electricity into hydrogen.

After electrolysis, hydrogen can be stored in pressurized vessels, liquid tanks, or metal-hydrides and porous carbon structures. Hydrogen can be directly injected up to certain limits into natural gas grids or converted into electricity in fuel cells, which can be very efficient, or adapted for use in gas-fired engines and turbines.

Methane, another PtG energy carrier, requires an additional conversion process called methanation, and a CO₂ supply. Although methane is three to four times more energy-dense than hydrogen, this conversion process makes PtG more complex, expensive, and less efficient for power-to-power applications. However, the advantage is that methane is fully compatible with existing natural gas structures and can replace fossil origin methane while conserving existing pipelines and being directly used in current gas-fueled appliances. Moreover, methanation requires carbon dioxide, which makes it possible to integrate PtG into biogas plants, upgrading biogas to biomethane or sewage, bioethanol, and other industrial plants that produce exhaust gas rich in CO₂.

Overall, PtG is a promising technology that offers long-term energy storage solutions, scalability to very large storage capacity sizes, and low self-discharge rates. With still some drawbacks in terms of efficiency and cost.

Figure 1.1 below shows an overview of the characteristics of these technologies in order to get an idea of the different solutions discussed previously.

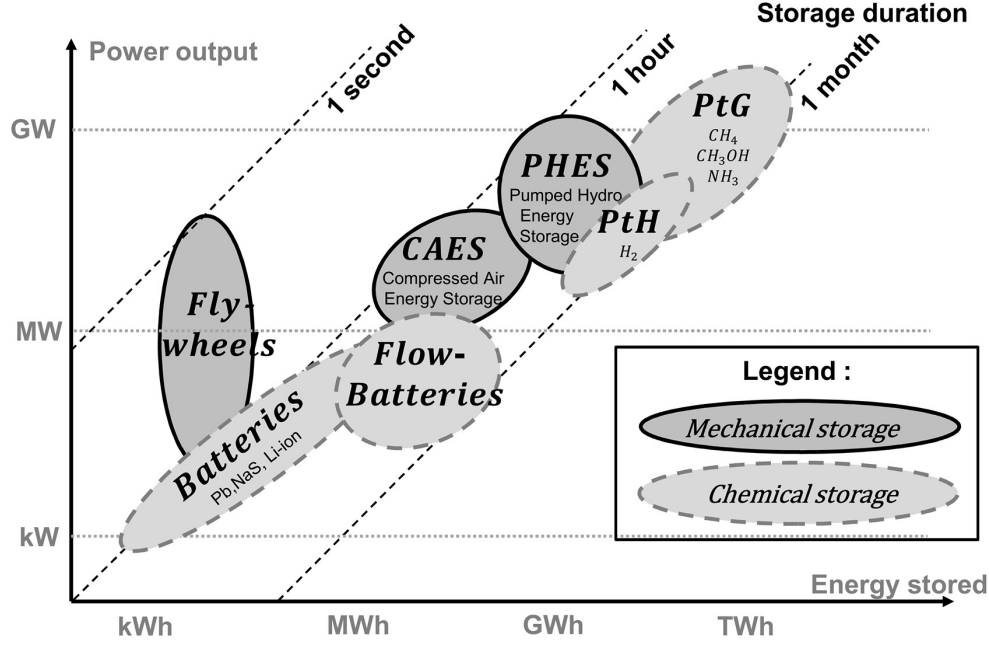


Figure 1.1: Difference in power output and energy stored for ES technologies [8]

The conclusion from this section is that there is no single ES technology that excels in all technical aspects, therefore selection should be based on a case-by-case analysis. Specifically, when it comes to the energy transition and the need for seasonal energy storage,... But the following two technologies show great promise: P2G, and P2L. The latter two have the advantage of integrating multiple energy markets and even the heavy duty transportation sector, allowing for a greater use of renewable sources in hydrocarbon-based applications, which is essential for the energy transition.

That's why, this work will examine power to gas and gas to power through an HCCI engine.

1.3 Fuel Production

The power-to-gas principle serves as the foundation of the generation of our fuel. Since obtaining methane is the ultimate goal of our fuel production, we must divide it into various steps. The first is obtaining renewable energy, where we will focus mostly on solar and wind power.

Hydrogen is then produced by electrolysis of water thanks to an electrolyser. The next step is first to capture carbon dioxide (CO_2) and then, to finally mix it with the hydrogen in order to produce methane. Recall that one of the key benefits of PtG is the ease with which energy may be transported as gas, particularly when that gas has a high energy density, as is the case with methane.

So we could afford to put our power plant far away from our energy source. But we decided to place them close to our power source. This is to may be, in future studies, be able to use the CO_2 from our exhaust for methanation and to be able to directly reuse the oxygen created during electrolysis for intake modifications of our engine.

1.3.1 Getting Electricity

As previously noted, we have selected wind and solar energy as (RES). These two energy sources are the ones that are taken into consideration in our situation because they are currently and according to forecasts, the most significant renewable resources for the future.

This may be seen in the graph below, which shows the amount of TWh produced by each resources in the world over time with a forecast presentation for 2030.

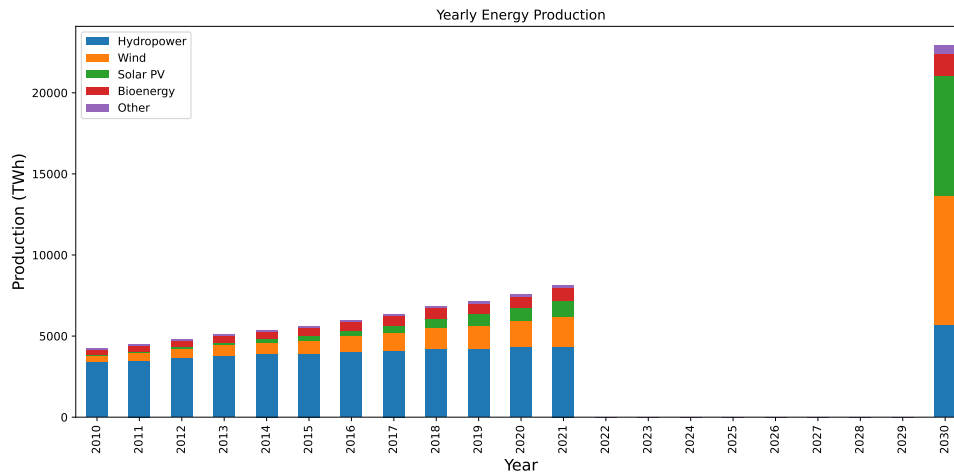


Figure 1.2: Evolution and difference of energy production between different RES [9]

Additionally, due to their modularity and flexibility of installation, these energy sources are considerably simpler to integrate into current energy systems. Whether it is a small village or the entire country's power grid, wind farms and solar installations can be customised to meet the unique requirements of a given region.

The first small-scale wind turbines were constructed in Belgium in the early 1980s, and the first solar photovoltaic systems were introduced in the early 1990s, marking the beginnings of sustainable wind and solar electricity. The demand for sustainable energy sources and an increasing awareness of climate change were to blame for this.

With the building of various wind farms, particularly in coastline and hilly regions, where wind resources are at their highest, wind energy development really got under way in the 1990s. In order to promote the installation of wind turbines, the government played a significant part in this by providing incentives and subsidies. A number of offshore wind farms were also constructed in the North Sea by the mid-2000s, further enhancing Belgium's renewable energy sources.

In the late 2000s, solar energy in Belgium had a tremendous boom. This was partly fueled by the government's generous green certificate programme, which ensured substantial returns for owners of solar photovoltaic (PV) systems. Due to Belgium's small size and high population density, large-scale solar farms were less practical, therefore rooftop solar PV installations received more attention.

Belgium had a total installed wind energy capacity of about 4 GW in 2021, with about 1.7 GW from offshore wind farms. The nation's installed PV capacity was around 5 GW on the solar front. Together,

these green energy sources met around 20% of Belgium’s overall demand for electricity, with wind making up a bigger portion than solar.

The complementarity between wind and solar energy in Belgium is an interesting characteristic of the country’s renewable energy industry. When there is less wind, there is frequently more sun, and vice versa, which helps to balance out the electricity generated from these sources over the course of a year.

The switch to renewable energy in Belgium has not been without difficulties, such as grid integration issues, worries about public acceptance, and the variable nature of wind and solar resources. However, the nation has advanced significantly in recent years. The future of sustainable wind and solar electricity in Belgium appears bright as a result of maintained technology breakthroughs and supportive policies.

1.3.2 Electrolysis

Nowadays, renewable-powered green hydrogen generation is one method that is increasingly being regarded as a means of lowering greenhouse gas emissions and environmental pollution in the transition towards global decarbonization. As a result, there is growing interest in developing a scalable and adaptable approach for producing and using this green hydrogen. This can be done by using renewable energy sources (solar, wind) to split water into hydrogen and oxygen like in Equation 1.1 and it is known as water electrolysis:



For this, four different types of water electrolysis technologies: alkaline water electrolysis, anion exchange membrane (AEM) water electrolysis, proton exchange membrane (PEM) water electrolysis, and solid oxide water electrolysis were developed based on their electrolyte, working conditions, and ionic agents (OH⁻, H⁺, O₂⁻). But in every situation, the fundamental principles are the same.

First the Alkaline water electrolysis. Alkaline water electrolysis is the most common technique. However, the major challenge associated with this technology is limited current densities due to moderate OH⁻ mobility and the usage of corrosive KOH electrolytes, which can form K₂CO₃ salt that decreases the number of hydroxyl ions and ion transferability, resulting in reduced hydrogen production. Additionally, the alkaline water electrolysis produces low-purity gases due to diaphragm inefficiencies.

The process involves the hydrogen evolution reaction at the cathode and the oxygen evolution reaction at the anode, with two moles of alkaline solution being reduced to produce one mole of hydrogen and two moles of hydroxyl-ions at the cathode. The hydroxyl-ions are then transferred to the anode through a porous separator under the influence of an electric circuit, where they are discharged to produce oxygen and water.

Secondly, AEM water electrolysis is a promising technique for water splitting, as it utilizes cost-effective transition metal catalysts and low-concentrated alkaline solutions as electrolytes, rather than more expensive noble metal catalysts and highly concentrated solutions. The process involves two half-cell reactions: the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER). Water molecules are reduced at the cathode to produce hydrogen and hydroxyl ions, while the hydroxyl ions are transported

through an anion exchange membrane to the anode, where they react to form oxygen and water. However, further investigation and improvement are still needed to ensure the stability and efficiency of the system for large-scale and commercial applications.

PEM (Proton Exchange Membrane) water electrolysis is an electrochemical process that splits water into hydrogen and oxygen with high purity using lower temperatures and higher current densities compared to alkaline water electrolysis. This is possible due to the fast kinetics of the hydrogen evolution reaction and the use of highly active metal surfaces in the Pt electrodes with a lower pH electrolyte. Furthermore, PEM is safer and more compact than alkaline water electrolysis. Despite the high stability of PEM, the cost of components, including electrode materials, current collectors, and bipolar plates, remains a major challenge. During PEMWE, the water molecule is decomposed to generate oxygen and protons at the anode, which is then transferred through the proton-conducting membrane to the cathode where protons and electrons recombine to produce hydrogen gas.

Then finally, The solid oxide water electrolysis cell (SOEC) is an electrochemical conversion cell that converts electrical energy into chemical energy by splitting water into hydrogen and oxygen. Unlike other electrolysis technologies, SOEC operates at high temperatures (500-850°C) and consumes water in the form of steam, resulting in improved energy efficiency and reduced hydrogen production costs. SOEC also offers the advantage of being thermally integrated with downstream chemical synthesis, making it an attractive option for industrial applications. However, the commercialization of SOEC has been hindered by insufficient long-term stability. Despite this, SOEC does not require the use of noble metal electrocatalysts and gives high conversion efficiency. During the SOEC process, water is initially reduced at the cathode side to produce hydrogen and oxide ions, which travel through the ion exchange membrane to the anode side. At the anode side, oxide ions are further reduced to generate oxygen and electrons, with the oxygen being released from the anodic surface and the electrons traveling through the external circuit to the cathode side.

Overall, the solid oxide water electrolysis cell offers a promising technology for producing green hydrogen and oxygen, with the potential for high energy efficiency and cost savings. However, further research is needed to improve the long-term stability of the technology and facilitate its commercialization.

To resume, Table 1.2 shows the different advantages and disadvantages of those 4 technologies.

Electrolysis technology	Advantages	Disadvantages
Alkaline Water electrolysis	-Well established Technology -Commercialized for industry applications -Noble metal-free electrocatalysts -Relatively low cost -Long-term stability	-Limited current densities -Crossover of the gasses -High concentrated liquid electrolyte
AEM Water electrolysis	-Noble metal-free electrocatalysts -Low concentrated liquid electrolyte	-Limited stability -Under development
PEM Water electrolysis	-Commercialized Technology -Operates higher current densities -High purity of the gases -Compact system design -Quick response	-Cost of the cell components -Noble metal electrocatalysts -Acidic electrolyte
AEM Water electrolysis	-High working temperature -High efficiency	-Limited stability -Under development

Table 1.2: Advantages and disadvantages of typical water electrolysis technologies [10]

In section 4.6 it is also possible to find the technical characteristics of typical water electrolysis technologies in detail.

In light of all these findings and the fact that the considered VRES are solar and wind energy, we frequently choose the technologies alkaline water for wind energy and PEM for solar energy. Because of this, a hybrid electrolyser that combines various technologies into one unit is now available. It can combine the advantages of both technologies to increase their flexibility and, consequently, their effectiveness. Due to its acceptance of variable voltage and relatively low cost, it may therefore employ an alkaline electrolytic cell to produce hydrogen when there is an excess of wind energy.

However, a PEM electrolytic cell can be used to generate hydrogen when solar energy is available since it runs at a relatively low temperature and does not require a lot of power. Its efficiency is consequently estimated to be 70%, making it the current solution of choice.

1.3.3 Hydrogenation of Carbon Dioxide to Methane

This subsection will cover the process by which hydrogen is changed into methane. However, in order to do this, carbon atoms must be absorbed from somewhere and combined with hydrogen. For this purpose, Carbon dioxide is an optimal source.

Carbon dioxide (CO_2) is a major contributor to the greenhouse effect, which is causing global climate changes. The world's population and improved living standards are increasing CO_2 levels, making it urgent to reduce emissions.

While there are techniques for fixing CO_2 , such as geological storage or afforestation, these approaches have drawbacks in terms of cost, safety, efficiency, and reliability.

Therefore, using CO_2 as a renewable and environmentally friendly source of carbon is an attractive solution.

By using CO_2 in a sustainable way, we can address the challenges posed by increasing CO_2 levels while also meeting our energy needs. This approach offers a promising path towards a more sustainable future, and it is up to us to explore its potential to the fullest. [11]

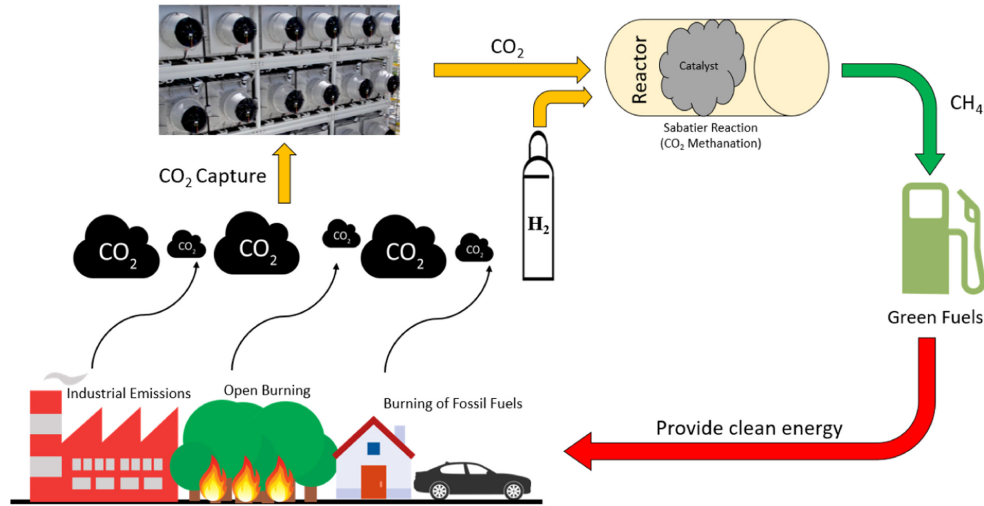


Figure 1.3: Scheme displaying the capture and recycling of CO_2 into green fuels and energy. [12]

So in Figure 1.3 we can see that recycling CO_2 as a source of carbon for fuels and chemicals should be viewed as a more sustainable use of the resources because it can actually reduce use of carbon-based fossil fuels without increasing global CO_2 emissions.

This Figure 1.3 corresponds well to our final objective of this part of the thesis because it is based on the creation of CH_4 . And we will use it as a guide in the explanation steps.

CO₂ Capture

First, the CO_2 capture. As shown in Figure 1.4, methods of post- or pre-combustion capture, or oxy-fuel combustion, are used to capture CO_2 from power plant exhausts.

Firstly, pre-combustion capture involves the partial oxidation of fossil fuel and the reaction of that fuel with steam to create syngas (CO and H_2O), which will then be further transformed into CO_2 and H_2 . H_2 can be used as fuel, and techniques are utilised to extract CO_2 before burning. The temperature is high and the operating pressure is between 20 and 30 bar.

Then, Oxy-fuel combustion involves burning the fuel in oxygen rather than air, and the flue gas is primarily made up of CO_2 and contaminants like SO_x . The oxy-fuel combustion interacts at high temperatures of 100–300 °C and pressures of 20–30 bar .

Oxy-fuel combustion has a very high oxygen concentration, which changes the chemical composition of the ash and causes a number of issues, including corrosion, fouling possible leaks into the plant, high maintenance costs,. There is a reported 8–12% loss in total net efficiency, which results in a 2–35% increase in fuel consumption since significant auxiliary power is needed to filter, liquefy, and separate oxygen from the air.

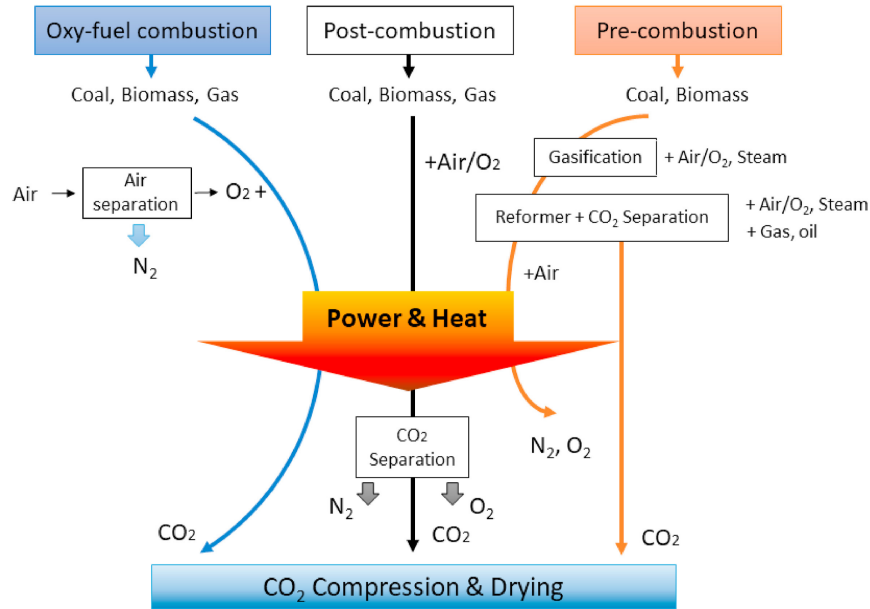
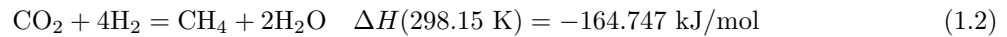


Figure 1.4: Different Carbon capture systems (CCS)[13]

Then we have the post-combustion CO₂ capture method. This works with a chemical solvent that will react with the CO₂ in the exhaust gases to capture it while releasing other gases such as nitrogen into the atmosphere. The purification of this CO₂ is done by a desorber which will separate it from the solvent in the form of a gas using heat or another regeneration technique. The post-combustion CO₂ abatement method is simple and serves as the foundation for the current CCS. It is true that pre-combustion and oxy-fuel capture each have different advantages, but it is unlikely that they will ever completely replace post-combustion capture on a worldwide scale.[14]

CO₂ Methanation

This part consists thus in combining the CO₂ and the hydrogen previously created or produced to make Methane and thus to obtain a more secure and much more practical final energy. This is possible thanks to the Sabatier reaction:



As shown in Equation 1.2 this reaction is very exothermic and also difficult to achieve due to the kinetic barrier of the 8 electron reduction. The numerous studies on this reaction are therefore often based on the type of metal catalyst such as nickel or cobalt used to make this reaction work. The aim is to find a catalyst that is firstly thermally stable so that it does not degrade at the temperature of the exothermic reaction and secondly that it can have a high activity at low temperatures. This last point is related to not wanting unwanted products in the reaction such as carbon deposits etc...

So the possibilities are firstly the noble metal ruthenium (Ru) who possesses high activity as well as other beneficial properties like excellent CH_4 selectivity, even at low temperatures, and high resistance to oxidising atmospheres. The biggest disadvantage is its expensive cost, which restricts its use. Additionally active in CO_2 methanation we can use iron (Fe) who is also relatively affordable. However, its CH_4 selectivity is modest. Then, the most used metal for CO_2 methanation is nickel (Ni). It is very active, highly CH_4 -selective, and inexpensive. Like the other non-noble metals Fe and Co, Ni has a strong propensity to oxidise in oxidising environments. One drawback is the high hazard posed by nickel carbonyl, which is a highly dangerous compound for human health. Finally the last, Cobalt (Co) is more expensive than nickel (Ni) and exhibits less activity so we generally pay little attention to it.

As far as the reactor is concerned, several reactors have been adapted to methanation but the ones most frequently used are the fixed-bed reactors. [15]

So to conclude, CO_2 methanation combines CO_2 and hydrogen to produce methane, a safer and more practical energy source, through the Sabatier reaction. Different metal catalysts like nickel, cobalt, ruthenium, and iron facilitate this process, with each having their own advantages and limitations. Nickel, despite its risks, is most common due to its high activity, methane selectivity, and affordability. These developments are key for enabling CO_2 methanation as a feasible route to sustainable energy.

1.4 From Gas to Power Technologies

To conclude this section, it would be valuable to engage in a succinct analysis of the diverse technologies of power generators currently available. Information available in the cited literature [16] provides insights into the efficiencies of other small scaled power generators, this information is also shown in Table 1.3.

Technology	Electrical eff. [%]	Total eff. [%]	Possible Biofuels
Conventional Rankine cycle	20-30	85-93	Most of solid, liquid or gaseous biofuels
Steam engines	12-20		Most of solid, liquid or gaseous biofuels
Gas turbines with HRSG	24-35	80-85	Gaseous biofuels, methanol, ethyl alcohol, RME
Microturbines	11-33	80	Possible to use methanol, ethanol, colza oil pyrolysis oil, biogas
Otto engines	35-40	80-90	Ethanol, methanol, gaseous biofuel
Diesel engines	40-45	85-90	Pyrolysis oil, pine tree oil, colza oil, RME gaseous biofuels
Stirling engines	20-40	90	Most of solid, liquid or gaseous biofuels Hydrogen methanol
Fuel cells: PAFC	40-45		Hydrogen , methanol
SOFC	45-60	80	Hydrogen, hydrogen+CO
MCFC	50-60		Hydrogen
PEFC	35-40		Methanol, hydrogen

Table 1.3: Characteristics of other comparable technologies

Even though a variety of technologies are listed in this Table 1.3, the main contenders of the HCCI engine being the fuel cells, the micro turbine and the piston engines will be considered in this analysis. They are the primary competitors due to the fact that they operate within similar output ranges and with comparable efficiencies.

Firstly the spark Ignition (SI) engines, also known as Otto engines, are common in small scale applications for generating heat and electricity, particularly in European countries. They are prized for their long lifespan, short start-up time of 5-10 minutes, and efficiency even at partial load, making them responsive to variable demand. However, these engines are not without flaws. They are quite loud, require frequent maintenance such as oil and spark plug changes, and only reach a brake thermal efficiency of up to 35% due to the need to keep the compression ratio low to avoid engine knock.

A variation, the lean burn spark-ignited engine, which runs on an excess of air, slightly improves brake thermal efficiency up to 38%. However, its combustion process is a significant source of nitrogen oxides (NO_x). Cost-effective after-treatment technologies like selective catalytic reduction (SCR) for this scale of units are currently unfeasible, limiting its use to areas with less strict emission standards.

In contrast, Compression Ignition (CI) engines, also utilized in small scale power production, are the most efficient prime movers available for small facilities with a typical brake thermal efficiency exceeding 40%. They have relatively low investment cost per kilowatt-electric power output and are responsive to variable demand. However, they naturally emit high levels of NO_x. The economic burden of requisite after-treatments complicates their use in cogeneration, but ongoing research and development aim to reduce these emissions below the imposed standard using catalytic converters and other technologies.

Next, micro-turbines are a type of small-scale combined heat and power (CHP) technology that generate heat and electricity from a gas turbine engine, making them ideal for structures or locations with significant electrical and heating needs. They operate by consuming fuel in the turbine's combustion chamber, producing hot exhaust gases which spin the turbine and create energy. The gases are then used via a heat exchanger to produce hot water or steam for heating or other activities, achieving overall efficiencies of up to 80%. Despite their high efficiency, small size, and low noise level, micro-turbine CHP systems tend to be costlier to construct and maintain than other small-scale CHP technologies, and they are less energy-efficient than alternatives such as fuel cells.

Fuel cell CHP systems produce electricity and heat by combining fuel (like hydrogen) with oxygen from the air in a fuel cell. They are highly efficient, clean, quiet, durable, and require low maintenance. They use fuel energy more effectively than traditional power generation methods and emit no greenhouse gases or other air pollutants. However, their high cost (3000\$ /kW) limits their commercialization.

Now that a clearer overview of the different technologies is given, we can turn our attention to the technology being examined in this dissertation: the HCCI engine.

2 Theoretical overview

This chapter aims to cover the entire theoretical concepts that underlie this technology. The unique combustion characteristics that define it and the challenges in controlling it are explained in detail, along with specific emissions, power, and efficiency aspects. A preliminary investigation of the potential of oxygen enrichment is then conducted based on several scientific articles. Thus, an initial analysis of the influence of this strategy on the engine's operating conditions is already carried out.

2.1 Principle of the HCCI

The master's thesis completed between 2015 and 2020 at UCLouvain served as some of the basis for the HCCI template created in this section [17] [18] [19] [20] [21] [22].

The base principle of an Homogeneous Charge Compression Ignition (HCCI) engine is to combine features and advantages of spark ignition (SI) engines and compression ignition (CI) engines through the spontaneous auto-ignition of an homogeneous mixture of air and fuel, resulting from its compression.

SI engines (also called gasoline or Otto engines) operate with a spark ignition system, where a spark plug ignites an homogeneous mixture of fuel and air in the engine's combustion chamber. The use of a stoichiometric mixture to ensure a good flame propagation speed and a good operation of the 3-way catalytic converter gives SI engines the advantage of low soot and nitrogen oxide (NO_x) emissions. However, the risk of knocking due to the auto-ignition of the mixture before the spark ignition limits the compression ratio of this type of engine, limiting its efficiency.

On the other hand, CI engines (also called diesel engines) use compression ignition, where the air in the combustion chamber is compressed until it becomes hot enough to inject the fuel, before the top dead center (TDC). The use of a high compression ratio (to ensure auto-ignition of the mixture) and an overall low equivalence ratio (to avoid a too high fraction of unburned gases) gives CI engines the advantage of high efficiency, allowing reduced fuel consumption and therefore, reduced CO_2 emissions. Yet, the mixture's inhomogeneity and high combustion temperature result in a significant output of soot, NO_x and unburned fuel.

Therefore, the HCCI engine is considered as a promising alternative for conventional gasoline and diesel engines due to its ability to increase fuel efficiency while lowering emissions of pollutants and greenhouse gases. However, because of the complexity of its implementation, there are still a lot of issues that need to be looked at before it can be used in practice.

2.1.1 Combustion Phenomenon

The combustion process in an HCCI engine differs from the combustion process in other internal combustion engines since it is controlled by the chemical kinetics evolving in the cylinder rather than by the ignition of a spark or the injection of fuel. Indeed, a homogeneous mixture of fuel and air enters the cylinder during the intake stroke. The temperature of the gases is then increased by the compression stroke, which causes a

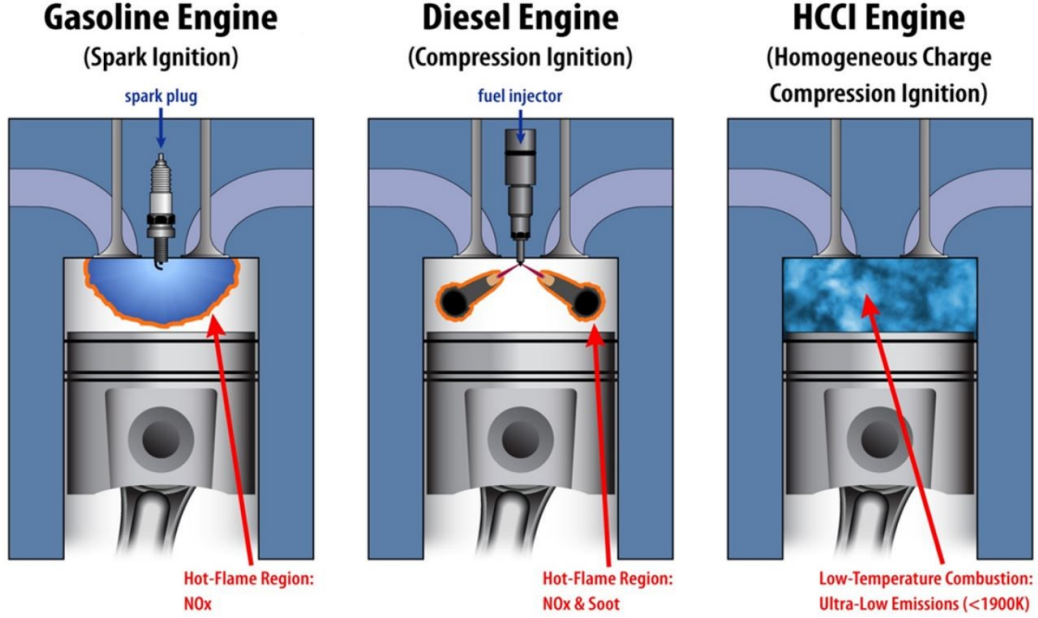


Figure 2.1: Representation illustrating the various combustion modes that can be observed in SI, CI, and HCCI engines found in [18].

chain reaction of free radicals produced by the thermal decomposition of the hydrocarbons and ultimately results in the combustion of the fuel. The resulting heat release causes the combustion products to expand during the engine's stroke expansion, which produces the mechanical energy. Considering a mixture as almost perfectly homogeneous, the temperature and pressure conditions inside the combustion chamber are nearly uniform, and the mixture almost instantly ignites. This causes a very sharp pressure peak, measured by the pressure rise rate (PRR), and a very quick heat release, measured by the heat release rate (HRR) (also known as the rate of heat release (RoHR)), which, if not carefully controlled, can cause mechanical damage to the engine. The first fundamental precaution to prevent this damage is the use of a high fuel dilution characterized by a limited equivalence ratio. The equivalence ratio is defined as the ratio between the fuel-air ratio used and the fuel-air ratio leading to stoichiometric combustion (Equation 2.1). We will see in subsection 2.2 that it is also possible to define it according to the fuel-oxygen ratio used. This ratio influences the behaviour of combustion since the chemical kinetics that govern it depends on the concentration of the fuel in the mixture. Because the speed of the combustion is proportional to the reactants concentration, decreasing the concentration of the fuel causes the combustion to slow down.

$$\phi = \frac{\frac{m_f}{m_{air}}}{\left(\frac{m_f}{m_{air}}\right)_{st}} \quad (2.1)$$

The nature of the combustion process in the HCCI engine, i.e. chemical kinetics, as well as the high speed at which it occurs (up to 6 times faster than in CI-SI engines [23]), make it extremely difficult to control the timing of auto-ignition of the mixture. In fact, this timing will depend on a variety of factors influencing, from near or far, the internal kinetics of the engine, in particular the equivalence ratio, compression ratio,

fuel composition, inlet temperature and pressure, the number of rotations per minute (RPM), etc as shown in Figure 2.2. The real challenge of combustion control is therefore to obtain auto-ignition of the mixture at the optimal time to maximize the mechanical work extracted from the chemical energy of the fuel while ensuring the safety of the engine.

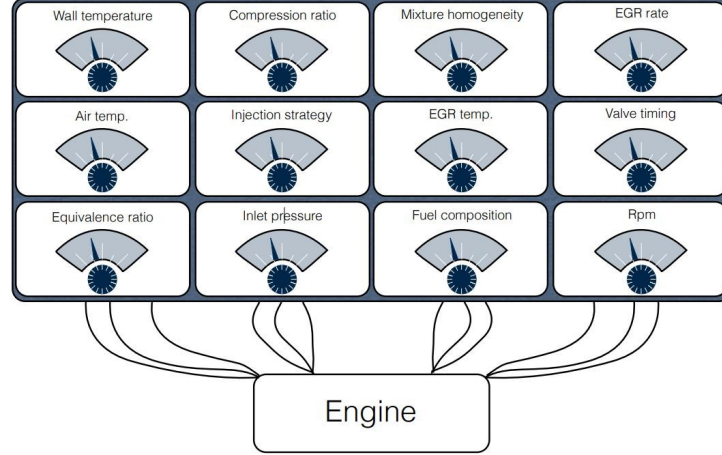


Figure 2.2: Indirect control through multiple parameters from [24]

A fundamental parameter essential to the concept of the HCCI engine is the so-called auto-ignition temperature. It is defined as the temperature to be reached to trigger the ignition of the fuel. As previously stated, this auto-ignition is dependent on a wide range of factors. However, due to its significant influence on the chemical kinetics, temperature is the factor that matters most. Indeed, a high temperature is the main trigger of the endothermic reactions of initiation and pre-ignition (cold flame) which set off the chain branching propagation reaction leading to the combustion. This auto-ignition temperature is specific to the fuel used because of the fuel's propensity to resist or not auto-ignite. This trend is reflected in the octane number, which is used to classify liquid fuels on a scale from 0 (for the least resistant fuel, i.e. n-heptane) to 100 (for the most resistant fuel, i.e. iso-octane). Methane, although a gaseous fuel, is considered one of the most resistant fuels to auto-ignition, which means that it needs to reach an activation energy, and therefore an auto-ignition temperature, higher than other fuels such as natural gas or biogas. In fact, natural gas is composed of methane but also of other hydrocarbons with low octane numbers. It promotes a more rapid auto-ignition, as does biogas, which is mainly composed of methane and carbon dioxide CO_2 . Its ability to operate with a wide range of fuels, both liquid and gaseous, is another key benefit of this technology, provided that all parameters are properly set to assure auto-ignition and prevent engine damage.

Returning to the engine cycle, it is necessary to highlight how the intake temperature affects combustion since it determines whether or not the mixture will be able to achieve its auto-ignition temperature. S. Aceves and D. Flowers shown that for a compression ratio of 18, the inlet temperature must be 380 K for natural gas to reach its auto-ignition temperature and 400 K for pure methane [25].

Ignition Timing

As said above, the combustion is characterized by the pressure rise rate and the heat release rate but also by the start of combustion (SOC) which is equal to CA10, the combustion midpoint, which is equal to CA50, and the duration of combustion (DOC), which is calculated as CA90–CA10. Using a Volkswagen TDI diesel engine adapted to operate in HCCI mode and fueled by a biogas composed of 60% CH₄ and 40% CO₂, Bedoya et al. [26] investigated the effects of the equivalence ratio as well as the pressure and temperature conditions at the intake on these various parameters. The 3 curves below are from their work. As the equivalence ratio rises, Figure 2.3 demonstrates that CA50 is globally advanced for all combinations of inlet pressure and temperature. This is due to the higher burning rate that characterizes richer mixtures and therefore induces a higher combustion speed. It is also clear that, for a given equivalence ratio, a higher input temperature promotes faster combustion since it allows the mixture to reach its auto-ignition conditions sooner. Figure 2.4 confirms this result by demonstrating that increasing the input temperature accelerates the start of combustion while decreasing the duration of combustion. The pressure and heat release rate peaks increase with inlet temperature and can reach extremely high levels. This highlights the need of carefully controlling the mixture's input conditions.

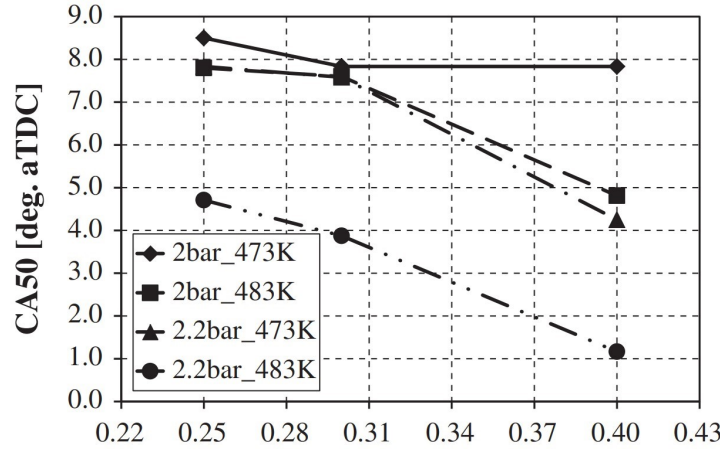


Figure 2.3: Crank angle at 50% cumulative heat release (CA50) related with the equivalence ratio for different inlet charge pressures and temperatures [26].

The difficulty of accurately predicting combustion timing does not allow the HCCI engine to vary load and speed as easily as in SI and CI engines since regulating all parameters simultaneously for optimized ignition timing is a relatively complicated task. This explains why these engines are rarely employed in the car industry, preferring instead to be used in stationary applications where they can be adjusted to operate at certain loads and speeds. Considering a constant rotational speed throughout this work, the real challenge is to determine the initial conditions that allow to adapt to a required load.

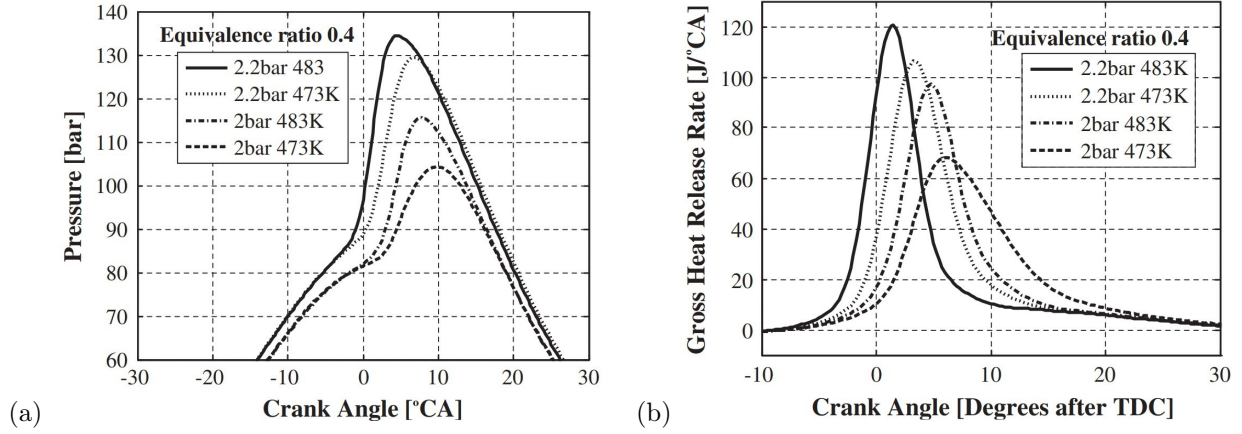


Figure 2.4: In-cylinder pressure (a) and gross heat release rate (b) at 0.4 equivalence ratio for different intake charge pressures and temperatures [26].

2.1.2 Limited Operating Range

As previously mentioned, maintaining combustion stability is one of the main obstacles for the HCCI engine. The intense sensitivity of this technology to variations in multiple parameters such as temperature and load significantly limits its operating range. Misfire and ringing are considered the 2 extreme limits for engine operation at low and high loads respectively. In the case of a stationary engine where the operating range only concerns the load range and not the speed range, the load is adjusted by the equivalence ratio and the input temperature, although the latter is less influential as observed by A. Gharehghani [27].

In the case of low load, i.e. when using a very lean air-fuel ratio, the small amount of chemical energy supplied by the fuel may not be sufficient to initiate and maintain the chain branching propagation reaction. This results in incomplete combustion due to partial fuel ignition failure, meaning reduced combustion efficiency as well as excessive CO and HC emissions. To avoid this, the combustion can be advanced by employing higher intake temperatures, for example. This would improve the burning rate of the fuel due to the higher pressure and temperature conditions closer to the TDC. The partial oxidation of the fuel leads to variations in the amount of energy produced from cycle to cycle which can be measured using the Coefficient of Variation (COV), expressed as a percentage. Misfire prevention necessitates a COV limit of 5%-10%, depending on the application.

At high load, the violence of combustion induces a fast rise in pressure which results in a ringing phenomenon, large pressure oscillations that can cause engine noise and mechanical damage. Figure 2.5 illustrates how HCCI engines and SI engines differ in terms of intensity and pressure rise. In SI engines, the fuel burns gradually, resulting in a smoother combustion and lower pressure rise rate and heat release rate values. This rapid pressure rise for HCCI is characterized by the maximum Pressure Rise Rate (MPRR) which should be limited to 10-20 [bar/CAD]. A limit can also be put on the maximum pressure reached by the mixture in the cylinder, the peak cylinder pressure (PCP), especially when utilizing a

turbocharger. The PCP and PRR could be reduced by delaying the combustion after the TDC, during the expansion period, by employing lower input temperatures. These values being reduced, it is then possible to enrich the air-fuel ratio and thus to enlarge the operating range at high load. Despite this potential improvement technique, the fuel dilution must generally remain high to avoid ringing and is the primary cause of the low power density characteristic of the HCCI engine.

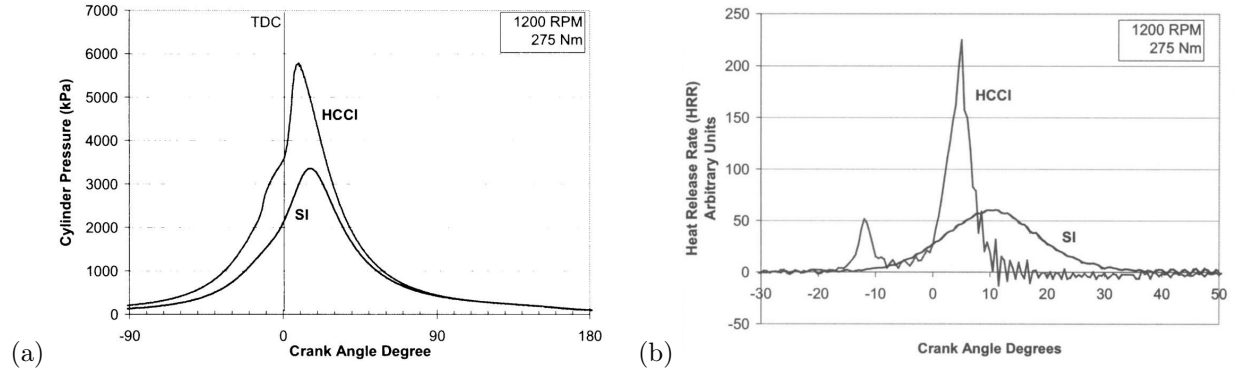


Figure 2.5: In-cylinder pressure (a) and Heat Release Rate (b) comparing HCCI and SI under same brake torque and same rotation speed [28].

As can be seen, the HCCI engine has a very small operating range, but the key issue for this technology is the potential to increase it and hence increase the power density. Different strategies such as fuel mixture [23], variable valve timing, variable compression ratio, charge pre-heating, turbocharging and exhaust gas recirculation (EGR) [17] [19], thermal stratification [21] or oxy-combustion [22] have already been investigated. Our work focuses on oxygen enrichment of air as a potential strategy to increase the power density of the HCCI engine.

2.1.3 Efficiencies and MEP

The transition from the fuel's chemical energy to the mechanical energy that the crankshaft can use is done through different stages of conversion of energy flows, each characterized by a corresponding efficiency. The mean effective pressure (MEP) values, which allow for the evaluation of the engine's energy performance regardless of its size, are therefore defined by normalizing these energy flows by the engine's displacement V_d . It is consequently expressed in [bar]. The succession of these MEP values and the efficiencies associated with the energy flow conversions are illustrated in Figure 2.6.

First, the FuelMEP characterizes the chemical energy available in the fuel. It can be calculated via the mass of fuel (m_f) fed into the cylinder per cycle and its Lower Heating Value (LHV).

$$\text{FuelMEP} = \frac{m_f \cdot \text{LHV}}{V_d} \quad (2.2)$$

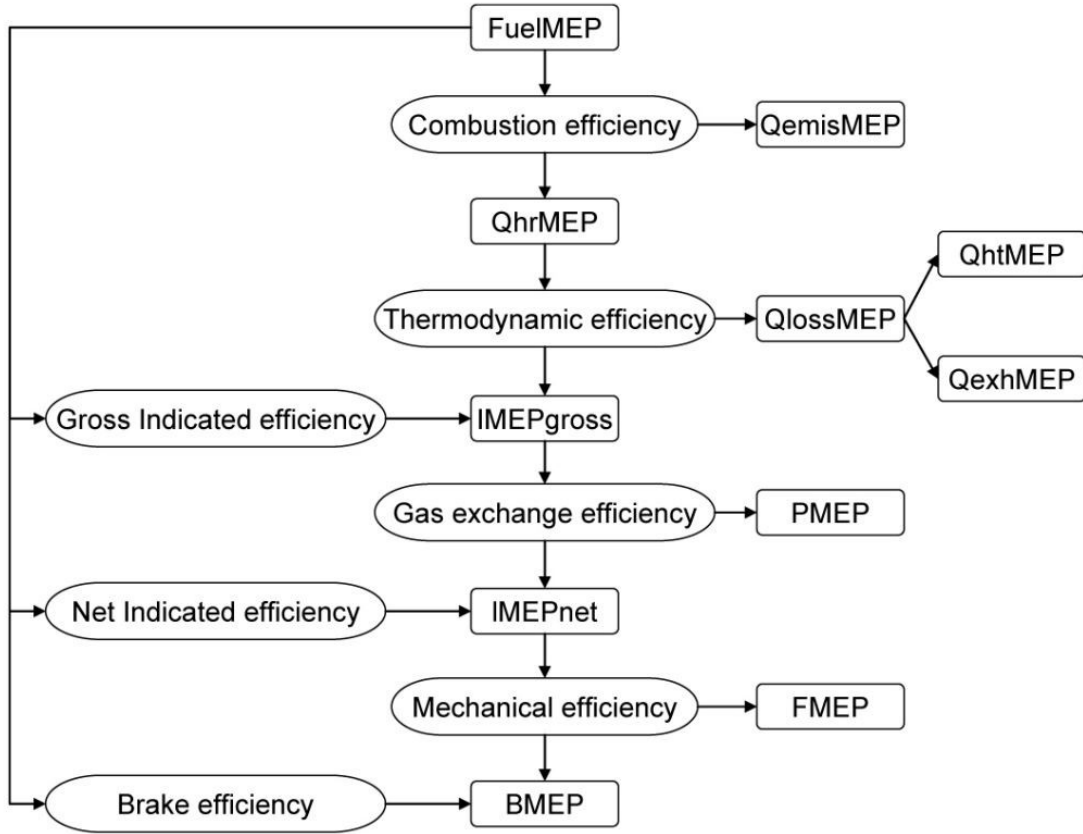


Figure 2.6: All the energy flows and their corresponding efficiencies, from the chemical energy of the fuel (FuelMEP) to the mechanical energy of the crankshaft (BMEP). [24]

Most of the fuel is then burned and the net heat released during combustion is expressed as $Q_{hr}MEP$, while the fraction of energy lost in the exhaust due to unburned fuels and incomplete combustion products is expressed as $Q_{emission}MEP$. η_c defines the efficiency of this combustion.

$$Q_{hr}MEP = FuelMEP - Q_{emis}MEP \quad (2.3)$$

$$\eta_c = \frac{Q_{hr}MEP}{FuelMEP} \quad (2.4)$$

This heat released by the hot source $Q_{hr}MEP$ is then converted into the internal work done on the piston, quantified by indicated MEP gross ($IMEP_g$). This conversion is accompanied by heat losses at the cold source which can be divided into 2 parts. The parietal heat losses and exhaust losses as measured by $Q_{ht}MEP$ and $Q_{exh}MEP$, respectively. The thermodynamic efficiency (η_{ti}) characterizes the efficiency of this conversion and can be multiplied by the combustion efficiency to obtain the gross indicated efficiency.

$$IMEP_g = Q_{hr}MEP - Q_{ht}MEP - Q_{ex}MEP \quad (2.5)$$

$$\eta_{ti} = \frac{\text{IMEP}_g}{\text{Q}_{hr}\text{MEP}} = 1 - \frac{\text{Q}_{ht}\text{MEP}}{\text{Q}_{hr}\text{MEP}} - \frac{\text{Q}_{exh}\text{MEP}}{\text{Q}_{hr}\text{MEP}} = 1 - \epsilon_{ht} - \epsilon_{ex} \quad (2.6)$$

With ϵ_{ht} and ϵ_{ex} , the parietal and exhaust loss coefficients respectively.

$$\eta_{ind,g} = \frac{\text{IMEP}_g}{\text{FuelMEP}} = \eta_c \cdot \eta_{ti} \quad (2.7)$$

To obtain the net work done on the piston during the entire engine cycle, we must take into account the pumping work done during the breathing phase. This work consumption is defined with the pumping MEP, P_{MEP}, and includes the head losses during the intake stroke and the pressure increase during the exhaust. It is expressed as the difference between mean in-cylinder pressures during the exhaust stroke P_{out} and the intake stroke P_{in} .

$$\text{PMEP} = P_{out} - P_{in} \quad (2.8)$$

By removing these pumping losses from the gross IMEP, the net indicated MEP is obtained, IMEP_n. The net indicated efficiency can thus therefore also be defined $\eta_{ind,n}$.

$$\text{IMEP}_n = \text{IMEP}_g - \text{PMEP} = \frac{-\oint p \cdot dV}{V_d} \quad (2.9)$$

$$\eta_{ind,n} = \frac{\text{IMEP}_n}{\text{FuelMEP}} \quad (2.10)$$

The last step takes into account the friction losses inside the engine when transmitting the net work done on the piston to the mechanical work available at the crankshaft. This mechanical work is quantified by the break MEP (BMEP), and is obtained by subtracting these friction losses FMEP from IMEP_n. This conversion is characterized by mechanical efficiency η_{mec}

$$\text{BMEP} = \text{IMEP}_n - \text{FMEP} \quad (2.11)$$

$$\eta_{mec} = \frac{\text{BMEP}}{\text{IMEP}_n} \quad (2.12)$$

Finally, the global efficiency with which the chemical energy of the fuel is converted into mechanical work that the crankshaft is capable of performing is referred to the break efficiency η_b .

$$\eta_b = \frac{\text{BMEP}}{\text{FuelMEP}} = \eta_{ind,n} \cdot \eta_{mec} \quad (2.13)$$

Intake Temperature and Equivalence Ratio Influence

The HCCI engine is able to extract more useful energy from the fuel than traditional internal combustion engines. This is due to the high combustion and thermodynamic efficiency that result from the simultaneous self-ignition of the fuel and the usage of high compression ratios, respectively. Indeed, the necessity to ensure the mixture ignites involves raising it to high temperatures, which requires the use of high compression ratios, especially for fuels with high octane numbers, such as methane. Because of the speed of combustion, the thermodynamic cycle of the HCCI engine is close to the theoretical cycle of Beau de Rochas, which is characterized by isentropic compression and expansion and ideal isochoric combustion.

The definition of this cycle's thermodynamic efficiency (Equation 2.14) is a first approximation that links an increase in efficiency to a higher compression ratio.

$$\eta_{th} = 1 - \frac{1}{\tau^\gamma} \quad (2.14)$$

As with CI engines, pumping losses are very low in the HCCI engine since it does not require a throttle valve. This reduces the gap between gross IMEP and net IMEP, ensuring better brake efficiency. This valve is essential to the SI engine to allow it to control the air flow, which is needed for using a stoichiometric air-fuel mixture. Since scavenging requires a lot of produced work, pumping losses during gas exchange are significantly increased.

The intake temperature and the equivalence ratio have an important impact on the different efficiencies. Figure 2.7, from Bedoyal et al., accurately captures this influence.

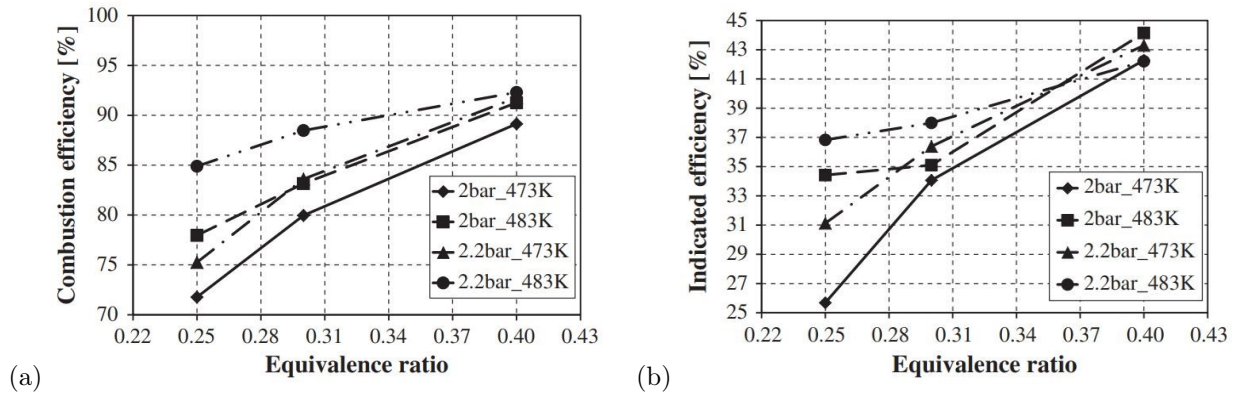


Figure 2.7: Combustion efficiency (a) and gross indicated efficiency (b) related with equivalence ratio for different intake charge pressures and temperatures [26].

First, the rise of combustion efficiency can be observed as the equivalence ratio does. Effectively, the rise in equivalence ratio advances the combustion process, which is subsequently carried out at higher in-cylinder temperatures, as explained in subsubsection 2.1.1 via Figure 2.3, allowing a more complete oxidation of fuel. Combustion is also improved by raising the intake temperature for a fixed equivalence ratio, although with a larger sensitivity for low equivalence ratios (0.25) than for high equivalence ratios (0.4).

The gross indicated efficiency $\eta_{ind,g}$, which combines the effects of combustion efficiency η_c and thermodynamic efficiency η_{ti} (Equation 2.7), follows the trend of the combustion efficiency to increase with the equivalence ratio as a result of the rise in in-cylinder temperature and burning rate. On the other hand, the impact of a higher inlet temperature only enhances the gross indicated efficiency at low equivalence ratios. For $\phi = 0.25$, an increase of 10[K] leads to an improvement in efficiency of 9% at 2 bar and 6% at 2.2 bar. This effect becomes less significant as the equivalence ratio rises, to the point that for $\phi = 0.4$, an improvement in the inlet conditions results in a reduction in efficiency. This can be explained by the fact that, for an already high equivalence ratio, a rise in temperature causes the combustion to occur

before the TDC, producing a negative work, as well as the fact that the heat transfer rate is intensified, increasing parietal losses. These two phenomena have the effect of lowering thermodynamic efficiency and, thus, gross indicated efficiency.

For the mechanical efficiency, increasing the amount of fuel is beneficial to the engine. Since the engine's size is unaffected, it does really allow for increased output without increasing mechanical friction losses. The relative importance of these friction losses is therefore reduced and the brake efficiency is increased. Regarding intake temperature, it affects brake efficiency in a number of ways. As was already said, increasing it leads to higher combustion efficiency, but decreasing it allows for a general decrease in the in-cylinder temperature, which reduces wall heat losses but also creates a denser load, allowing for the burning of more fuel, at the same equivalence ratio.

2.1.4 Emissions

HCCI engines are also of great interest because of their clean combustion. The emissions produced are lower than those of CI and SI engines, particularly in terms of nitrogen oxides (NO_x) and soot molecules.

The reaction of NO_x molecules in the atmosphere leads to the formation of other pollutants responsible for respiratory problems, environmentally destructive acid rain, or global warming through the formation of ozone in the lower atmosphere. Therefore, reducing these pollutants is crucial for both human and environmental health. The formation of nitrogen oxides occurs according to the Zeldovich mechanism and is strongly temperature dependent due to the energy required to break the bonds of N_2 . Figure 2.8 depicts the increase in NO_x at temperatures higher than 2000 [K]. In addition to a high temperature, the availability of oxygen, and a slow combustion process are also favorable conditions for the release of these molecules.



Despite the fuel being burned at temperatures that are suitable for the generation of these emissions, stoichiometric air-fuel mixtures used in SI engines restrict the amount of oxygen that is available and enable a 3 way catalyst to significantly reduce NO_x emissions. On the other hand, for CI engines, these conditions are particularly confirmed in the poor zones near the flame's diffusion. Because of the low temperatures (1500-1800 [K]) at which HCCI engines burn fuel, no NO_x emissions are produced.

Soot particles are the result of non-optimal combustion. They are mostly composed of solid carbon particles that combine with other molecules like unburned hydrocarbons (HC), nitrogen oxides, or metals from engine component wear. These compounds might be poisonous and contribute to air pollution, which might be harmful to both the environment and people's health. These pollutants develop in local areas of rich mixture, where the amount of oxygen is insufficient to complete the combustion. The non-uniform composition of the mixture in a CI engine leads to the creation of these particles, especially during the

premixed combustion phase where the local equivalence ratios are high. Using a homogenous, stoichiometric mixture prevents these particles from developing in SI engines, while using a homogeneous, lean mixture prevents these particles from forming in HCCI engines, as shown in Figure 2.8.

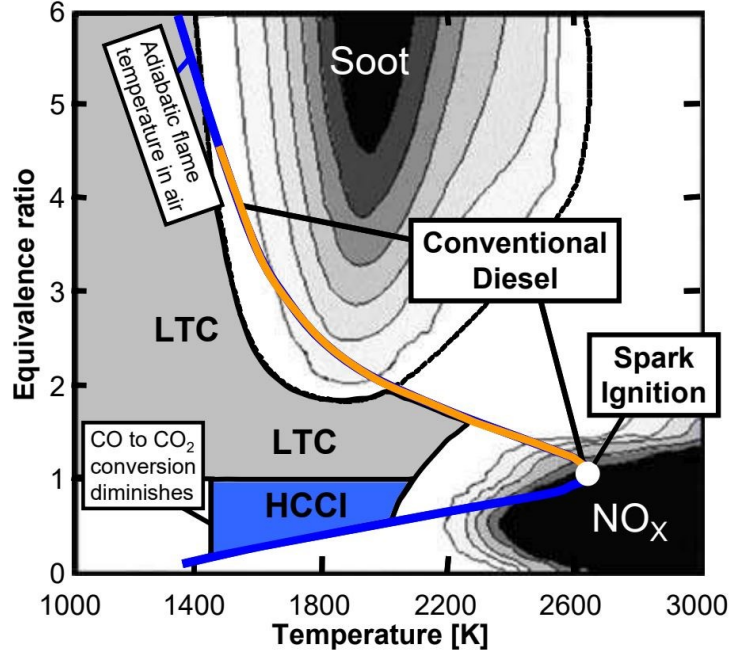


Figure 2.8: Temperature and equivalence ratio conditions leading to soot and NO formation for conventional diesel, LTC diesel, SI and HCCI engines [24]

Although the combustion process of HCCI engines offers significant advantages in soot and nitrogen oxide emissions, the low temperatures employed can result in partial combustion of the mixture, particularly in the cooler regions of the engine such as the cylinder walls. This phenomenon leads to the formation of unburned hydrocarbons such as methane, whose pure release produces an impact on the greenhouse effect equivalent to 23 times that of CO₂ [24]. The low in-cylinder temperatures can also prevent the oxidation of CO to CO₂ (2.18). The carbon monoxides are then lost in the exhaust gases and harm human and environmental health due to their toxicity and contribution to global warming. SI engines also generate a significant amount of unburned fuel and CO as a result of a fuel-rich mixture and halted combustion when the spark reaches cold surfaces like walls or fissures. The residual energy in the unburned HC and CO is lost in the exhaust gases, which results in lower combustion efficiency for HCCI engines, in the range of 90-95%, whereas CI engines are able to achieve values near to 100%.



2.2 HCCI Amelioration : Oxygen Enrichment

As explained in subsubsection 2.1.2, one of the main limitations of the HCCI engine is the low achievable power density. Indeed, the high inlet temperatures necessary for the fuel to reach its auto-ignition point limit the quantity of fuel that can be injected according to the following perfect gas law (Equation 2.19):

$$\frac{p}{\rho} = R^* T \quad (2.19)$$

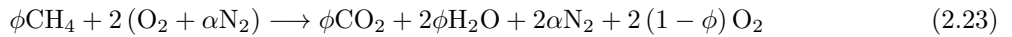
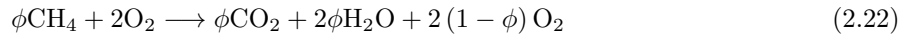
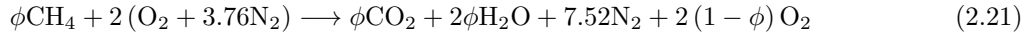
This limits the operating range of the engine (as well as its efficiency due to the high heat losses in the wall and in the flue gas. Dr. Pochet suggests the valorization of oxygen as a solution, especially for a fuel like methane that is auto-ignition resistant [23]. Due to its effect on the mixture's intake temperature, it would allow us to increase the amount of fuel we inject into the engine without substantially increasing the violence of the combustion.

2.2.1 Equivalence Ratio

The intake temperature of the mixture is an important parameter to determine which will depend on the oxidizer used during combustion. If pure air is the most frequent oxidizer, it is also possible to modify its properties by using different oxygen percentage rates. This phenomenon is known as oxygen-enrichment of the air and refers to the partial or complete substitution of nitrogen molecules with oxygen molecules. Let's analyze the impact of oxygen enrichment on the equivalence ratio:

$$\phi = \frac{\frac{m_f}{m_{air}}}{\left(\frac{m_f}{m_{air}}\right)_{st}} = \frac{\frac{n_f \cancel{M_f}}{n_{O_2} M_{O_2} + n_{N_2} M_{N_2}}}{\left(\frac{n_f \cancel{M_f}}{n_{O_2} M_{O_2} + n_{N_2} M_{N_2}}\right)_{st}} = \frac{\frac{n_f}{n_{O_2} (M_{O_2} + \alpha M_{N_2})}}{\left(\frac{n_f}{n_{O_2} (M_{O_2} + \alpha M_{N_2})}\right)_{st}} = \frac{\frac{n_f}{n_{O_2}}}{\left(\frac{n_f}{n_{O_2}}\right)_{st}} = \frac{\frac{n_f}{n_{O_2}}}{\frac{1}{2}} = 2 \frac{n_f}{n_{O_2}} \quad (2.20)$$

Using the fact that whatever the percentage of oxygen χ , the number of moles of N_2 will always be related to the number of moles of O_2 : $n_{N_2} = \alpha \cdot n_{O_2}$ and that $\left(\frac{n_f}{n_{O_2}}\right)_{st}$ will always be equivalent to $\frac{1}{2}$ at stoichiometry ($\phi = 1$) whether it is a combustion with pure air (2.21), a combustion with 100% oxygen (2.22) or a combustion with α mol of N_2 for one mol of O_2 (2.23).



The definition of the equivalence ratio does not change whatever the percentage of oxygen used in the oxidizer and its value only depends on its numerator, i.e. the quantity of fuel and oxygen injected.

In order to better understand its influence, it could be interesting to redefine this equivalency ratio in terms of oxygen percentage χ rather than n_{O_2} . Assuming that there is only oxygen and nitrogen in the oxidizer, the number of moles of O_2 and N_2 are related by χ according to Equation 2.24.

$$n_{N_2} = \alpha \cdot n_{O_2} = \left(\frac{1 - \chi}{\chi} \right) \cdot n_{O_2} \quad (2.24)$$

Based on the total number of moles present in the mixture initially, and knowing that $n_{O_2} = \frac{2}{\phi} n_f$, from 2.20, we have :

$$\begin{aligned} n_{tot} &= n_f + n_{O_2} + n_{N_2} \\ &= n_f + n_{O_2} + \left(\frac{1 - \chi}{\chi} \right) \cdot n_{O_2} \\ &= n_f + \left(\frac{1}{\chi} \right) \cdot \frac{2}{\phi} n_f \end{aligned} \quad (2.25)$$

And finally :

$$\phi = \frac{2n_f}{\chi \cdot (n_{tot} - n_f)} \quad (2.26)$$

This relationship enables the equivalence ratio to be adjusted in accordance with the input of fuel MEP and oxygen rate, the total number of moles being fixed by the initial conditions according to the perfect gas law. This relation implies logically that increasing the oxygen rate decreases the equivalence ratio while raising the fuel injection into the cylinder increases it.

2.2.2 Intake Temperature

The chemistry and kinetics that cause combustion in the HCCI engine provide an explanation for the relationship between oxygen enrichment and intake temperature. When oxygen is substituted for nitrogen, the partial pressure of oxygen in the mixture rises, enabling methane and oxygen to react with each other more quickly and increasing the mixture's reactivity. Because the mixture ignites more easily, its intake temperature can be lowered while still assuring auto-ignition.

Spano et al. [29] investigated how oxygen could be used more effectively for the HCCI engine's methane combustion. They maintained a constant fuel level throughout their work and studied the effects of changing air oxygen levels on various parameters, including intake temperature, ignition timing, and MPRR. Here is an overview of the conclusions they made. First, they demonstrated that it is possible to achieve stable combustion by reducing the intake temperature by 30 K with an oxygen enrichment from 21% up to 49% as shown in Figure 2.9. At greater O_2 percentages, the combustion's sensitivity to the addition of oxygen is reduced. It means that a wider variety of oxygen concentrations can be used for combustion while maintaining the same intake temperature.

Second, they illustrated that peak combustion was influenced by the oxygen consumption rate, as indicated in Figure 2.10 (a). When the quantity of oxygen is increased, the peak is closer to top dead center, which reduces the ignition delay. Again, at high oxygen concentrations, where a significant variation in

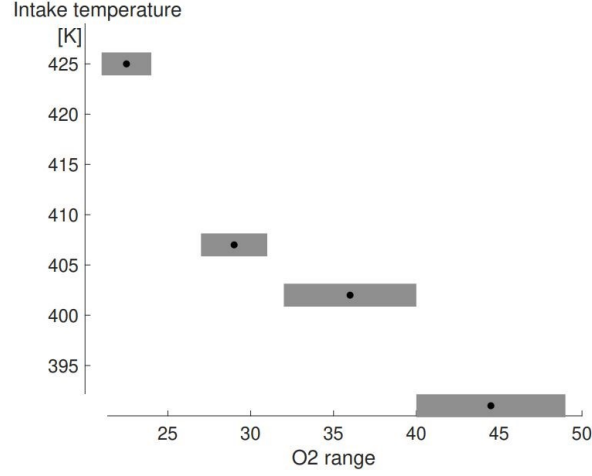


Figure 2.9: Intake temperature of the mixture as a function of the oxygen percentage. Enriching the mixture with oxygen allows to decrease the intake temperature by almost 30 K [29].

oxygen causes a smaller advance of the combustion peak, this sensitivity is weaker. Similar results are applicable to the MPRR depicted in Figure 2.10 (b) since it changes much more dramatically with the oxygen concentration for low oxygen levels (from 5 to 17 [bar/CAD] for a 4% boost in oxygen content) compared to high oxygen levels (from 5 to 11 [bar/CAD] for a 8% boost in oxygen content).

In addition to increasing the power density by increasing the mixture’s density, lowering the input temperature enables the reduction of the heat needed to preheat the mixture, which results in savings through the heat exchanger. In order to evaluate the effects of oxygen enrichment, our analysis will be based on a trade-off between the cost of producing the oxygen as well as the cost of replacing the nitrogen molecules with oxygen molecules as well as the potential increase in power density, the efficiency improvement, and the reduction of heat given to the mixture.

2.2.3 Power to Fuel Context

With regard to the power-to-fuel context in which the HCCI engine is positioned, the approach of oxygen enrichment appears to be ideally suited. Indeed, half a mol of oxygen is produced as a byproduct of the electrolysis of water for every mole of hydrogen produced as indicated in the Equation 1.1. Using oxygen from the electrolysis of water would therefore reduce the nominal cost of hydrogen used to produce methane through the Sabatier reaction presented in subsubsection 1.3.3. This pure oxygen source removes the primary energy drawback of oxygen enrichment, which is the separation of oxygen from nitrogen through an air separator, which generally consumes 190 [kWh/ t_{O_2}] [30]. The exhaust gases’ simple chemical composition is another key benefit in P2F context because it simplifies and lowers the cost of their after-treatment. In the case of an ideal complete stoichiometric oxy-combustion, Equation 2.22 becomes reaction

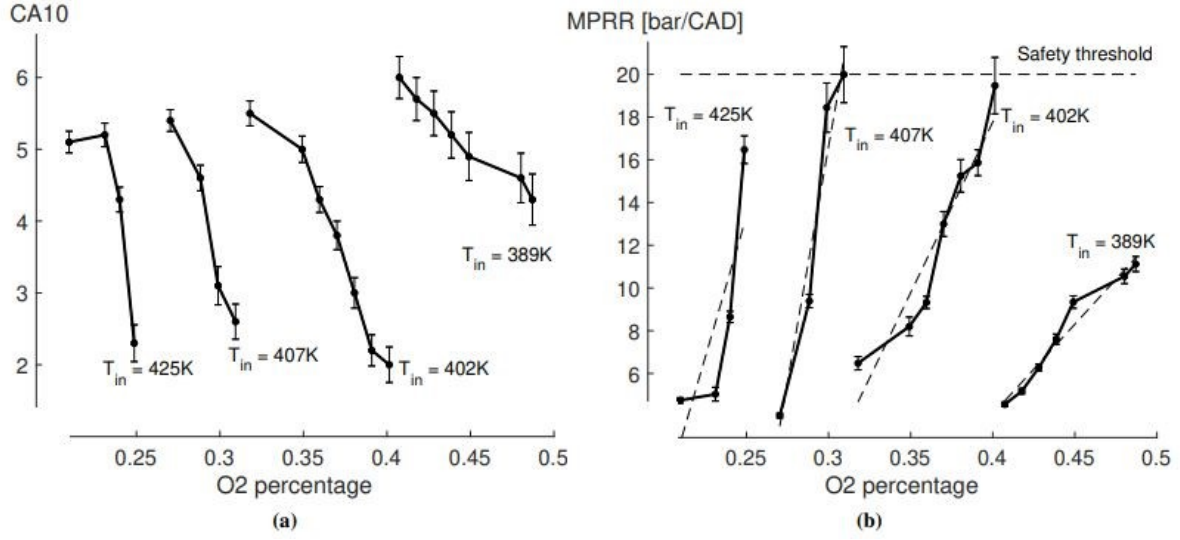


Figure 2.10: Influence of oxygen percentage on (a) ignition timing, and (b) on MPRR [29]

Equation 2.27 and the exhaust gases consists only of water (H_2O) and carbon dioxide (CO_2) :



A pure CO_2 stream can then be obtained only by condensation. All of this can be condensed into a closed-cycle power storage system with net-zero emissions as shown in Figure 2.11.

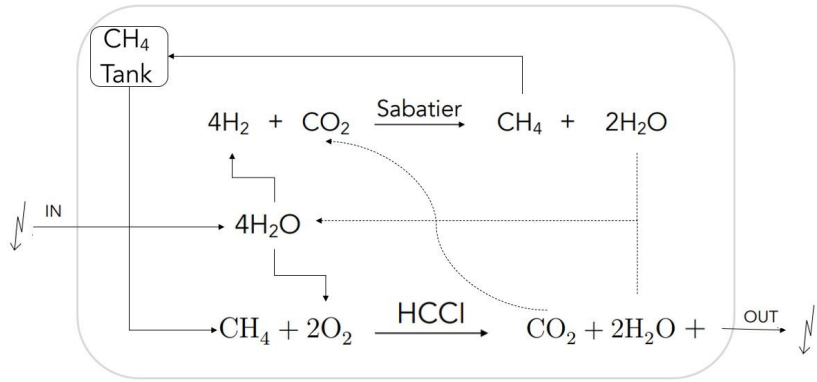


Figure 2.11: Oxy-combustion in closed-cycle power storage system without EGR, inspired from [23]

2.2.4 Oxygen-Enriched Combustion Emissions

Contrary to the just discussed part with oxy-combustion, the analysis of the combustion behavior for oxygen enrichment is more difficult due to the involvement of nitrogen molecules in the reaction and the non-simplicity of the flue gas composition. Bedoya et al. [31] have studied the effect of oxygen enrichment with a 1.9L Volkswagen turbocharged direct injection (TDI) engine modified to run in HCCI mode. They used a typical biogas containing 60 % of CH_4 and 40 % of CO_2 . They decided to maintain a steady fuel injection rate at each engine cycle to maintain a constant fuel MEP throughout the research for oxygen content in air of 21%, 22% and 27%. As Spano et al have shown for pure methane [29], they showed that the oxygen enrichment allowed an advance of the combustion at constant intake temperature (approximately 1.5 CAD from 21% to 27%) and thus a decrease of the ignition delay. Biogas having a lower CH_4 content, its combustion peak will be more advanced than that of pure methane due to a lower resistance to auto-ignition. Regarding HC and CO emissions, which are the characteristic emissions of HCCI engines as described in subsubsection 2.1.4, they increase when the oxygen content in the air goes from 21% to 22% and then decrease when it goes from 22% to 27% but with a general trend of increase between 21% and 27% as shown in Figure 2.12 (a) and Figure 2.12 (b) from their work. The experiment was performed at different inlet pressures and different fuel flows and we can observe on Figure 2.12 that the overall HC and CO emissions decrease for higher inlet pressures and higher biogas flows. This is because adding more fuel typically results in higher in-cylinder temperatures, which are unfavorable for the production of carbon monoxide CO and hydrocarbon HC.

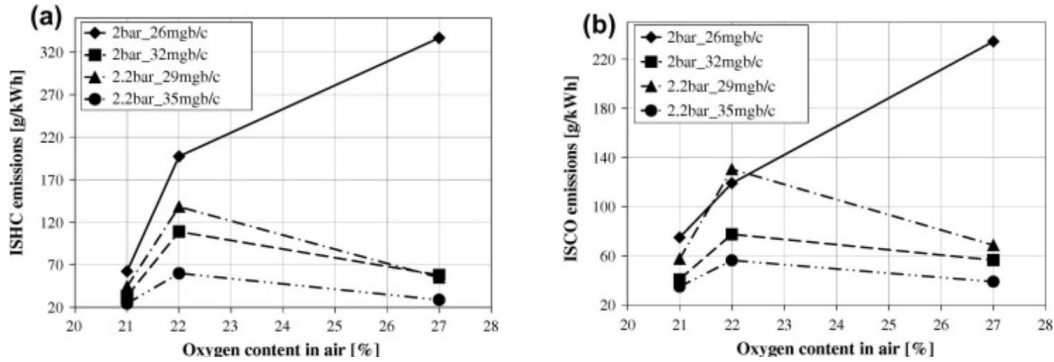


Figure 2.12: Indicated specific HC (a) and CO (b) emissions related with the oxygen content in air. The tests were performed at 473 K inlet charge temperature for different inlet pressure and inlet biogas flow rate [31].

3 HCCI Modeling : 0D Model

This chapter aims at explaining the modeling that our simulation follows as well as all the thermodynamic concepts that are behind it. It starts with a review of the geometrical and thermodynamic principles useful to study the behavior of a gas in an HCCI engine. subsection 3.2 goes into detail about the complete modeling process, starting with a representative explanation that links the model to reality before explaining how it operates. After this, the limitations that this 0D model can face will be explained. And at the end of the chapter, our primary focus will be directed towards understanding the experimental values that we've received. We will then delve into the adaptations we've had to implement in response to these values. Finally, we will conclude with a detailed explanation of how we calibrated our model in accordance with these experimental values.

The modeling of the HCCI engine in the power to fuel system chain is a fundamental task in our thesis, especially for the analysis of the effects of the oxygen enrichment method on engine performance. This allows us to evaluate the importance of key parameters such as the chemical compositions of the fuel and the oxidizer, or the initial conditions of temperature and pressure, on the behavior of the combustion. All this is made possible through the prediction of the auto-ignition timing (CA10) which is the main objective of this model.

Effectively, the initial goal of our thesis is to analyze the possibility of improving the power density of the HCCI engine through the enrichment of air with oxygen, while respecting the operating limits of this engine. These limits, seen in section subsection 2.1.2, are largely influenced by the ignition timing because of its significant correlation with the MPRR. The basis of our research therefore consists of a 0D model, capable of predicting the CA10, and therefore the MPRR, on the basis of the initial conditions provided such as the intake temperature and the equivalence ratio.

The 0D model, or single zone model, considers uniform conditions for the entire volume of the combustion chamber, without taking into account spatial variations. In addition to offering a reduced computation time and consequently faster simulations, this model is particularly adapted to the context of HCCI engine given the quasi-homogeneity of the mixture inducing a quasi-simultaneous ignition of the whole space occupied by the combustion chamber. The absence of flame propagation and the low impact of fluid dynamics on the ignition of a homogeneous charge also play in favor of using this model for the HCCI context.

The 0D model uses the free and open-source CANTERA software library initially developed in C++ but accessible for many other programming languages, including Python, the code language used for this thesis. This software provides a full range of tools for simulation and analysis of chemical processes and thus provides all the information to solve the chemical kinetics of gases in the cylinder with detailed combustion mechanisms. By giving only a few parameters of the gas such as its temperature and pressure as input, CANTERA provides all the information on the thermodynamic state of this gas and is able, on the basis of the chemical reaction rates that take place, to calculate the evolution of the different chemical components involved in the combustion and the consequent heat release. It thus allows to fully characterize the new thermodynamic state of the gas at the time step $t+1$, according to the given reaction conditions.

The chemical reaction kinetic mechanism generally used via CANTERA is GRI-Mech 3.0 [32] for its simplicity based on 53 species and 325 chemical reactions available. However, it may be preferable to adopt a kinetic process that is better suited to the scenario being modeled, in this case, the combustion of methane. Due to its expertise in the combustion based on experimental data specific to light hydrocarbon fuels, particularly methane, and its greater accuracy for this particular system type, the USC-Mech 2.0 [33] kinetic mechanism was ultimately chosen. As explained by A.Pankini, this mechanism "integrates recent thermodynamic, kinetic, and species transport updates related to high-temperature oxidation of hydrogen, carbon monoxide, and C1–C4 hydrocarbons" [34]. The 111 species and 784 reactions it includes make it just as simple and fast as GRI-Mech 3.0. It contains data on the thermodynamic properties of the chemical species such as heat capacity, formation temperature or reaction enthalpies. It is therefore perfectly adapted to the simulation of methane combustion performed for this thesis. This simulation tool is also available through other software such as CHEMKIN or FLUENT but CANTERA was chosen because of its easy access through the python programming language.

3.1 Mathematical and Thermodynamic Relations Necessary for the Model

3.1.1 Geometric Principles

The investigation of the engine geometry and its evolution is one of the initial stages of our modeling for its influence on the gas behavior. As the engine cycle consists of 4 strokes, the crankshaft makes 2 rotations for a total range of 720 [CAD]. We choose to utilize 0 [CAD] at top dead center, which is the end of compression, as a reference. The bottom dead center at the beginning of compression is therefore located at -180 [CAD] and marks the start of the cycle, which lasts until 540 [CAD]. The timing of the opening and closing of the valves plays an important role since it defines the CAD range during which the gas inside the cylinder exchanges mass, or not, with the external environment. Indeed, the system is closed between the intake valve closing (IVC) and the exhaust valve opening (EVO) and its mass can be considered as constant. The intake valve opening (IVO) and exhaust valve closing (EVC) will also have to be defined to mark the beginning of the intake phase and the end of the exhaust phase.

The compression ratio τ and the cylinder displacement V_d also characterize the geometry of the engine and allow to know the volume of the cylinder at the top and bottom dead center according to the following relations :

$$\tau = \frac{V_{BDC}}{V_{TDC}} \quad V_d = V_{BDC} - V_{TDC} \quad \implies \quad V_{TDC} = \frac{V_d}{\tau - 1} \quad V_{BDC} = V_d + \frac{V_d}{\tau - 1} \quad (3.1)$$

To describe the variation of volume in which the gas is located according to the angle of rotation of the crank, it is necessary to express the geometrical position of the piston according to this angle. By convention, the piston position is set to 0 when it is at TDC. This position only depends on the engine's geometrical elements, such as the conrod's length L and the crankshaft's radius r , which corresponds to half the stroke S (Figure 3.1).

A trigonometric development leads to the exact position of the piston as a function of the crank angle θ :

$$z(\theta) = r \left(\frac{L}{r} + 1 - \cos(\theta) - \sqrt{\left(\frac{L}{r}\right)^2 - \sin^2(\theta)} \right) \quad (3.2)$$

Then, multiply this relation by the piston area A and add the volume at TDC allows to determine the volume occupied by the gas according to the crank angle. This instantaneous volume and its derivative are essential for the calculation of heat release presented in the next section.

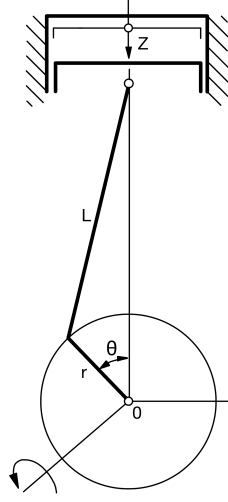


Figure 3.1: Schematic representation of the piston's position according to θ in an internal combustion engine with a connecting rod length L and a crank length r .

$$V(\theta) = V_{TDC} + \frac{S}{2} A \left(\frac{L}{r} + 1 - \cos(\theta) - \sqrt{\left(\frac{L}{r}\right)^2 - \sin^2(\theta)} \right) \quad (3.3)$$

$$= \frac{V_d}{\tau - 1} + \frac{V_d}{2} \left(\frac{L}{r} + 1 - \cos(\theta) - \sqrt{\left(\frac{L}{r}\right)^2 - \sin^2(\theta)} \right) \quad (3.4)$$

$$\frac{dV}{d\theta} = \frac{V_d \sin \theta}{2} \left(1 + \frac{\cos \theta}{\sqrt{\left(\frac{L}{r}\right)^2 - \sin^2 \theta}} \right) \quad (3.5)$$

3.1.2 Thermodynamic Principles

Heat Release Calculation

The thermodynamic parameters that characterize a gas or a gas mixture, such as pressure p , temperature T , volume V , number of moles n , or even internal energy U , define its state. Our simulation of the mixture in the HCCI cylinder depends critically on our ability to forecast its evolution given our understanding of its thermodynamic condition and the physical principles guiding its behavior. Considering the cylinder as being closed between the IVC and the EVO, a first physical principle known as the "first law of thermodynamics" can be applied. This one states that the variation of the internal energy for a closed system (one that does not exchange matter with the environment) is equal to the amount of energy exchanged with the external environment through thermal transfer (in the form of heat) and by mechanical transfer (in the form of work). The signs in Equation 3.6 indicate that the quantity of heat Q is received by the load and the quantity of work W is performed by it on its environment.

$$\Delta U = Q - W \quad (3.6)$$

This formula is important because it is the basis of the development leading to the relationship between the rate of heat released by combustion and the evolution of the in-cylinder pressure. To achieve this relationship, it is necessary to start by differentiating this first law with respect to the crank angle θ :

$$nc_v \frac{dT}{d\theta} = \frac{dQ}{d\theta} - p \frac{dV}{d\theta} \quad (3.7)$$

Then, it is required to apply the law of perfect gases $pV = nRT$, a second physical law to be differentiated in order to characterize the evolution of the gas mixture according to θ .

$$\frac{d}{d\theta}(pV) = \frac{d}{d\theta}(nRT) \quad (3.8)$$

$$p \frac{dV}{d\theta} + V \frac{dp}{d\theta} = nR \frac{dT}{d\theta} \quad (3.9)$$

Injecting Equation 3.9 into Equation 3.7, we obtain an expression of the heat variation $\frac{dQ}{d\theta}$ available for the load :

$$\frac{dQ}{d\theta} = p \frac{dV}{d\theta} + nc_v \frac{dT}{d\theta} \quad (3.10)$$

$$= p \frac{dV}{d\theta} + \frac{c_v}{R} \left(p \frac{dV}{d\theta} + V \frac{dp}{d\theta} \right) \quad (3.11)$$

$$= \left(1 + \frac{c_v}{R} \right) p \frac{dV}{d\theta} + \left(\frac{c_v}{R} \right) V \frac{dp}{d\theta} \quad (3.12)$$

Remembering the adiabatic coefficient $\gamma = \frac{c_p}{c_v}$ and Mayer's relation $R = c_p - c_v$ with c_p and c_v , the specific molar heat capacities at constant pressure and constant volume respectively :

$$\frac{dQ}{d\theta} = \frac{\gamma}{\gamma - 1} p \frac{dV}{d\theta} + \frac{1}{\gamma - 1} V \frac{dp}{d\theta} \quad (3.13)$$

It is important to note that this heat Q corresponds to the the total heat exchange between the charge and the environment, Q_{net} , which is composed of the heat released by combustion Q_{gross} and the heat lost through the cylinder walls by convection, Q_{loss} .

$$Q_{\text{net}} = Q_{\text{gross}} - Q_{\text{loss}} \quad (3.14)$$

The rate of heat released by combustion is thus obtained by incorporating combustion heat release and heat losses in Equation 3.13 :

$$\frac{dQ_{\text{gross}}}{d\theta} = \frac{\gamma}{\gamma - 1} p \frac{dV}{d\theta} + \frac{1}{\gamma - 1} V \frac{dp}{d\theta} + \frac{dQ_{\text{loss}}}{d\theta} \quad (3.15)$$

This HRR relation links the variation, with respect to the crank angle degree, of the heat released by mixture's combustion with the variation of pressure, volume and heat lost in the walls. The evolution of the heat released by combustion as a function of angular position, $Q_{\text{gross}}(\theta)$, is the result of the integration of Equation 3.15 over the range of crankshaft angles during which combustion occurs. An example for characteristic curves of the heat release rate and the cumulative heat release is shown in Figure 3.2.

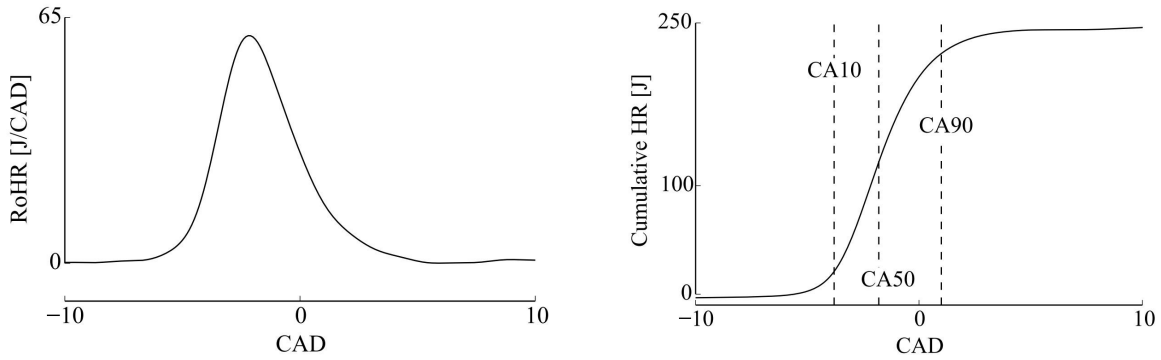


Figure 3.2: Typical HCCI HRR and $Q_{\text{gross}}(\theta)$ profiles [35]

Once the cumulative heat release is known, we can easily determine the crankshaft angle, in [CAD], that corresponds to the various combustion events, such as the start (CA10), middle (CA50), and end (CA90), since the CA_X represents the angle for which $X\%$ of the total heat has been released by the combustion :

$$Q_X = \frac{X}{100} (Q_{\text{gross},\text{max}} - Q_{\text{gross},\text{min}}) \quad (3.16)$$

The combustion duration (DOC) is referred as the time (in CAD) required to transition from 10% to 90% of the total heat generated, CA90-CA10. It provides an idea of how rapidly combustion happens.

Heat Losses Estimation

The determination of heat losses is another fundamental aspect of our engine modeling, especially in the case of 0D simulations. Indeed, the objective of this model is to predict the combustion behavior as well as possible, in particular via the determination of the CA10. For this, it is vital to describe the engine's core

temperature since it controls the combustion for fuels with single-stage ignition, such methane. However, given the uniform scalar field of temperature characteristic of the 0D model, it is the whole volume of gas that will mimic this high temperature of the core implying a much shorter and more intense heat peak than if the boundary layers were taken into account. How these in-cylinder heat losses are estimated is critical for the estimation of the combustion peak and the correct replication of the core temperature.

In general, the heat transfer from the gas to the walls of the combustion chamber is considered convective for the entire exchange surface A :

$$\frac{dQ_{\text{loss}}}{dt} = h \cdot A \cdot (T - T_{\text{wall}}) \quad (3.17)$$

A consists of the surface of the piston, the head of the cylinder, as well as the lateral surface of the cylinder which evolves according to the position of the piston, and thus to the angular position of the crankshaft. A new simplification is made here considering an equal and uniform temperature for all surfaces included in A, while in reality, some areas like the piston or the exhaust are hotter than others. This uniform temperature indicated by T_{wall} , in [K], remains constant throughout the cycle, unlike T, the in-cylinder gases temperature, which changes throughout the cycle.

The parameter h represents the Newton convective heat transfer coefficient and constitutes a very large field of study on its own. It can be characterized in accordance with a number of correlations, the most popular ones being those of Woschni, Hohenberg, Annand, and Chang in the context of the HCCI engine. These correlations are very representative of the heat transfer between the gas boundary layer and the walls of the cylinder, leading to a hotter core temperature that 0D model can't reach. Using them do not provide a very good representation of the core temperature that we seek to simulate. However, it is possible to adjust the scaling factor α to suit the results predicting the combustion behavior to the experimental results. Indeed, α_{scaling} is set to 130 for these correlations but this value leads to an overestimation of the losses in 0D model because boundary layers are hotter in 0D simulation than in reality. Decreasing its value would allow to obtain a better estimation of the heat fluxes at the TDC despite an under estimation of the heat losses during compression. In any case, this correction of the convection coefficient through the scaling factor must be adapted according to the working conditions in which we are and α must therefore necessarily be recalibrated so that the model fits the experimental data. We choose to perform this calibration with the Hohenberg correlation since it better fits the HCCI conditions [36] and its ease of calculation based on instantaneous parameters :

$$h = \alpha_{\text{scaling}} \cdot \left(\frac{p}{10^5} \right)^{0.8} \cdot L^{-0.06} \cdot T^{-0.4} \cdot \left(\frac{S \cdot RPM}{30} + 1.4 \right)^{0.8} \quad (3.18)$$

With α , the scaling factor. p, the instantaneous in-cylinder pressure [Pa]. T, the instantaneous temperature of the gas [K], and S the stroke of the piston [m]. The characteristic length L often corresponds to the instantaneous cylinder volume V [m³] in most cases even if the original Hohenberg correlation takes into account the cubic root of the instantaneous cylinder volume $\sqrt[3]{V}$ [36].

Piston Work

At an instantaneous pressure p , the rate of work performed by the burning gas on the piston, or by the piston on the gas, implies a variation of volume according to the relation 3.19. This quantity is defined as negative when the mixture gives energy to the piston and positive when the mixture receives energy from the engine.

$$\frac{dW}{d\theta} = -p \frac{dV}{D\theta} = -(p_{cyl} - p_{atm}) \frac{dV}{d\theta} \quad (3.19)$$

The integration of the instantaneous work over the whole cycle allows to calculate the total net work done by the gases which should have a negative final value. Next, the absolute value of this quantity is calculated and divided by the engine's displacement to determine the engine's net IMEP (Equation 2.9) and the efficiencies that follow (see Section 2.1.3).

3.2 0D Model

3.2.1 Model Representation

CANTERA made possible the simulation of the gas evolution within the HCCI engine providing all the tools necessary to characterize the combustion and the heat and mass transfer through chemical reaction mechanisms, etc. This software enables the realistic modeling of numerous physical events, including those that take place in an HCCI engine. To do this, we had to start by creating a set of 9 interconnected objects: 4 reservoirs, 2 valves, 1 reactor and 2 walls (see Figure 3.3).

In CANTERA, reservoirs are considered as infinitely large volumes that maintain a constant state, meaning that their temperature, pressure and chemical composition never change from the initial values imposed. The first reservoir corresponds to the ambient air below the lower surface of the piston. It consists of a gas composed of 21% oxygen and 79% nitrogen, at ambient temperature and pressure, i.e. 300 [K] and 101325 [Pa] respectively. The second reservoir represents the environment responsible for heat losses within the cylinder, since Cantera does not allow heat exchange between a reactor and a wall, but only between 2 reactors separated by a wall, or between a reactor and a reservoir separated by a wall. The gas in this tank is air maintained at a pressure of 1 atmosphere. Nevertheless, these characteristics are mostly unimportant since the crucial element for heat transfer is the temperature, which will be set at a constant value equivalent to T_{wall} for this reservoir. The third reservoir corresponds to the gas exhaust area. It is thus once again air composed of 79% oxygen and 21% nitrogen. Its temperature and pressure conditions are set at 300 [K] and 1 [bar]. Finally, the last reservoir corresponds to the inlet of the system. It is through this inlet that we will set all our input parameters to characterize the mixture in its initial state, at time $t=0$, just before launching the simulation. In this reservoir, CANTERA enables the creation of a combination of fuel and oxidizer while allowing the user to choose several input conditions like temperature, pressure, oxygen rate and fuel quantity (fuel MEP).

The reactor is then created. It represents a reaction volume where the thermodynamic state and the chemical species evolve when the simulation is running. It therefore corresponds to the cylinder of the HCCI engine and all its geometrical characteristics are provided by the engine specifications (see subsubsection 3.4.1). It is initially empty but, as soon as the simulation starts, it is immediately made up of the mixture and the thermodynamic conditions which characterize it at the beginning of compression, since it is at this moment that the simulation starts (-180 [CAD]).

Valves are CANTERA objects that represent flow devices with a mass flow rate calculated according to the pressure drop across them. The first one establishes a link between the reactor and input reservoir. It symbolizes the intake valve. The second one serves as the exhaust valve and joins the reactor to the outlet reservoir. It is possible to link the behavior of these valves to the simulation time and thus to define an admission time between IVO and IVC as well as an exhaust time between EVO and EVC.

As said before, walls are stateless objects in Cantera, meaning that no differential equation is integrated to determine any wall property. The first wall separates the reactor from the second reservoir. It is possible to give it a certain surface area [m^2] (top and bottom surfaces added to linear surface of the cylinder) and an overall heat transfer coefficient [$\frac{W}{m^2K}$], which both change as the simulation progresses. Finally, the second wall represents the piston which separates the ambient air and the in-cylinder reactor. It is defined by the head cylinder's surface and a speed that is imposed according to Equation 3.5 in order to cause the cylinder's volume to change throughout the course of the simulation.

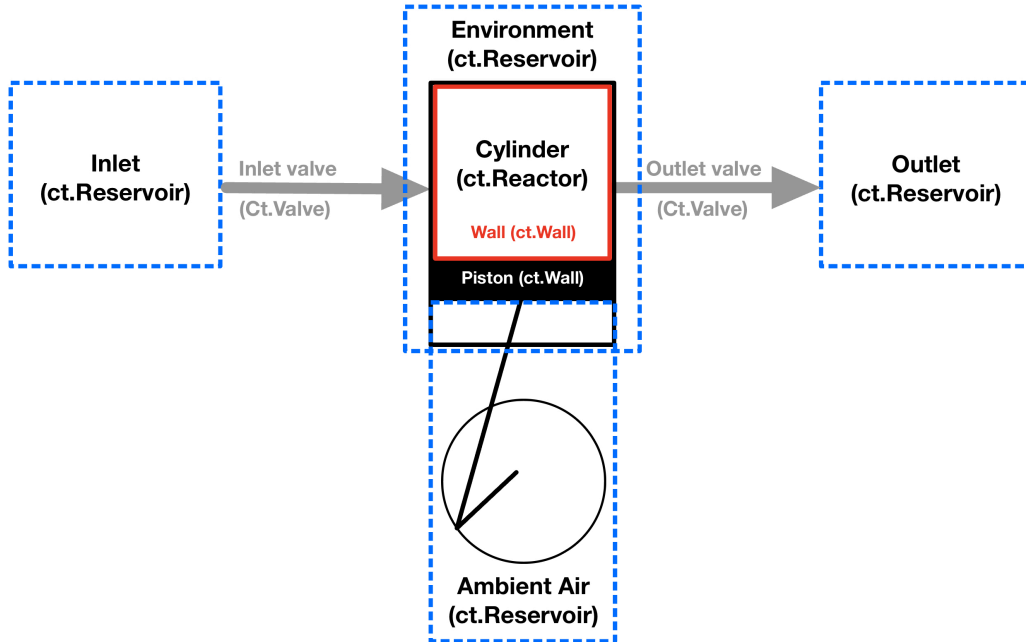


Figure 3.3: Set of 7 interconnected CANTERA objects for the HCCI engine simulation.

3.2.2 Model Explanation

The 0D model considers a fuel-oxidizer mixture as an ideal gas, contained in a combustion chamber of volume V with uniform temperature and pressure fields across the volume. The thermodynamic state of the mixture is therefore the same at each point in the space occupied by the gas.

The objective is to model the thermodynamic evolution of the gas throughout the cycle based only on the engine specifications and the initial state of the mixture. Starting from these input conditions such as the type of fuel, the composition of the oxidizer, the amount of fuel, the temperature and the pressure, the model predicts the thermodynamic state of the gas at the next time step based on the first principle of thermodynamics for closed systems as well as on the reaction rates of species involved in the kinetic mechanics of methane combustion. The single-zone model considers therefore a closed system from -180 [CAD] to 180 [CAD], i.e. during the compression and expansion phases, with no trapped residual gases. Throughout the simulation, the model imposes an instantaneous volume $V(t)$, calculated as a function of the crank angle according to Equation 3.4, based on piston motion.

The differential form of the first law of thermodynamics for closed systems (Equation 3.7) is the ODE that will guide the evolution of the gas throughout the cycle, specifying the separation of the net heat release into its two components $Q_{\text{net}} = Q_{\text{gross}} - Q_{\text{loss}}$:

$$\frac{dU}{dt} = n c_v \frac{dT}{dt} = \frac{dQ_{\text{gross}}}{dt} - \frac{dQ_{\text{loss}}}{dt} - p \frac{dV}{dt} \quad (3.20)$$

The CVODES solver of CANTERA is used to integrate this ODE at each time step with a defined absolute and relative error, which will be discussed in subsubsection 4.5.2. This solver also allows for predicting the mass evolution m_k of each specie according to their rate of change (known from USC 2.0) at instantaneous thermodynamic conditions, as well as the total heat release by the reactions Q_{gross} during this time step. The average mole number n [mol] and the constant volume heat capacity c_v [$\frac{\text{J}}{\text{mol K}}$] of the mixture are known directly from the instantaneous thermodynamic conditions prevailing at time t .

The term dQ_{loss} , representing parietal heat losses, is modeled by Relation 3.21 as explained in Section 3.1.2 :

$$\frac{dQ_{\text{loss}}}{dt} = h A (T - T_{\text{wall}}) \quad (3.21)$$

The Hohenberg correlation (3.18) gives the convection coefficient h for instantaneous temperature, pressure and volume parameters. T_{wall} is constant throughout the simulation and uniform across the wall surface. Its value is provided by the experimental data and depends on the different cases studied.

The pressure p represents the instantaneous pressure inside the cylinder, and the volume variation dV/dt is calculated using Equation 3.5 based on the piston speed and taking into account the angular velocity ω :

$$\frac{dV}{dt} = \frac{dV}{d\theta} \cdot \frac{d\theta}{dt} = \frac{dV}{d\theta} \cdot \omega.$$

Now, it is possible to predict the gas's state at time $t+1$. In fact, the internal energy increment is used to determine the temperature increment $dT = dU/(n c_v)$ from which we obtain $T(t+1)$. The piston speed at this new time step determines the volume, and the ideal gas law is used to get the pressure. The algorithm used during the compression and expansion phases is shown in Figure 3.4. It is observable that the choice of the initial conditions is determining for the accuracy of our model since they are the real starting point of it.

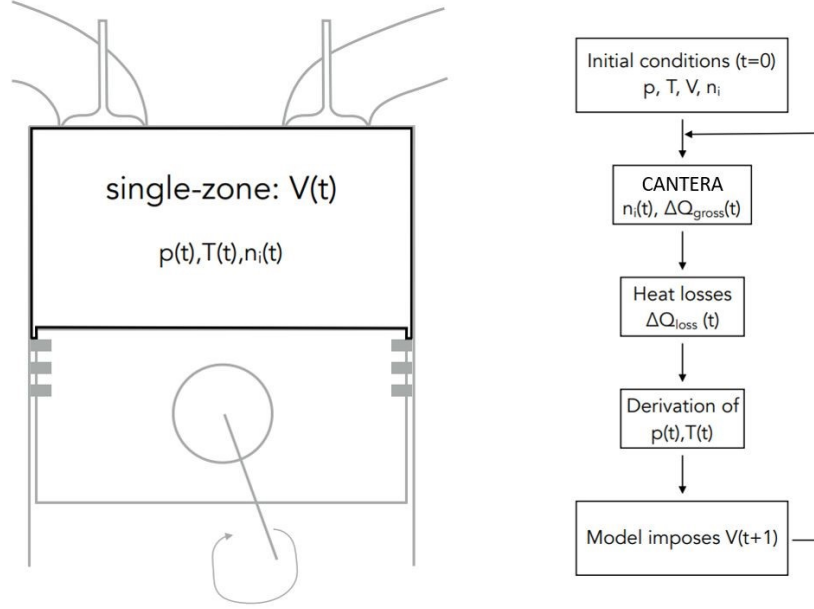


Figure 3.4: Schematic representation of the algorithm used for the single-zone model inspired by [23].

3.3 Model Limitations

A 0D model, as its name might suggest, has certain inherent limitations that we must consider to effectively use it for simulating aspects of combustion. To start with, both temperature and pressure within the cylinder are represented as scalars, encompassing the entire mixture of the cylinder. Therefore, thermodynamic conditions and species concentration are assumed to be uniform throughout the cylinder's volume. This uniformity has to be taken in account during the hole modeling. For example it plays a crucial role when simulating heat losses, as heat losses are mainly affected by the temperature of the outer layers, rather than the temperature of the core.

Another consequence of the constant thermodynamic conditions across the volume is that we won't observe any stratification during the combustion process. This is because the entire piston is assumed to have the same temperature, leading to a very abrupt combustion as a function of crank angle degree (CAD). When we refer to rapid combustion, it corresponds to the fact that our model often predicts a significantly exaggerated heat release rate. This overestimation can be observed in Figure 3.5, which contrasts our heat release rate prediction with the experimental data for equivalent baseline conditions.

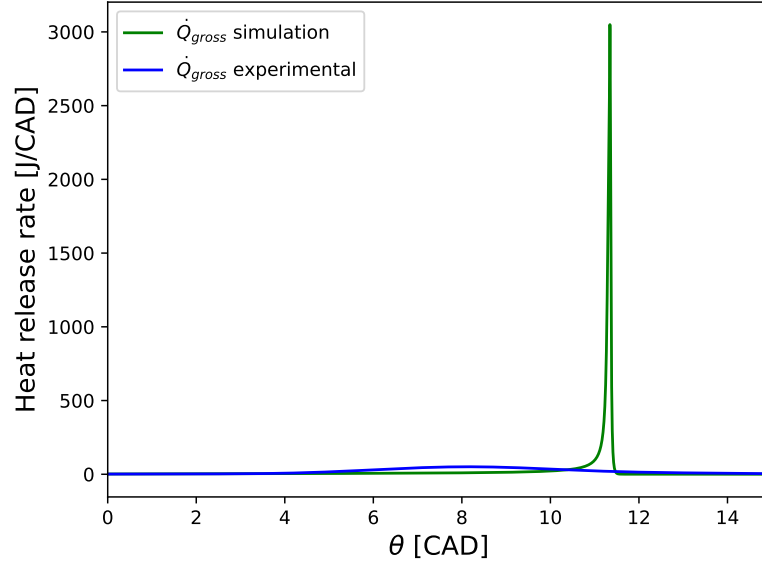


Figure 3.5: Comparison between experimental and simulation heat release rate

On this figure, it's plainly evident that our model predicts combustion to occur very instantaneously, in stark contrast to the experimental curve. The experimental data maintain a relatively low heat release rate over a much longer period, which is the opposite behavior of our model.

This overestimation correlates with an inflated Maximum Pressure Rise Rate (MPRR), which may lead to complications in our analysis. As a result, we had to develop a different approach to accurately determine the MPRR under specific combustion conditions, as explained in subsection 4.2).

Apart from the uniformity of our cylinder attributed to our 0D model, it's also crucial to note that one of our assumption for the working of our model is that our temperature, pressure, and mixture composition are interconnected through the ideal gas law.

While it's true that a 0D model has numerous limitations, we noticed that by formulating constructive hypotheses based on values this model can predict, it's possible for the 0D model to yield significant insights, as evidenced by the findings of this study.

3.4 Experimental Data

3.4.1 Experiment Specification

The majority of this thesis's work is devoted to a numerical analysis of a combustion cylinder, whose specifications were acquired from the UCL research engine used to provide the experimental data that served as the foundation for our model calibration (see subsection 3.5). This engine is the Yanmar L100V (Figure 3.6), originally designed as a 4-stroke CI engine. Numerous modifications have been made to this engine over the years to enable new experimental settings and further HCCI engine investigations. Actual engine specifications are given in Table 3.1.

UCL HCCI research engine	
Engine type	Air-cooled Four-stroke Single-cylinder
Displacement volume, V_d	435 [cm ³]
Geometric compression ratio, τ	21.2 : 1
Effective compression ratio, τ_{eff}	19.64 : 1
Cylinder bore, B	86[mm]
Piston stroke, S	75[mm]
Crank radius, r	37.5[mm]
Connecting rod length, L	120.5[mm]
Rotation speed	1500[RPM]
Intake valve closing, IVC	-127[CAD]
Exhaust valve opening, EVO	127[CAD]

Table 3.1: Actual HCCI engine specifications

The experimental data come from experiments carried out by S. Spano in the IMMC laboratory of UCLouvain to investigate the impact of oxygen enrichment on engine performance. Various initial conditions were tested by imposing the composition of the methane-oxidizer mixture, its inlet temperature, mass flow, etc., in order to measure the experimental pressure prevailing inside the cylinder throughout the experiment. Each test corresponds to 100 engine cycles. Post-processing via the MATLAB interface is then performed to deduce the cumulative heat release Q_{gross} (via Equation 3.20), the start of combustion (CA10) and the Maximum pressure Rise Rate for each of the 100 cycles based on the pressure measurements. These 3 data sets are then averaged to observe their evolution as a function of input conditions. The Hohenberg correlation is used in the convective heat transfer model to calculate the post-processed losses dQ_{loss} , with the engine cooling fan maintaining a constant temperature T_{wall} . Typical experimental data are shown in Table 3.2:

$O_2[\%]$	$T_{in} [K]$	$T_{\text{body}} [K]$	FuelMEP[bar]	$Q_{\text{gross,max}} [J]$	CA10 [°CAD]	MPRR[bar/CAD]
20.88	476.2	423.2	9.31	291	6.70	3.63
26.44	459.2	409.9	8.25	286	6.30	3.45
35.88	446.5	416.6	8.79	258	5.70	3.97

Table 3.2: Experimental results from S.Spano : $Q_{\text{gross,max}}$, CA10, MPRR



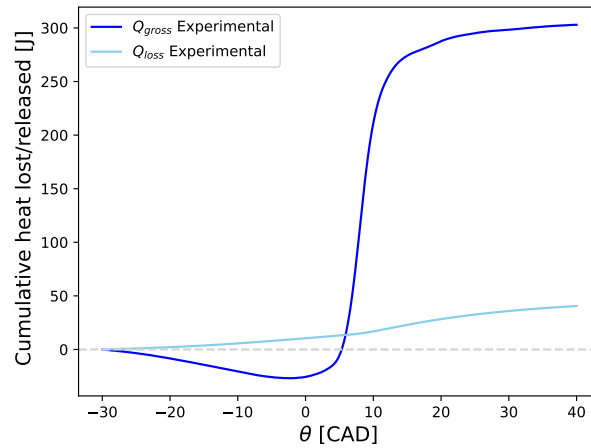
Figure 3.6: YANMAR L100V [37]



Figure 3.7: UCL HCCI research engine

3.4.2 Experimental Results Analysis/Correction

This part focuses on understanding experimental data. It is crucial to ensure that these values are accurate and reliable to prevent any misleading outcomes in our subsequent results. Firstly, since our calibration will be essentially based on combustion timing, We concentrate on examining the cumulative experimental heat release and the cumulative experimental heat losses. These are shown in the Figure 3.8 It is worth noting that the conditions under which this graph is displayed are currently insignificant as our main focus is on its visual representation.

Figure 3.8: Experimental Q_{gross} and Q_{loss}

The initial aspect to notice is the negative part of the curve preceding combustion. This might appear peculiar since heat discharged during combustion can only be positive. We attempted to understand this irregularity in the experimental curve through the following reasoning.

Firstly, there could simply be endothermic reactions occurring just before combustion, causing a part of the decrease in the internal cylinder heat.

Another plausible reasoning could be related to the error on the clearance volume or on the top dead center. This presumption stems from a research [38][39] that asserts the Pressure-Volume phase lag to be a significant source of inaccuracies in thermodynamic computations. The Pressure-Volume (P-V) phase lag in an internal combustion engine refers to the temporal offset or discrepancy between the peak pressure and the top dead center position of the piston. The time it takes for the flame to spread across the combustion chamber, the delay caused by auto-ignition, and other intricate physical and chemical processes that take place during combustion all contribute to the fact that there is frequently a phase lag in practise.

The approach covered by Tazerout et Al in order to calculate the proper value of TDC, which is necessary to precisely determine the thermodynamic characteristics, is based on the compression ratio and the T-S diagram when the engine is in motoring conditions. According to this study, the T-S diagram in a case with a proper TDC calibration must be symmetrical with respect to the peak temperature as shown in Figure 3.9. In contrast, an experimental TDC that has been improperly calibrated will exhibit a loop with a cross point in its (T-S) diagram, as seen in Figure 3.10.

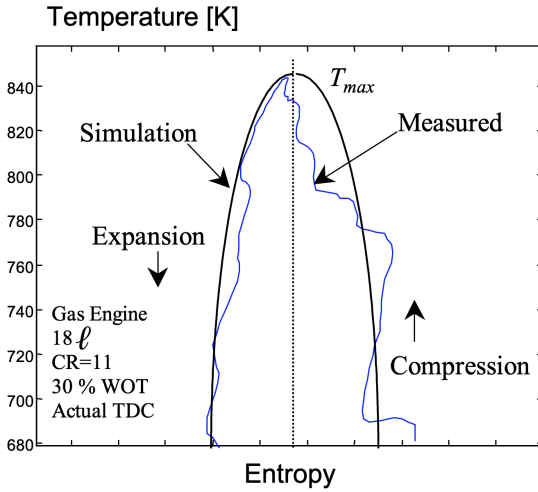


Figure 3.9: Example of (T,S) diagram with a correct TDC calibration [39]

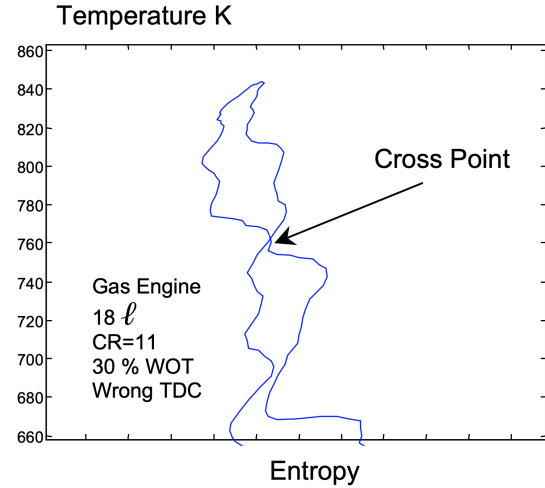


Figure 3.10: Example of (T,S) diagram with wrong TDC calibration [39]

To get an idea of the offset of the experimental TDC, we can look at the pressure curve at motoring conditions. Figure 3.11 clearly illustrates that the pressure peak doesn't precisely coincide with the crank angle degree (CAD) zero, i.e. top dead center. If the post-processing of the experimental pressure curve does not take into account this volume-pressure lag, it could lead to incorrect CHR curves.

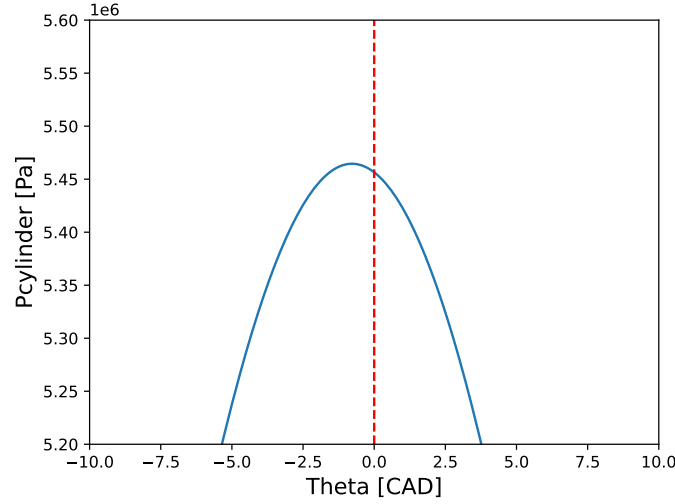


Figure 3.11: Pressure curve with a peak before the actual TDC

Finally, other errors related to experimental post-processing could explain this phenomenon. Towards the end of our work, we received new experimental data that were more consistent. The shape of heat release and heat loss curves derived from these new data is presented in Figure 3.12. The error discussed regarding the negative part of CHR curve in Figure 3.8 was found to be associated with the improper utilization of the effective compression ratio in post-processing. Unfortunately, these new experimental data, due to their limited quantity and diversity (few tested conditions), do not form a sufficient dataset to calibrate our model. Additionally, we still observe a small negative portion (although reduced compared to before) on the curve derived from the new data, which could be explained by what has been previously mentioned.

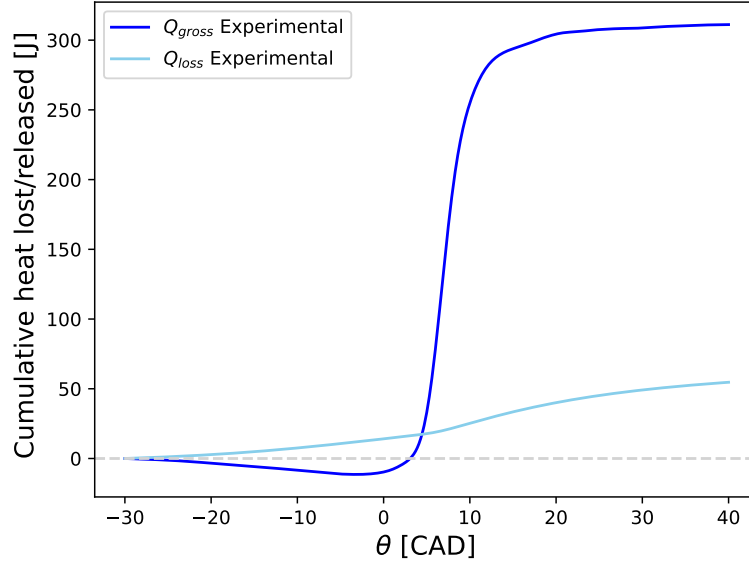


Figure 3.12: Experimental Q_{gross} and Q_{loss} for new data.

However, reliable results can be obtained from calibration with the first data set by incorporating the negative portion of the cumulative heat release curves into the combustion timing prediction process. Consequently, we postulated that combustion initiates at the lowest point of the Q_{gross} experimental curve. This assumption seems logical, as the rise in this curve can only be attributed to the methane combustion. Hence, we will calculate the combustion timings from this point onward. Nevertheless, this reference point might not be perfectly accurate, as combustion take place slightly before this point to "balance" the negative slope of the CHR of the pre-combustion phase. However, we consider this discrepancy as close to negligible due to the small size of the negative slope before the combustion compared to the maximum slope during combustion.

3.5 Model Calibration and Validation

This section focuses on the calibration of our model to best fit the initial parameters given as input to the model. As presented in subsubsection 3.2.2, the model inputs are fuelMEP, the amount of oxygen in the oxidizer, the starting temperature and pressure, the relative time-step error, the alpha scaling factor, and the engine specifications. By meticulously processing the experimental data and calibrating the input parameters, we can fine-tune our model to ensure it mirrors reality as closely as possible.

As previously mentioned, the calibration of the 0D model is based on experimental results of oxygen-enriched methane combustion obtained by S. Spano. We have simply changed the way of calculating the start of combustion with the correction explained in the previous section to obtain the results available in Table 3.3. Additionally, we chose to utilize CA05 rather than CA10 as reference variable representing

the start of combustion. This choice is justified by the quasi-instantaneous combustion of the 0D model. Indeed, it makes more sense to think of CA05 as the commencement of combustion than CA10 given the almost vertical slope of the cumulative heat release. The CA05 values derived from the experiments must therefore be known. They are computed in post-processing from the experimental cumulative heat release Q_{gross} curve taking into account its negative part. They are obtained by averaging over all 100 cycles of 1 experiment, to avoid basing our analysis on a single experimental cycle and thus ensure more robust post-processed values of CA05 generalized over several cycles.

$O_2[\%]$	$T_{in} [K]$	$T_{\text{body}} [K]$	FuelMEP[bar]	CA05 [$^{\circ}$ CAD]	MPRR[bar/CAD]
20.88	476.2	423	9.31	4.70	3.63
26.65	460.5	423	9.32	3.40	5.44
56.15	420.37	423	9.43	3.60	4.59

Table 3.3: Experimental results from S.Spano : $Q_{\text{gross}_{\text{max}}}$, CA05, MPRR

3.5.1 Bottom Dead Center State Calibration

Since we are employing a single-zone closed-system model to simulate a real engine, the initial thermodynamic state of the reactor in the model must coincide with the initial thermodynamic state of the experimental cylinder when the latter turns into a closed system, i.e. when the intake valve closes. Therefore it would make sense to start our simulation with the CAD that corresponds to the IVC of the experimental cylinder, which is -127 [CAD]. Given the difficulties of calculating p_{IVC} and T_{IVC} on the basis of input values, this choice could, however, result in quick inaccuracies. Consequently, it was determined that the bottom dead center would serve as the simulation's starting point.

When developing his 0D model, Dr. Pochet [23] already conducted a research of the interaction between intake and BDC parameters in order to look into the connection between intake conditions and the resulting auto-ignition timing. Its aim was to estimate the input parameters that would allow CA10 to occur at the top dead center. Although we will perform the reverse procedure, i.e. estimate the CA05 on the basis of the input parameters, we will rely on his explanations for what follows.

For the pressure, we consider the difference between p_{intake} and p_{BDC} to be negligible, even though the intake valve is still open at BDC. This approximation is confirmed by experimental results, which show only a very slight difference between these 2 pressures. Note that this assumption, considering $p_{in} = p_{\text{BDC}}$, is not always true for models that go the other way round, i.e. estimating p_{in} on the basis of p_{BDC} . The inlet pressure can be deduced as equivalent to the BDC pressure from the simulation only for a IVC that occurs before 157 CAD before TDC.

Due to heat exchange, mixing with residual gases and gas dynamic effects, the temperature of the engine at bottom dead center is very different from the intake temperature. Various correlations are proposed, and it will be necessary to choose the one best suited to our case. The first correlation results from research done on the Orleans HCCI engine by Contino et al. [40], who examined the influence of these 3 phenomena. This relation (Equation 3.22) was created using a cooling system of 90 [$^{\circ}$ C] and an equivalence ratio of

0.3 for valeric biofuels, such as methyl, ethyl, propyl, butyl, and pentyl. It is considered valid for input temperatures from 40 to 200°C.

$$T_{BDC} = 0.652 \cdot T_{in} + 138[K] \quad (3.22)$$

The geometric parameters of the engine under study are too dissimilar from ours, despite the fact that this correlation holds true for input temperatures matching those of methane combustion. A valid correlation should then be sought for the UCLouvain research engine. Fortunately, Dr. Pochet [23] has created experimental correlations for measuring the BDC temperature from the intake one with this specific engine. The first one was developed for hydrogen combustion at an equivalence ratio of 0.2 and intake temperatures ranging from 53 to 115°C :

$$T_{BDC} = 0.548 \cdot T_{in} + 49.835[C] \quad (3.23)$$

Unfortunately, this correlation is valid for temperatures a little too low compared with those we are assessing. A second correlation was developed, again on the UCLouvain research engine, for an ammonia-hydrogen mixture at an equivalence ratio of 0.35 and temperatures between 49 and 233°C.

$$T_{BDC} = 0.657 \cdot T_{in} + 57.917[C] \quad (3.24)$$

This correlation is the one that best suits the experimental conditions on which we are basing our work, and will therefore be incorporated into the 0D model in order to best estimate the temperature at the start of the simulation on the basis of the intake temperature studied. We make this approximation since no correlation has been shown for methane combustion using the experimental engine at UCLouvain. Given the importance of a correct BDC temperature estimation on the accuracy of our model, the use of this correlation is a non-trivial assumption that must be taken into account when analyzing the results. Developing this correlation for methane combustion with the UCLouvain engine could be an interesting challenge to investigate in future work.

The last parameter to be adjusted, provided as input to our model, is the compression ratio. Because the intake valve closes later than the BDC, compression begins while the valve is still open, resulting in a lower experimental in-cylinder pressure. The effective compression ratio, which is by definition lower than the geometric one, serves as a defining characteristic of this real compression. This experimentally found parameter is provided in Table 3.1 and is used to account for the delayed IVC. Because of this, the simulated volume at the top dead center is larger than the geometric volume : $V_{TDC} = \frac{V_d}{\tau_{eff}-1}$. The total number of moles calculated at the beginning of the simulation is thus:

$$n_{tot,BDC} = \frac{p_{in} \cdot V_{BDC}}{R \cdot T_{BDC}} \quad (3.25)$$

3.5.2 Ignition Timing Calibration : Scaling Factor Alpha

Now that the thermodynamic conditions at the start of the simulation (BDC) are linked to the initial conditions measured in the intake manifold, we'll proceed with the analysis of the last essential parameter for calibrating our model, namely the Hohenberg scaling factor alpha. As explained in the part on heat losses estimation, this parameter can be adjusted to align combustion timing perfectly with experimental results. To achieve realistic ignition timing, a lower alpha than the 130 used in the Hohenberg correlation (Equation 3.18) should be used, although this underestimates the actual heat losses in the cylinder for different temperature conditions.

In order to obtain an accurate prediction of the combustion start, the alpha factor should be adjusted based on inlet conditions, particularly the intake temperature, using experimental results. The calibration of the alpha factor aims to simulate heat losses in order to provide the best possible prediction of CA05 compared to the experimental CA05. If the input intake temperature is different, the simulation of losses is affected by this new intake temperature and must be adjusted to consistently provide a correct prediction of CA05 compared to the experimental one. Therefore, the scaling factor needs to be modified.

Even if the experimental wall temperature is not always equal to 423K, the effect of this temperature is reflected in the experimental CA05 and is considered in the choice of the alpha factor of the model which aims to achieve a CA05 as close as possible to the experimental one, with a constant simulated wall temperature. Table 3.4 shows the alpha settings that result in the best agreement for same, experimental and simulated, intake conditions.

$O_2[\%]$	$T_{in}[K]$	$T_{BDC,sim}[K]$	$T_{wall,exp}[K]$	$T_{wall,sim}[K]$	α_{sim}	CA05 _{exp} [CAD]	CA05 _{sim} [CAD]
20.88	476.2	464.5	423	423	103	4.70	4.62
26.65	460.5	454.2	423	423	100	3.40	3.43
56.15	420.37	427.79	423	423	97	3.60	3.56

Table 3.4: CA05 comparison for different temperature conditions

Figure 3.13 shows the evolution of CA05 as a function of the chosen alpha for the case of combustion with 20.88% oxygen for temperature conditions $T_{in}, T_{body} = 476, 423$ K. We can observe how making the wrong alpha choice could cause an ignition timing mistake. For example, choosing $\alpha = 90$ would lead to an ignition timing CA05 = 2.11 instead of CA05 = 4.62. Above a value of 108, heat losses are too high and the model leads to ignition failure for these operating conditions. As the aim of this thesis is to investigate the potential of oxygen enrichment to increase power density, different oxygen levels, fuelMEP levels and temperature conditions will be tested. This suggests that the alpha factor should be recalibrated in order to account for the conditions tested through the experimental data in order to prevent the inaccuracy mentioned above. This recalibration is explained in more detail in subsubsection 4.4.1.

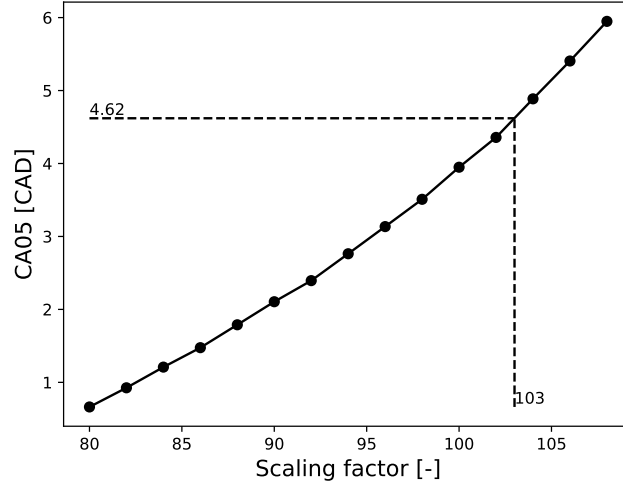


Figure 3.13: Evolution of CA05 as a function of α for $(T_{in}, T_{body})=(476,423)$ [K]

To illustrate the calibration process, we have chosen to display the results for the first row of Table 3.4 (with an O₂ percentage of 20.88%) in Figure 3.14. In this figure, we can observe that the calibration of α at 103 has been done effectively to match the combustion timing. This successful calibration is evident by the close values of the experimental and simulated CA5, which stand at 4.70 and 4.62 respectively, indicating a high degree of proximity.

As previously stated, to accomplish this, α was deliberately underrepresented to more effectively model the core temperature, which is hotter than the temperature near the wall.

Due to the fact that the cylinder is considered a closed system from the bottom dead center. This inherent assumption coupled with an underestimated α in our model consequently leads to a slight overpressure in the cylinder. The solution for having a correct evaluation of the in-cylinder pressure is explained in subsubsection 3.5.3. This calibration is the approach adopted for this thesis because of the aim to predict the MPRR based on an accurate CA5 rather than relying on the pressure curve which, in a 0D model, has a derivative that does not accurately reflect the true PRR.

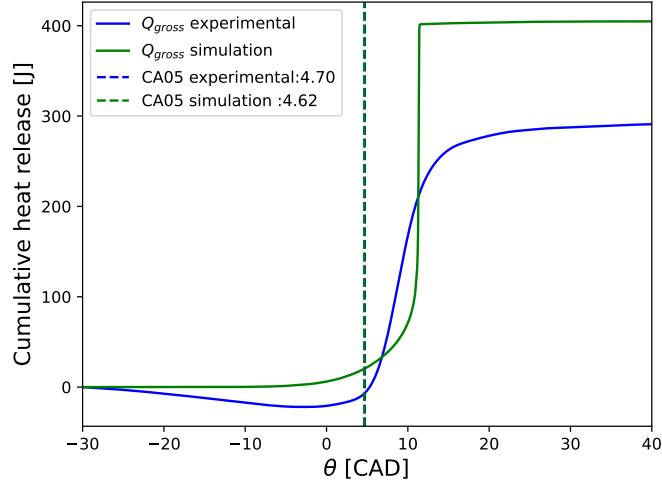


Figure 3.14: Experimental and simulated CA05 and Q_{gross} for combustion timing fitting

3.5.3 Pressure Calibration

As previously mentioned, here is a brief section on pressure calibration. This is aimed at providing a thorough understanding of two key aspects: firstly, the impact of α on our cumulative heat release, and secondly, the effect of heat loss phenomenon in a cylinder for a 0D model.

For this calibration to take place, several aspects need to be managed.

The first one is that in this particular case, the consideration of a closed system has to be only from the effective IVC (-152 [CAD]) of our engine [22] and no more from BDC (-180 [CAD]). To recall, $V_{IVC} = \tau_{eff} \cdot V_{TDC}$ denotes the effective IVC. Another important point is the fact that in this situation, no correlation could be utilized for T_{IVC} .

The second aspect that must be controlled for the calibration to be as accurate as possible is indeed the α factor, which needs to be increased in order to better represent the losses. This improved depiction of losses is crucial since it has a non negligible effect on the pressure evolution.

So to close the loop, since the α has to be increased to model the pressure evolution in the cylinder accurately, we are now dealing with a situation where there's more heat loss. This consequently underestimates the center core temperature and thus delays combustion. This, combined with the fact that the effective IVC is used as the starting point for the closed system, differentiates the combustion timing from reality. Hence, it is infeasible for our model to accurately represent both the combustion timing and the evolution of pressure concurrently.

4 Results and Discussions

This chapter presents a detailed analysis of the obtained results. Firstly, we explain the calibration choices made based on the provided experimental data. Then, an investigation of the correlation between MPRR, start of combustion, and fuelMEP is conducted using a statistical tool, since it is essential to enable the simulation to analyze the influence of operating conditions while guaranteeing engine safety by avoiding ringing. The initial findings include an analysis of the load's influence on the combustion delay and an approximate evaluation of the engine's performance for methane-air combustion.

The main focus of this study lies in the impact of oxygen addition, which is extensively covered in the following chapter. After establishing a correlation for alpha that allows for a combustion timing fitting of the model depending on the intake parameters, we follow a well-defined methodology to observe the influence of oxygen on the achievable operating conditions of the engine such as intake power density. Performance parameters are then widely estimated to get a quantitative idea of their evolution with the addition of oxygen. Additionally, an analysis of the uncertainty associated with input parameters provided to the model is carried out, allowing us to assess the robustness of the obtained results.

Finally, this chapter concludes with a brief comparison of the energy efficiencies with the technologies presented in the state of the art.

4.1 Data Choices Justification

This section has been added to help readers understand the choices made during the rest of the work, particularly the decision to not use the newly post-processed experimental curves and the impact it has on the subsequent results. Firstly, it is important to distinguish between the first set of experimental data we worked with and the second set received shortly before submitting the work. Regardless of the dataset used, the pressure curves, being directly measured and not calculated, reflect the experimental reality. However, the post-processing calculations used to obtain cumulative heat release curves, wall losses, etc., can contain errors that result in post-processed curves that no longer reflect the experimental reality. In the case of the first set of experimental data, the provided post-processed curves were calculated with an effective compression ratio ($\tau_{eff} = 19.64$) different from that of the engine (18.47). Having access only to this incorrect compression ratio and the resulting Q_{gross} curves, the model also uses 19.64 as the effective compression ratio and has been calibrated based on combustion fitting with the experimental Q_{gross} curves also calculated with 19.64.

To obtain reliable pressure curves, it is necessary to rely on pressure fitting as explained in Section 3.5.3 using a different alpha value. However, this approach loses its meaning because performing pressure fitting between a model with $\tau_{eff} = 19.64$ and experimental pressure curves with $\tau_{eff} = 18.47$ does not yield consistent alpha values. Therefore, meaningful pressure fitting becomes very challenging.

The use of an effective compression ratio of 18.47 would have allowed for meaningful pressure fitting, but the limited quantity and diversity of data provided for this compression ratio would have hindered the achievement of accurate combustion timing fitting.

Therefore, the decision was made to retain the first dataset and base all our results on combustion timing

fitting since the primary goal of this work is to accurately predict CA05. Due to the difference in effective compression ratios between the simulated and experimental pressure curves, these variables are never directly compared in this work.

4.2 MPRR/CA05-FuelMEP Correlation

This particular segment plays a crucial role in analyzing the effects of FuelMEP modifications. It is essential because it helps us determine the point at which MPRR exceeds a certain threshold during the enhancement of FuelMEP in our engine cylinder.

To refresh our memories, this MPRR value (Maximum Pressure Rise Rate) is a fairly significant factor to ascertain the thresholds of an engine that should not be breached.

This portion is crucial to our numerical analysis because, given that we are working with a 0D model, our MPRR is unfeasible to model due to the virtually instantaneous combustion of such a model. We therefore had to innovate a solution so that we can still estimate our MPRR based on certain parameters.

The first significant parameter is the combustion timing. This influences the combustion as the volume and speed of the piston at the moment of combustion will significantly impact the pressure increase. It can be fairly easily predicted that the closer the combustion occurs to the top dead center, the smaller the volume and slower the piston descent, thus resulting in a greater pressure increase.

And finally, our second significant parameter for modeling the MPRR is the FuelMEP. It is significant as it represents the mean effective pressure of the fuel in the engine, which is a direct indicator of combustion efficiency, and thus of overall engine performance. Indeed, the higher the FuelMEP, the more efficiently the fuel is used, which means not only better engine performance, but also a higher MPRR value.

Our methodology for predicting MPRR is based on the experimental data available to us. After collecting numerous CA5 data calculated from experimental rate of heat release, as well as corresponding FuelMEP and MPRR values, we utilized statsmodels [41], who is a powerful Python library for statistical modeling and analysis, to perform multiple linear regression and analyze the relationship between the dependent variable (MPRR) and the two independent variables (CA5 and FuelMep).

The regression model is adjusted using the Ordinary Least Squares (OLS) method from the statsmodels library, a statistical technique that aims to minimize the sum of the squared residuals, which are the differences between the observed and predicted values provided by the model. The core principle behind this method is to optimize the model's predictions by reducing the discrepancy between these observed and estimated values.

The OLS method, through its mechanism of minimizing these residuals, establishes an optimal line of best fit for the data. This line is considered the best because it is the line where the sum of the squared vertical distances of each data point from the line is the smallest. These distances, also known as residuals or errors, are crucial in understanding how well our model has performed.

The outcome of this process is a set of coefficients for the independent variables, the calculated values that best fit the model. Each of these coefficients represents the change in the dependent variable for each one-unit change in the corresponding independent variable, assuming all other variables are held constant. This set of coefficients thus formulates a mathematical representation of the relationships within the data,

creating a blueprint that can be used to predict the dependent variable based on a given set of independent variables.

In Figure 4.1, we can perceive the dependence of the experimental MPRRmean on its corresponding parameters, CA05mean (displayed on the left) and FuelMEP (displayed on the right). It's imperative to highlight that for each subplot, all other independent variables, apart from the one under analysis, are assumed to be constant. However, this use of the term "constant" does not imply that the value of the variable remains unchanged across all observations. Rather, it suggests that we are controlling or adjusting for the effects of that variable, allowing the graph to portray the impact of the independent variable under scrutiny on the dependent variable, regardless of the influence of the other independent variables.

Another noteworthy aspect is that this analysis is solely based on the experimental data received. We utilize the term 'MEAN' as the data that we provide to our statistical tool are averages derived from 100 experimental cycles conducted under specific conditions. Consequently, the results of this statistical analysis should be understood within the context of these averaged measurements, recognizing the inherent variability that may arise from the experimental process.

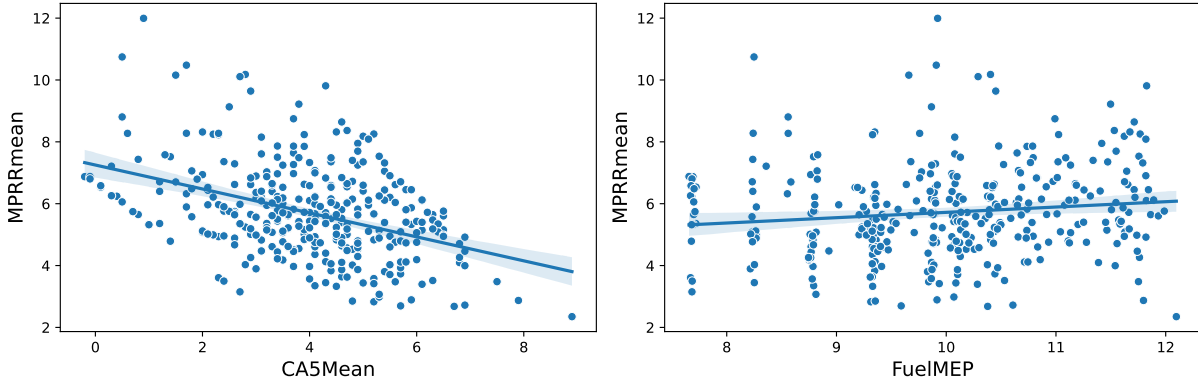


Figure 4.1: MPRR correlation with CA5MEAN (Left), FuelMEP (Right) assuming the other independent variable constant

So based on the Ordinary Least Squares (OLS) regression analysis performed on only our experimental dataset, we've determined a reliable mathematical relationship linking our dependent variable, MPRRmean, to the independent variables, namely CA5Mean and FuelMEP. This relationship can be neatly summarized by the following regression equation 4.1:

$$\text{MPRR} = (-1.571 \cdot \text{CA05}) + (2.025 \cdot \text{FuelMEP}) - 8.275 \quad (4.1)$$

The coefficients in the regression equation imply that for each unit increase in CA5Mean, there is an associated decrease of 1.571 units in the MPRRmean, keeping the other variables constant. Similarly, for each unit increase in FuelMEP, we observe an increase of 2.025 units in the MPRRmean, while holding other variables constant. The constant term of -8.275 represents the baseline value of MPRRmean when

both CA5Mean and FuelMEP are zero. Even if this constant value seems to be nonphysical and non-probable, it is necessary for the mathematical calculation of linear regression because it gives the model additional flexibility to adapt to the data, by shifting the regression line up or down.

All variables in the model are statistically significant, as indicated by their p-values, which are well below the commonly used threshold of 0.05. The model's F-statistic is 1036, and the associated p-value is near zero, which suggests that the model as a whole is statistically significant.

However, as with all statistical models, it is essential to keep in mind that these results are subject to certain assumptions about the data, such as linearity, homoscedasticity, and independence of errors. It is thus recommended to use caution when generalizing these results to different contexts.

4.3 Methane-Air Combustion

This section aims to analyze the influence of engine load on the ignition timing and power output for methane combustion with air consisting of 21% oxygen and 79% nitrogen. The perfectly calibrated scaling factor α for this percentage of O_2 is 103. Since the intake temperature and equivalence ratio for a stationary engine application determine the input charge, these two variables will be the focus of our investigation.

4.3.1 Ignition Timing

Let's start with the impact of intake temperature. The quantity of fuel, and therefore the equivalence ratio, is kept constant by choosing a FuelMEP equivalent to 9.31 bar ($\phi = 0.43$ for $T_{in} = 486$ K) as model input. The tested temperature range is limited by minimum ignition temperature (471 K). As expected, the increase in intake temperature leads to an increase in in-cylinder temperature during compression, allowing for a faster ignition. Figure 4.2 clearly shows that the start of combustion is advanced with the increase in intake temperature.

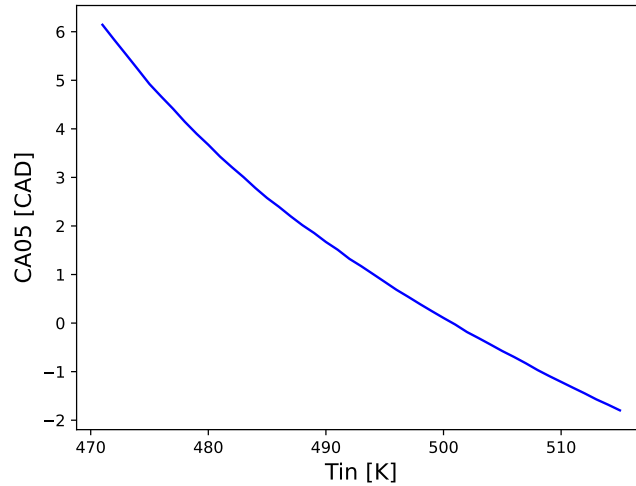


Figure 4.2: Influence of intake temperature T_{in} [K] on combustion timing CA05 for FuelMEP = 9.31 [bar]

The influence of temperature cannot be totally dissociated from that of the equivalence ratio, since a change in temperature at the model input modifies the initial number of moles present in the model. Figure 4.3 and Figure 4.4 depict this impact. Since the quantity of fuel is kept constant, this decrease in the initial number of moles of the mixture due to the increase in inlet temperature results in a reduction in the number of moles of air in the mixture. As a result, there is an increase in the equivalence ratio and the molar fraction of fuel. Recalling the ideal gas law (Equation 4.2) and Equation 4.3 illustrated in subsection 2.2 is useful to examine this phenomenon. For a constant oxygen ratio χ and a fixed quantity of fuel moles n_{fuel} , the increase in temperature at bottom dead center (caused by the rise in intake temperature according to Equation 3.24) results in a richer air-fuel mixture.

$$pV_{\text{BDC}} = n_{\text{tot}}RT_{\text{BDC}} \quad (4.2)$$

$$\phi = \frac{2n_f}{n_{O_2}} = \frac{2n_f}{\chi \cdot (n_{\text{tot}} - n_f)} \quad (4.3)$$

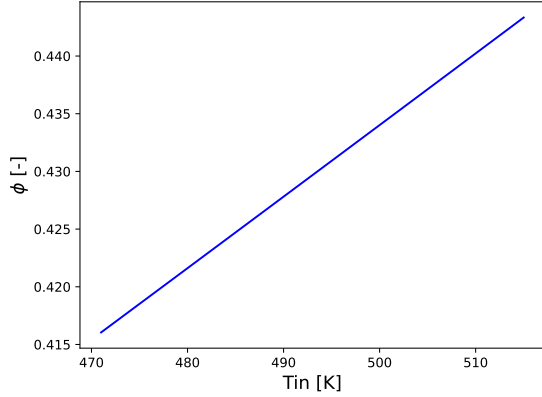


Figure 4.3: Equivalence ratio evolution in function of T_{in} with a constant FuelMEP

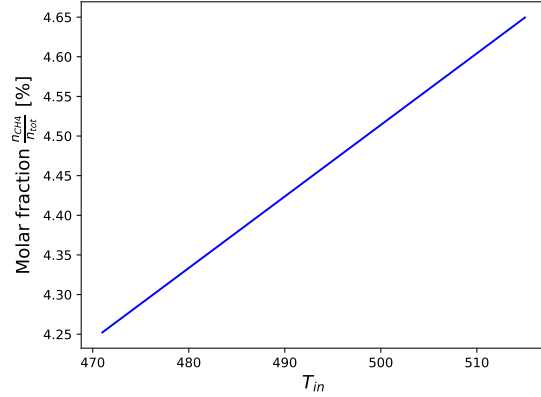


Figure 4.4: CH4 molar fraction evolution in function in function of T_{in}

It is a little less obvious how the equivalence ratio affects the beginning of combustion in the 0D model for a fixed intake temperature. Indeed, Figure 4.5 and 4.6 demonstrate that, contrary to our projections, combustion is delayed as quantity of fuel injected increases.

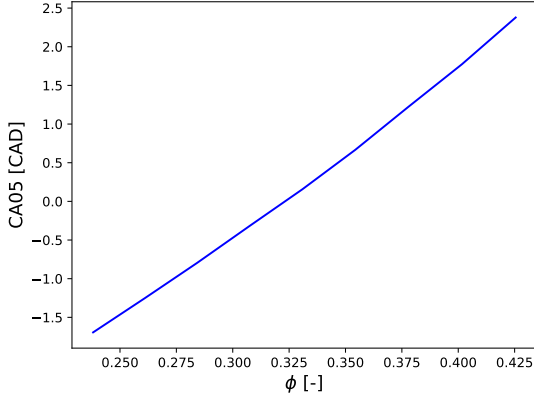


Figure 4.5: Influence of ϕ on combustion timing for $T_{in} = 486.2$ [K]

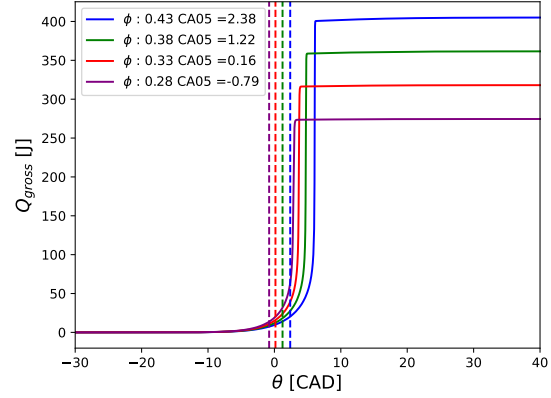


Figure 4.6: Influence of ϕ on heat release for $T_{in} = 486.2$ [K]

To better understand this phenomenon, P. Kongsereparpb dissociated the engine load from thermodynamic properties when analyzing the impact of equivalence ratio on the onset of combustion in his PhD [42].

Increasing the equivalence ratio results in a more intense combustion process, generating a higher thermal load and releasing more heat. The increased heat release leads to elevated wall temperatures within the combustion chamber, which, in turn, affects the temperature of the residual gases. As a result, the in-cylinder temperatures at the beginning of the compression stroke will be hotter, despite an equivalent temperature at bottom dead center (due to a temperature-controlled intake charge), thereby inducing earlier ignition. However, from a thermodynamic perspective, the opposite occurs. The molecules of fuel and combustion products are larger than air molecules. Increasing the quantity of fuel, therefore, increases the overall thermal capacity of the mixture. This implies that more energy is required to raise the temperature of the mixture, resulting in a delayed combustion process. A P. Kongsereparpb said : " If only thermodynamics effects were considered, riching the mixture would tend to retard the SOC timing". Since the OD model simulates only a single cycle, the increase in thermal load due to the rise in wall temperature is not considered, which justifies the increase in CA05 with the equivalence ratio.

4.3.2 Power Output

The main advantage of the 0D model is the reliable and fast estimation of combustion timing based on the heat release derived from the chemical kinetics of the gases involved in the model with a scaling factor calibrated for this purpose. However, as mentioned earlier, this calibration overestimates the pressure because, firstly, the calibrated scaling factor for ignition fitting underestimates the heat losses, resulting in elevated in-cylinder temperatures and pressures, and secondly, the model considers a closed system from

bottom dead center instead of intake valve closing CAD. Therefore, the model does not allow a reliable study of pressure curves and the related parameters, such as mean effective pressure and efficiencies discussed in subsubsection 2.1.3. These pressure curves will be overestimated compared to the experimental curves they should approximate.

Nevertheless, an analysis based on the 0D model, although calibrated for combustion timing, provides an idea of the quantitative evolution of these parameters and the influence of operating conditions on them. Figure 4.8 illustrates the influence of the equivalence ratio for the same inlet temperature. As expected, a higher load induces a more intense pressure peak. It is important to note that the evolution of the peaks with ϕ is underestimated due to the contrary influence of the equivalence ratio on the combustion onset with the model. Indeed, the increase in the equivalence ratio delays the combustion onset when it should advance it, thus producing even more intense pressure peaks.

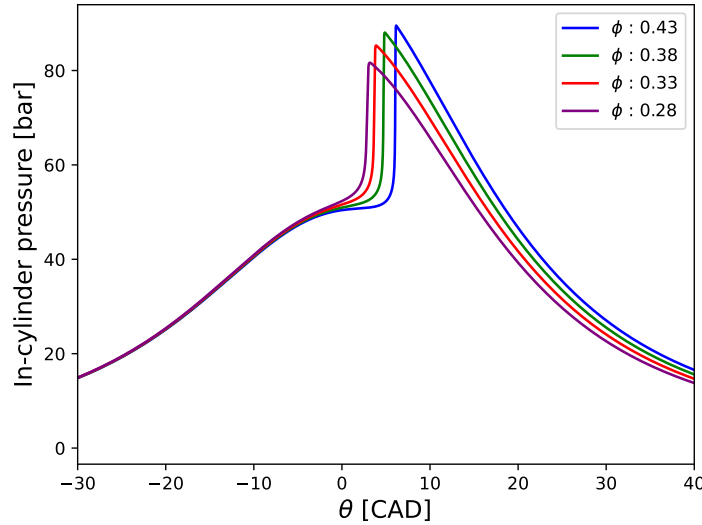


Figure 4.7: Pressure curves comparison at 4 different ϕ for $T_{in} = 486$ K

Given that the maximum pressure is overestimated, the simulated IMEP is also overestimated. Indeed, by imposing exactly the same operating conditions (Intake temperature of 471 K and fuelMEP of 9.31 bar), the simulated $IMEP_{gross}$ (4.0431 [bar]) overestimates the experimental $IMEP_{gross}$ (3.6572 [bar]) by 9.54%. Since the model only considers two engine strokes, pumping losses due to intake and exhaust are not taken into account, and the IMEP calculated based on work (Equation 3.19) corresponds to the gross IMEP. The net IMEP is then obtained by simply subtracting the pumping losses, which are typically low in the case of an HCCI engine, between 0.5 and 2% of the $IMEP_{gross}$ according to experimental data. Assuming pumping losses as 1% of $IMEP_{gross}$, it gives an indicated efficiency of :

$$\eta_{ind,net} = \frac{IMEP_{net}}{FuelMEP} = \frac{IMEP_{gross} - \frac{IMEP_{gross}}{100}}{FuelMEP} = \frac{4}{9.31} = 43\% \quad (4.4)$$

Experimental net indicated efficiency is given to be 38.44 %. The overestimation of simulated IMEP compared to the experimental one lead to an overestimation of the net indicated efficiency for the same fuel content.

Although the simulated $\text{IMEP}_{\text{gross}}$ is not very reliable, it is interesting to observe how it evolves with the quantity of injected fuel. Figure 4.8 clearly shows that to increase the engine power, logically, the amount of fuel injected must be increased. The only limit to increasing the fuel content is the resulting increase in MPRR and maximum pressure.

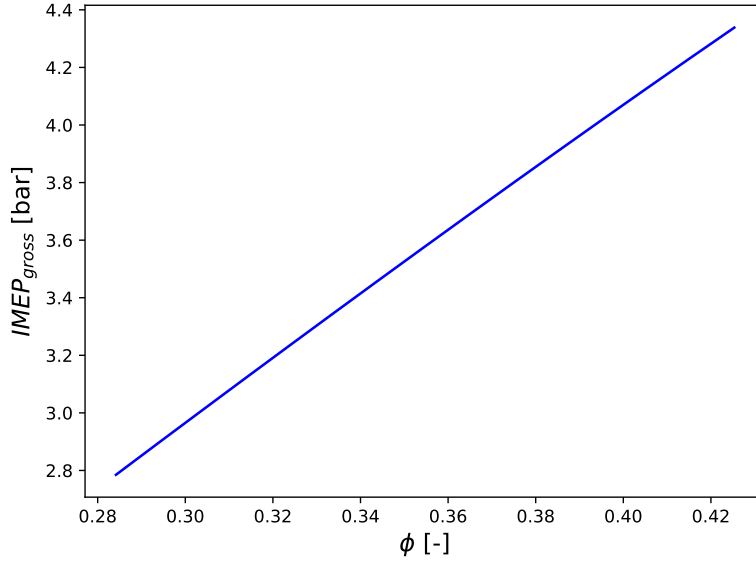


Figure 4.8: Evolution of $\text{IMEP}_{\text{gross}}$ with ϕ for $T_{in} = 486$ K

4.4 Oxygen Enrichment

4.4.1 Alpha and MPRR Limit Choices

As explained in subsection 3.5.2, determining the optimal alpha for accurate combustion timing prediction depends on the input conditions from which it is calibrated. For simulation conditions that are exactly the same as the experimental conditions, manually adjusting this parameter is sufficient to fine-tune the heat losses and obtain a CA05 value very close to the experimental CA05, as demonstrated in Table 3.4. Since the goal of this thesis is to test settings that are not the same as the experimental conditions, a correlation that enables determining alpha based on these initial conditions is required. In addition to the intake temperature, the FuelMEP also influences the determination of alpha.

The "best" α has therefore been calculated for the entire set of experimental data, and a correlation could subsequently be established with FuelMEP and inlet temperature using a method similar to the one used for the MPRR correlation. The relationship obtained is as follows:

$$\alpha = (0.173499 \cdot T_{in}) - (0.000149 \cdot \text{fuelMEP}) + 165.702140 \quad (4.5)$$

With T_{in} in [K] and FuelMEP in [Pa].

In order to avoid any risk of engine damage, the model must ensure that it remains below the safety threshold of the Maximum Pressure Rise Rate (MPRR) as the tested conditions evolve. This threshold is set at 8 [bar/CAD] for the UCLouvain research engine and its specifications presented in Table 3.1. By inverting Equation 4.1 and incorporating this MPRR limit of 8 [bar/CAD], it is possible to determine the start of combustion that must not be exceeded based on the amount of fuel injected into the engine.

$$\text{CA05} = (-0.6365 \cdot \text{MPRR}) + (1.289 \cdot \text{FuelMEP}) - 5.267 \quad (4.6)$$

$$\text{CA05} = 1.289 \cdot \text{FuelMEP} - 10.359 \quad (4.7)$$

This limit on combustion timing will therefore be adjusted as the quantity of fuel injected and therefore the power density increases.

4.4.2 Method

This section explains the cyclic method that was employed to obtain our results in order to analyze the influence of oxygen concentration on the engine power density. Figure 4.9 provides a clear understanding of this methodology. The input parameters of the model that vary throughout the process are the inlet temperature T_{in} , oxygen concentration χ , scaling factor α , and the fuel quantity n_f (derived from FuelMEP) or equivalence ratio ϕ . Providing both of these parameters as inputs to the model is impossible since they are interconnected by Equation 4.3. The chosen starting conditions correspond to the methane-air mixture studied in subsection 4.3 with the corresponding temperature and composition conditions. As this mixture was tested experimentally, the calibrated value of α for these conditions is obtained from Table 3.4 instead of Equation 4.5. Since the fuelMEP is known, the combustion start limit that should not be exceeded, denoted as CA05_{lim} , is also known.

The first step involves increasing the oxygen concentration while ensuring that the ignition timing does not exceed the previously set limit. This is done by keeping the fuel quantity constant. The second step is to decrease the inlet temperature of the mixture until reaching the necessary ignition temperature limit, $T_{in,min}$. The equivalence ratio is kept constant through a proportional increase in the number of moles of fuel and oxidants (including oxygen) induced by the temperature decrease. These two steps lead us to a new state of conditions characterized by a lower inlet temperature and a higher fuel quantity. Consequently, these new conditions require recalibration of the α parameter based on Equation 4.5 to adapt the simulation of heat losses for predicting the CA05 for the new range of tested conditions that will follow. The increase in FuelMEP also necessitates adjusting the combustion timing limit to be respected,

considering its influence on the MPRR: a higher FuelMEP results in a higher MPRR, necessitating a delay in combustion to stay below the fixed threshold of 8 bar/CAD. This limit on combustion timing will therefore be adjusted as the quantity of fuel injected and therefore the power density increases.

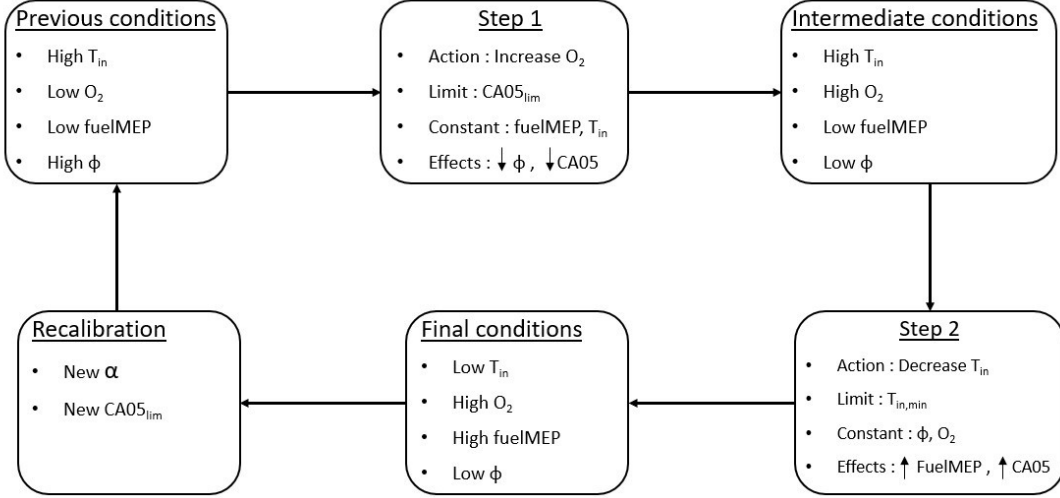


Figure 4.9: Cyclic method of test condition evolution

Due to the repetitive nature of this method, only the first two sets of conditions were commented upon, while the subsequent results were simply displayed and summarized in tables.

4.4.3 Results

Table 4.1 below summarizes all the operating conditions that were investigated using the 0D model according to the method described above. For each range of oxygen percentage investigated, the associated inlet temperature corresponds to the minimum temperature required for mixture ignition for the lowest oxidant in the range, while the upper limit (26,33,40,49,67,100) was chosen to stay below the maximum MPRR limit. For each range of inlet temperature investigated, the associated oxygen ratio corresponds to the maximum ratio before reaching the MPRR limit for the highest temperature, while the lower limit (456, 442, 428, 415, 403, 397) was chosen to ensure ignition.

O_2 [%]	ϕ	T_{intake} [K]	FuelMEP [Bar]
21 - 26 %	0.414 - 0.334	471	9.31
26 %	0.334	471 - 456	9.31 - 9.51
26 - 33 %	0.334 - 0.263	456	9.51
33 %	0.263	456 - 442	9.51 - 9.71
33 - 40 %	0.263 - 0.217	442	9.71
40 %	0.217	442 - 428	9.71 - 9.92
40 - 49 %	0.217 - 0.177	428	9.92
49 %	0.177	428 - 415	9.92 - 10.12
49 - 67 %	0.177 - 0.130	415	10.12
67 %	0.130	415 - 403	10.12 - 10.31
67 - 100 %	0.130 - 0.087	403	10.31
100 %	0.087	403 - 397	10.31 - 10.41

Table 4.1: Set of operating conditions investigated

[21% - 26%]

As explained above, the first set of conditions corresponds to the previously studied combustion of methane with air, specifically oxygen at 21% and a FuelMEP of 9.31 bar. Since these data have been experimentally tested, they can be directly inputted into our model, and the start of combustion CA05 can be aligned "manually" by calibrating the alpha parameter. On the other hand, correlation 4.5 will be used for the subsequent oxygen ranges.

According to Equation 4.7, the limit for the ignition timing is $CA05_{lim} = 1.64$ [CAD]. The minimum temperature required for ignition is $T_{i,min} = 471$ K for an oxygen concentration of 21%. It is necessary to increase this oxygen concentration until reaching the aforementioned $CA05_{lim}$ without exceeding it. As shown in Figure 4.10, increasing the oxygen concentration, and thus replacing nitrogen molecules with oxygen molecules, leads to faster combustion. It can also be observed that an oxygen concentration exceeding 26% results in exceeding the CA05 limit and therefore the MPRR limit.

The second step is illustrated in Figure 4.11 and involves decreasing the inlet temperature while keeping the equivalence ratio constant. The objective is to increase the power density, so instead of maintaining a constant fuel injection quantity, it is possible to increase it by reducing the inlet temperature until just before ignition failure occurs. Reading Figure 4.11 from right to left, we can observe the delayed ignition timing and the increase in FuelMEP. The minimum temperature required for ignition is 4 $T_{i,min} = 456$ K, and the corresponding FuelMEP is 9.51 [bar]. Going from 9.31 to 9.51, the increase in oxygen already results in a 3.22% improvement in input power density.

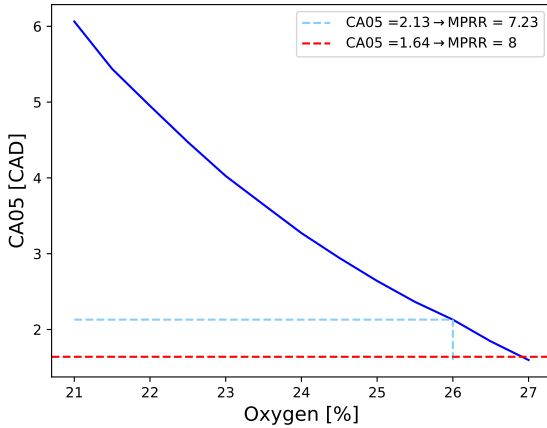


Figure 4.10: CA05 evolution in function of an increase of the O_2 percentage

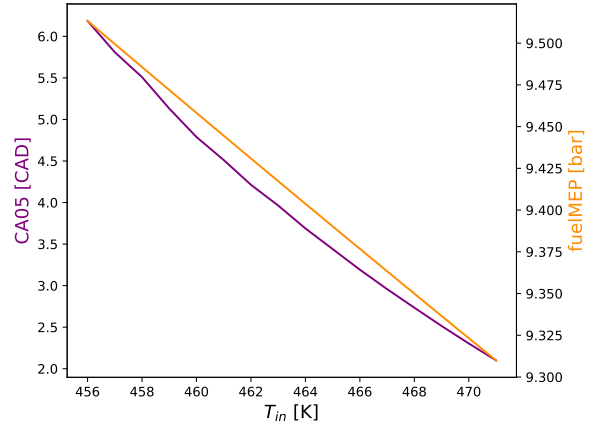


Figure 4.11: CA05 and FuelMEP evolution in function of a decreasing T_{in}

The values for this first oxygen range are summarized in the Table 4.2:

alpha	CA05 _{lim} [CAD]	O ₂ [%]	T _{in} [K]	FuelMEP [bar]	ϕ [-]	Input power density improvement [%]
103	1.64	21%	471	9.31	0.414	-
103	1.64	26%	456	9.51	0.334	3.22

Table 4.2: Summary of values for oxygen range [21-26]%

[26% - 33%]

Now that the temperature has been lowered to its minimum value, we can once again increase the oxygen levels. Due to the dependence of MPRR on fuelMEP and the increase in fuelMEP up to 9.51 bar, the CA05 limit to prevent an MPRR of 8 bar/CAD is slightly delayed and is now CA05_{lim} = 1.90 CAD. Given that these are new conditions, the scaling factor needs to be recalibrated. For a fuelMEP of 9.51 bar and a temperature of 456 K, equation (refalphaCOrrrelation) allows calibrating the scaling factor to a value of 103.

The oxygen concentration can now be increased for a constant temperature of 456 K and a constant fuelMEP of 9.51, up to the limit CA05_{lim} = 1.90 [CAD], while ensuring not to exceed it. Figure ?? illustrates that the maximum percentage to stay below this limit is 33%. In the next step, we examine the fuelMEP that can be achieved by decreasing the temperature until ignition failure. This failure occurs just below T_{in,min} = 442 K. The corresponding fuelMEP value is 9.71 bar. This reasoning is summarized again in Table 4.3, as well as in Figures 4.12 and 4.13.

alpha	CA05 _{lim} [CAD]	O ₂ [%]	T _{in} [K]	FuelMEP [bar]	ϕ [-]	Density improvement [%]
103	1.90	26%	456	9.51	0.334	-
103	1.90	33%	442	9.71	0.263	4.21

Table 4.3: Summary of values for oxygen range [26-33]%

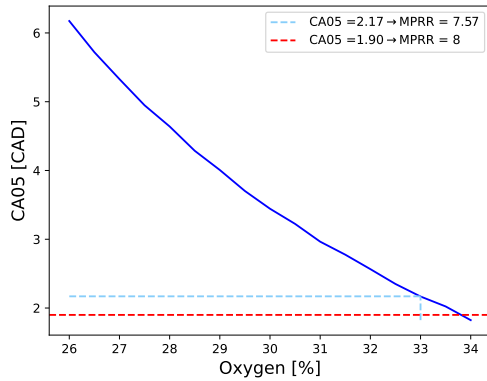


Figure 4.12: CA05 evolution in function of an increase of the O₂ percentage

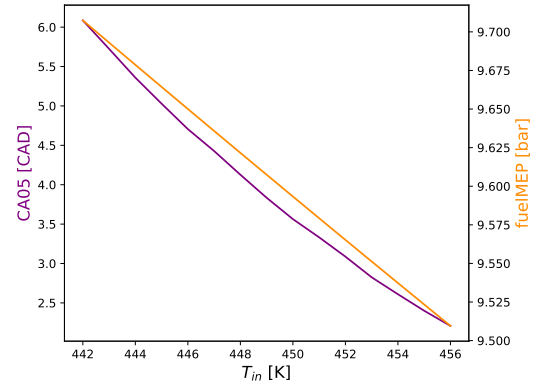
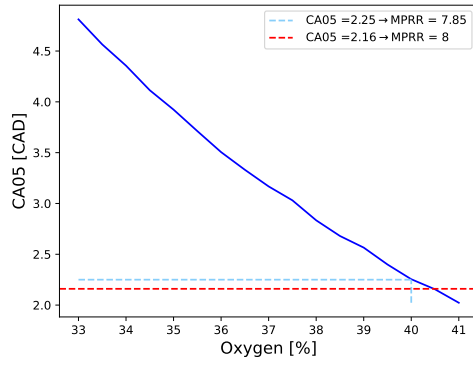
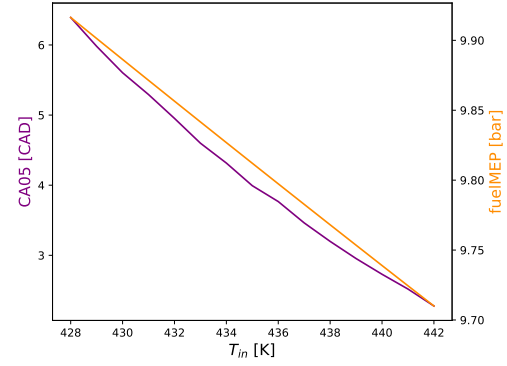


Figure 4.13: CA05 and FuelMEP evolution in function of a decreasing T_{in}

[33% - 40%]

alpha	CA05 _{lim} [CAD]	O ₂ [%]	T _{in} [K]	FuelMEP [bar]	ϕ [-]	Density improvement [%]
98	2.16	33%	442	9.71	0.263	-
98	2.16	40%	428	9.92	0.217	6.55

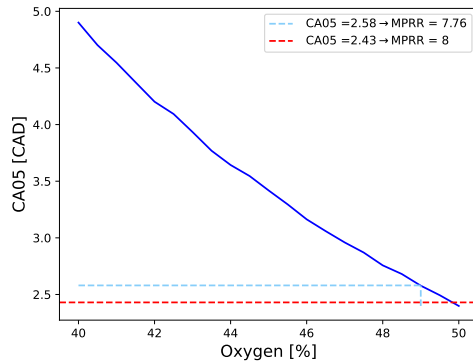
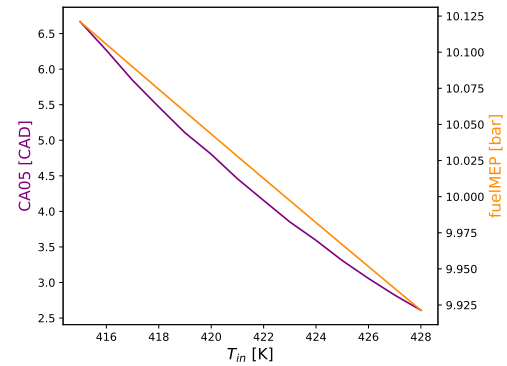
Table 4.4: Summary of values for oxygen range [33-40]%

Figure 4.14: CA05 evolution in function of an increase of the O₂ percentageFigure 4.15: CA05 and FuelMEP evolution in function of a decreasing T_{in}

[40% - 49%]

alpha	CA05 _{lim} [CAD]	O ₂ [%]	T _{in} [K]	FuelMEP [bar]	ϕ [-]	Density improvement [%]
92	2.43	40%	428	9.92	0.217	-
92	2.43	49%	415	10.12	0.177	8.70

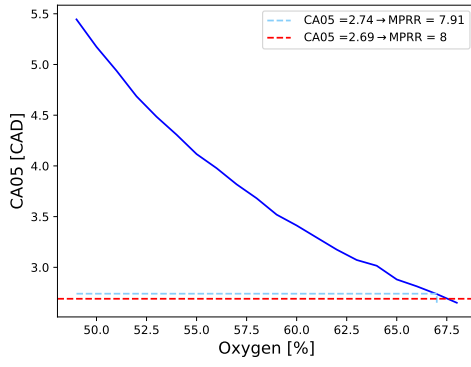
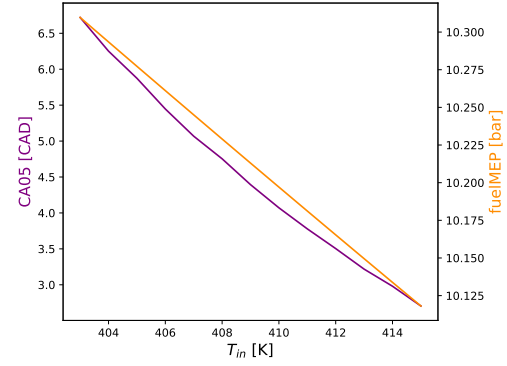
Table 4.5: Summary of values for oxygen range [40-49]%

Figure 4.16: CA05 evolution in function of an increase of the O₂ percentageFigure 4.17: CA05 and FuelMEP evolution in function of a decreasing T_{in}

[49% - 67%]

alpha	CA05 _{lim} [CAD]	O ₂ [%]	T _{in} [K]	FuelMEP [bar]	ϕ [-]	Density improvement [%]
87	2.69	49%	415	10.12	0.177	-
87	2.69	67%	403	10.31	0.130	10.74

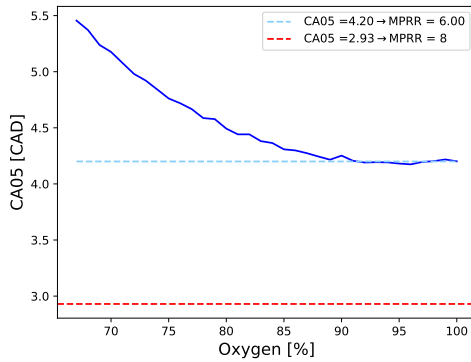
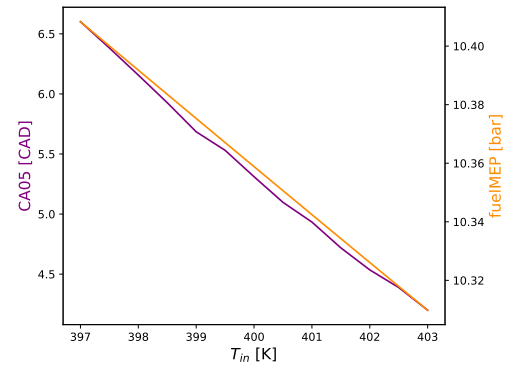
Table 4.6: Summary of values for oxygen range [49-67]%

Figure 4.18: CA05 evolution in function of an increase of the O₂ percentageFigure 4.19: CA05 and FuelMEP evolution in function of a decreasing T_{in}

[67% - 100%]

alpha	CA05 _{lim} [CAD]	O ₂ [%]	T _{in} [K]	FuelMEP [bar]	ϕ [-]	Density improvement [%]
82	2.93	67%	403	10.31	0.130	-
82	2.93	100%	397	10.41	0.087	11.82

Table 4.7: Summary of values for oxygen range [67-100]%

Figure 4.20: CA05 evolution in function of an increase of the O₂ percentageFigure 4.21: CA05 and FuelMEP evolution in function of a decreasing T_{in}

4.4.4 Discussion

The findings from Table 4.4.3 provide clear evidence that the presence of oxygen has a significant impact on reducing the ignition delay. This effect is further illustrated in Figure 4.22, which clearly demonstrates the trend of oxygen enrichment improving combustion because of the mixture becoming more reactive. As a result, a lower intake temperature is required to achieve ignition of the mixture. Specifically, increasing the oxygen concentration in the oxidizer up to 100% reduces the minimum temperature required for ignition by 74 K.

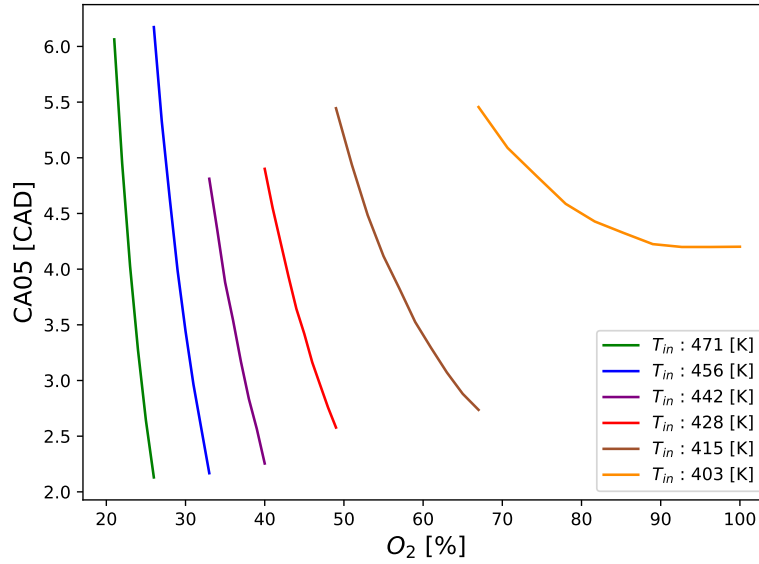


Figure 4.22: Influence of oxygen percentage on ignition timing

Figure 4.23 illustrates the influence of oxygen concentration on the Maximum Pressure Rise Rate (MPRR), taking into account the variation in the injected fuel quantity resulting from the temperature decrease. Firstly, the figure clearly shows that all tested conditions remain below the previously set threshold of 8 bar/CAD, indicating that they are within acceptable limits. The figure also indicates that the range of oxygen percentages for which the intake temperature does not lead to ignition failure or knocking phenomenon is larger for high oxygen concentrations. Accordingly, at increasing oxygen concentrations, the combustion timing is less sensitive to oxygen enrichment, to the extent that between after 88%, oxygen enrichment no longer affects the start of combustion. On the other hand, for lower oxygen concentrations, the combustion is significantly advanced even with a slight variation in oxygen content, resulting in a substantial increase in MPRR. This highlights that lower oxygen concentrations have a stronger influence on combustion violence, leading to higher MPRR values.

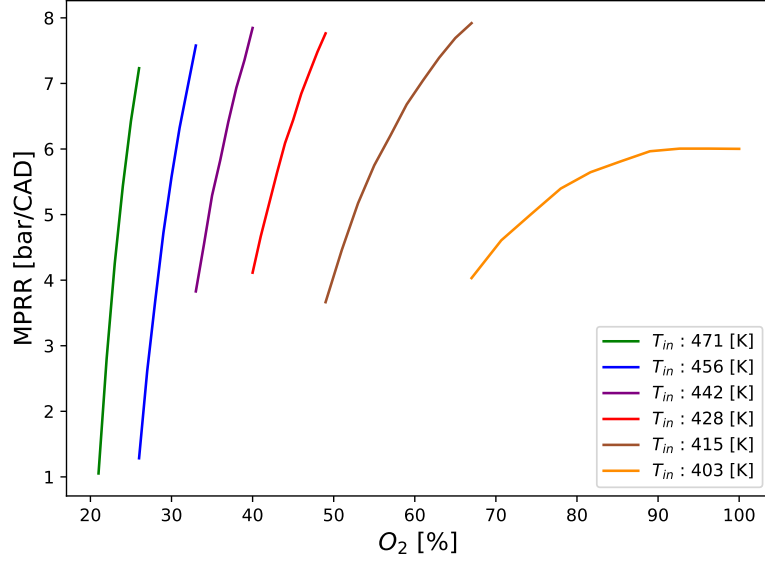


Figure 4.23: Influence of oxygen percentage on MPRR

The influence of oxygen on the fuel quantity and, consequently, on the achievable power density at the engine inlet is presented in Figure 4.24. The maximum temperature decrease of 74 K results in a maximum increase of 11.82% in the input power density for combustion performed with oxygen as the sole oxidant, compared to methane-air combustion. This increase is achieved while preventing any material damage caused by excessively high MPRR. Figure 4.25 provides a clearer understanding of the safe input conditions that can be provided to the engine. The maximum limit of the attainable power density at the inlet is determined by the minimum temperature required for mixture ignition, which is 397 K. Any temperature below 397 K, regardless of the oxygen concentration in the oxidant, will result in ignition failure.

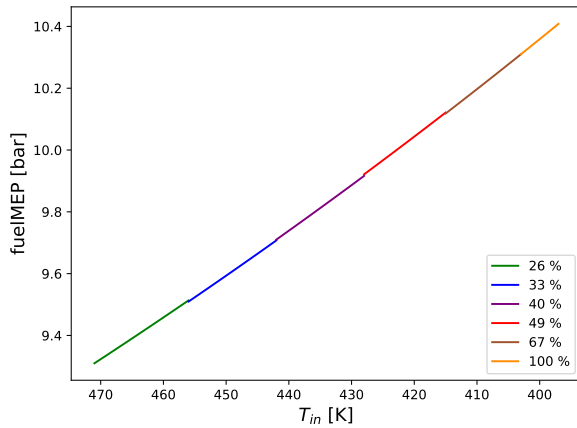


Figure 4.24

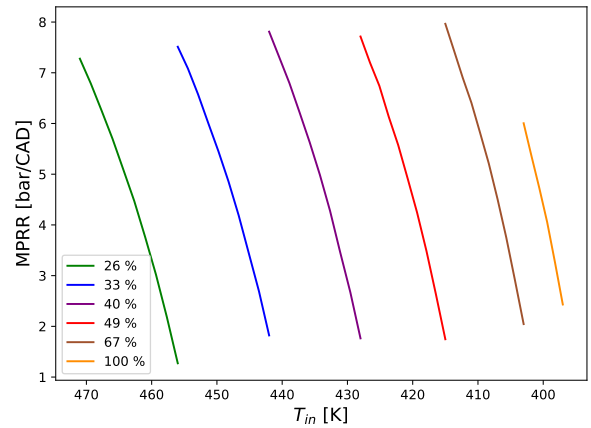


Figure 4.25

4.4.5 Power output

Similar to the case of methane-air combustion, this section aims to provide a quantitative understanding of MEP values, efficiencies, and the influence of oxygen on the evolution of these parameters.

Indeed, fitting the parameter α based on the ignition timing leads to an overestimation of all the parameters calculated from pressure curves and their derived values. The complete set of operating conditions and corresponding outputs are summarized in Table 4.8.

O_2 [%]	T_{in} [K]	FuelMEP [Bar]	IMEP _{gross} [Bar]	Gross indicated efficiency [%]
33	456	9.51	4.48	47.13
33	442	9.71	4.59	47.31
40	442	9.71	4.65	47.88
40	428	9.92	4.77	48.11
49	428	9.92	4.83	48.68
49	415	10.12	4.90	48.40
67	415	10.12	4.98	49.22
67	403	10.31	5.04	48.9
100	403	10.31	5.07	49.21

Table 4.8: Evolution of IMEP and efficiency for different operating conditions

Despite the low reliability of the obtained values, the trend of gross MEP increasing with oxygen concentration is clearly visible in Figure 4.26. This is because, at a constant fuel quantity, an increase in oxygen concentration shifts the combustion towards the left, resulting in higher power output. This effect is more pronounced for lower oxygen levels due to the high sensitivity of combustion timing at these concentrations. For higher concentrations, adding a large amount of oxygen (from 67 to 100%) only induces a slight increase in power density (from 5.04 to 5.07 bar). Additionally, at a fixed oxygen quantity, the decrease in temperature naturally leads to an increase in fuel MEP, resulting in higher power output.

The true advantage of increasing power density through oxygen lies in the improvement of mechanical efficiency due to the reduced relative importance of friction losses, leading to higher BMEP and, consequently, higher brake efficiency.

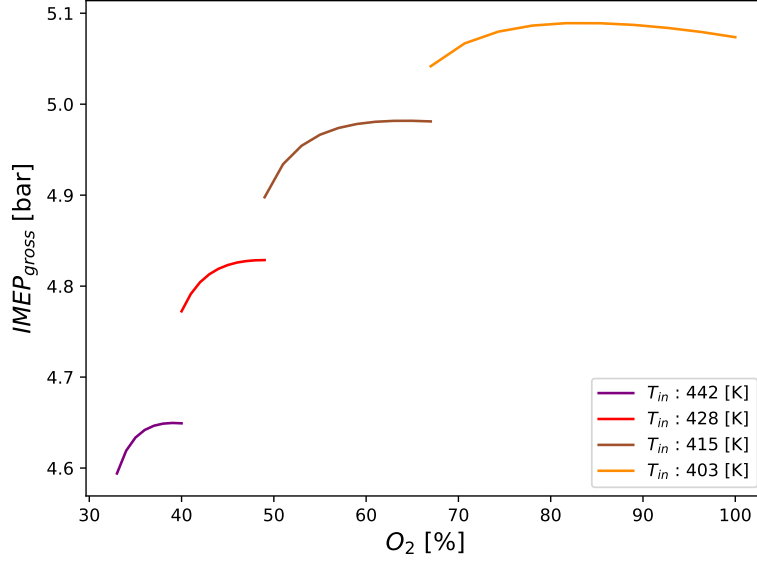


Figure 4.26: Evolution of $IMEP_{gross}$ with the oxygen percentage for different intake temperatures

4.5 Uncertainty Analysis

Completing our model's section and the presentation of its outcomes necessitates a critical step: performing an uncertainty analysis. This analysis shows the effect of not accurately knowing the input parameters on the output of the model.

The ultimate objective of this process is to provide range of possible outcomes of the actual installation in reality, and the probability of those outcomes. And this without resorting to the widely used approach of only considering mean values as valid if they have been tested multiple times under identical conditions. The pursuit of this analysis aids us in understanding and assessing the reliability and validity of our model, ensuring that we maintain transparency in our approach and thoroughness in our conclusions.

4.5.1 Uncertainty of the Inlet Conditions of the Model

In this section, the impact of uncertainty from various input parameters of our model on a specific output is assessed. For this purpose, the Rheia library [43], in conjunction with a Python interpreter is used.

This library calculates the mean, standard deviation of the target variable, and the Sobol' indices of the parameters by constructing a Polynomial Chaos Expansion (PCE). The PCE, with its representative equation shown below 4.8, is a replacement of the Monte Carlo Simulation, which needs roughly 10^4 training samples to get statistical moments and Sobol indices on the output, while now only a handful of points is enough. It is thus way faster than his predecessor. It Involves expressing the model as a series of orthogonal polynomials Ψ_i along with their corresponding coefficients u_i . The type of polynomials used depends on the type of distribution analyzed.

In our case, we assume a Gaussian (normal) distribution, which therefore necessitates the use of a type of polynomial known as Hermite polynomials (Legendre polynomials for an uniform distributions).

$$\mathcal{M}^{\text{PCE}}(\mathbf{X}) = \sum_{\alpha \in \mathcal{A}} u_{\alpha} \Psi_{\alpha}(\mathbf{X}) \approx \mathcal{M}(\mathbf{X}) \quad (4.8)$$

In this equation, α are the multi-indices, and $\mathcal{A}$ is the designated set of multi-indices. The size of this set is determined by a truncation scheme.

To quantify these $|\mathcal{A}^{M,p}|$ coefficients, with p representing the polynomial order and M the stochastic dimension, least-square minimization is applied based on actual system model evaluations.

As explained earlier, this model does more than just compute the mean and standard deviation. It also returns the contribution of each stochastic parameter to the variance of our output. This is the contribution that our Sobol index, the equation for which is provided below (see equation 4.9), quantifies.

Thus, the total-order Sobol indices quantify the overall impact of a stochastic parameter in the input, taking into account mutual interactions as well.

$$S_i^{T,\text{PC}} = \sum_{\alpha \in A_i^T} u_{\alpha}^2 / \sum_{i=1}^P u_i^2 \quad A_i^T = \{\alpha \in A | \alpha_i > 0\} \quad (4.9)$$

The next step is therefore to quantify the uncertainties of the crucial parameters in the model. For the UCLouvain test bench, the uncertainties related to engine inputs of interest, such as the intake temperature and the bottom dead center temperature, the FuelMEP, the O_2 percentages and the rotational speed of the crankshaft are determined using the comprehensive methodology developed in the Ph.D. thesis of M. Pochet [23]. This methodology takes into account the influence of sensors, post-processing techniques, and engine setup.

It is also important to consider the uncertainties in the prediction of first the α value and the T_{wall} . The alpha value uncertainty is calculated by the Statsmodel package in Python. In our model, the T_{Wall} is assumed to be constant and is set equal to the mean of the experimental values. Consequently, we also had to determine its standard deviation.

In Table 4.9, all these uncertainties are gathered. Those are the values that will be incorporated into our Rheia tool. We also take into account that $u = U_{95}/1.96$ because in a normal distribution, around 95% of observations fall within 1.96 times the standard deviation of the mean. It is important to note that the values expressed in percentage are relative errors compared to the others, which are absolute errors.

Parameter	U_{95}	σ
T_{in}	0.4 [%]	0.204
T_{BDC}	2 [%]	1.0204
T_{Wall}	12.9164 [K]	6.59
$FuelMEP$	2 [%]	1.0204
%O ₂	< 0.1 [%O ₂]	0.000510
RPM	0.024 [RPM]	0.012
α	6.792	3.447

Table 4.9: Parameters uncertainty

By generating $2*|\mathcal{A}^{M,p}| = \frac{(p+M)!}{p!M!}$ samples (the factor 2 is to ensure a well-posed Least-Square Minimization), and by taking the combustion timing as objective of interest, Rheia provides a standard deviation of $\sigma = 2.795$ and a mean of $\mu = 3.546$ [CAD] for the CA5 (Case with 84% of O₂ and $T_{in} = 409$ [K]). As mentioned earlier, it also provides the Sobol indices represented in Figure 4.27 and a probability density curve in Figure 4.28.

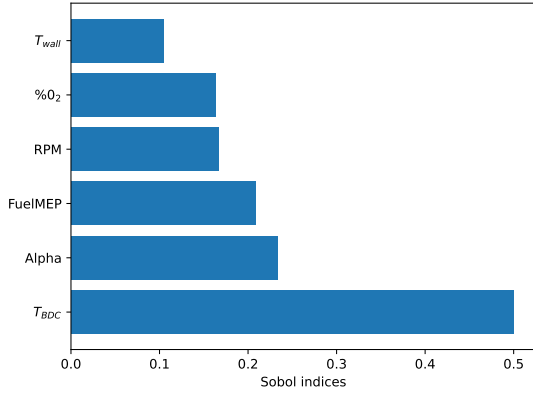


Figure 4.27: Residuals

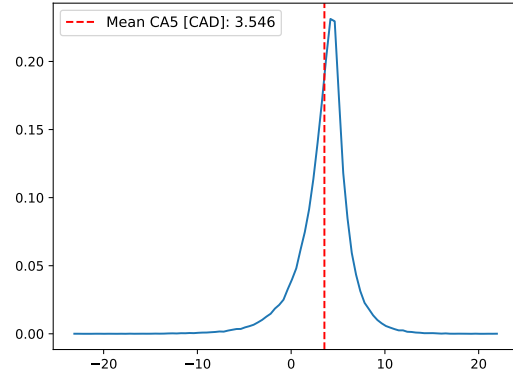


Figure 4.28: Probability density function

The impact of parameter uncertainties on the combustion timing is clearly illustrated in Figure 4.27. It is evident and reasonable that the uncertainties in the predicted values have a significant influence on the majority of the variance in the final efficiency. One other point worth mentioning is that the assumption of maintaining T_{wall} is validated because its error only has a slight effect on our combustion timing. The reason behind the high influence of the uncertainty in T_{BDC} on the final efficiency can be attributed to the equation used for its prediction. This equation, in addition of being a prediction equation rather than an experimental measurement, is derived for a mixture of ammonia and hydrogen, not methane. Therefore, while it provides a quantitative estimate, it lacks precision for our specific situation. As mentioned in Section 3.5.1, the search for a prediction equation tailored to our specific conditions remains an avenue for improvement in the future.

In Figure 4.28, the probability density function (PDF) is displayed. It exhibits a distinct shape compared to a typical PDF. This difference arises due to the significant influence of the uncertainty in T_{BDC} on our heat losses through the Hohenberg formula. As a consequence, combustion does not occur in these cases. This is evident from the left side of the curve, where the density of probability is non-zero when the CA5 is way too low. This explains why the standard deviation we obtained is significantly large. Thus, it would be prudent in future endeavors to find a more accurate correlation for the bottom dead center (BDC) temperature. This would allow for a reanalysis and subsequently, more coherent values, while ensuring combustion is occurring.

4.5.2 Uncertainty Analysis on Cantera Integration

In this subsection, the goal is to explain the impact of error tolerances in our model during the integration of reactor equations (Equation 3.20) using the Cantera solver (CVODES).

The objective is twofold: first, to observe the convergence of the model data for validation purposes, and second, to reduce simulation times without significantly impacting the results. To examine these two aspects, Figure 4.29 illustrates the different combustion timings (CA5) based on the imposed value of tolerance in the model. By analyzing the figure, a clear convergence can be observed between $rtol = 10^{-9}$ and $rtol = 10^{-10}$, as the CA5 output values, below these tolerances, no longer exhibits significant variations.

Thus, these tolerance values are deemed acceptable for achieving the lowest possible simulation time while maintaining an acceptable level of precision.

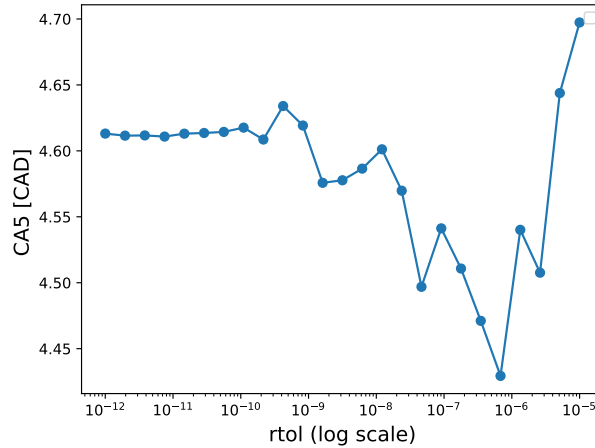


Figure 4.29: The effect of $rtol$ on accuracy of combustion timing

It is noteworthy that the relative tolerance values used in many other cases of engine modelling are larger than those in this situation. This discrepancy arises from the nearly instantaneous combustion in the model, which necessitates the solver to employ very small tolerances in order to accurately describe the reality of the system.

4.6 Technologies Comparison

The purpose of this section is to conclude our thesis by having a rough evaluation of how our findings, particularly the impact of enhancing power density via increasing O_2 percentage, re-situates the HCCI engine between the technologies analysed in Section 1.4. We can accomplish this by tracing the route of electricity from its generation to its reintegration into the grid through our engine. To begin developing a clear understanding of this process, we can start with the transformation of energy to methane (refer to Figure 4.30).

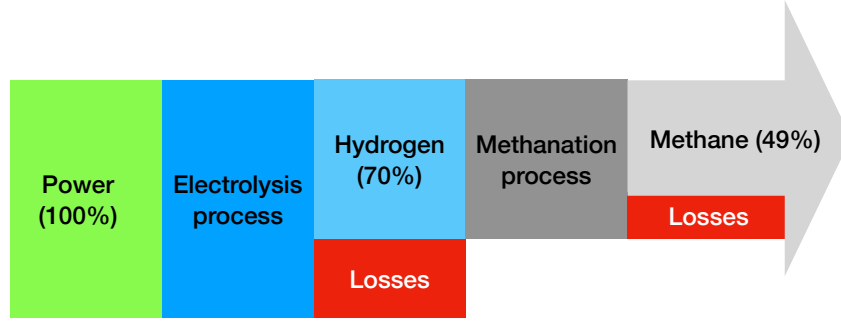


Figure 4.30: Efficiencies from power-to-gas

In Figure 4.30, we can observe the progression of renewable energy through various processes to produce methane, with methane generation accounting for approximately 49% of the base energy.

Combining this proportion with the electrical efficiencies of different technologies is indeed intriguing. These efficiencies are presented in Table 1.4.

Regarding the efficiency of the HCCI engine with 21% oxygen, we initially considered a mechanical efficiency (η_{mec}) of 0.90 (Typical value for a diesel kind engine). In Section 4.3.2, the $IMEP_{gross}$ value is calculated, which first had to lose 1% due to pumping losses (small for a HCCI). Then, this $IMEP_{net}$ obtained, when multiplied by η_{mec} , it provides the break mean efficiency (BMEP), making it comparable to other technologies if we divide it by the FuelMEP to obtain the total efficiency. We thus obtain an electrical efficiency of 38.66% which seems to be a credible value due to the close gap with the diesel engine efficiency. When employing oxygen enrichment in the combustion process, we maintain a constant Fuel Mean Effective Pressure (FMEP) value of 0.403 [Bar], which was previously calculated by subtracting Indicated Mean Effective Pressure (IMEP) from Break Mean Effective Pressure (BMEP). However, with the introduction of oxygen, the IMEP typically increases compared to lower oxygen concentrations. Consequently, we recalculate the BMEP using this new $IMEP_{net}$ value.

In the specific case of using 67% oxygen, as shown in Table 4.8, the new efficiency can be determined. By dividing the recalculated BMEP by the FuelMEP, an efficiency value of 44.5% is obtained. It becomes apparent that there is a clear increase in efficiency with the addition of oxygen. This is primarily due to the fact that when power density is increased, friction losses associated with engine size do not increase. Therefore, oxygen enrichment becomes advantageous in terms of efficiency.

Another factor contributing to the increased efficiency with oxygen enrichment is the lower inlet temperature. With less preheating energy required for the gases, the overall efficiency is improved. These effects demonstrate the benefits of oxygen enrichment in enhancing engine efficiency but this is not taken in account in this representation due to the lack of information in amounts of the engine.

By considering these factors, we can observe a notable rise in efficiency as oxygen concentration increases, resulting in improved performance and energy utilization in the engine.

	SI engine	CI engine	Micro-turbine	Fuelcell	HCCI engine with O_2(21%)	HCCI engine with O_2(67%)
η_{ptp} [%]	16.66	19.6	10.78	36.0	18.94	21.8

Table 4.10: Efficiencies from power-to-power

The different values of overall efficiency can be represented in Table 4.10. It is important to note that we are solely concerned with electrical efficiencies in this case. The HCCI engine and the other mentioned technologies have significant cogeneration capabilities. The recoverable heat from cogeneration can significantly increase efficiencies (see total efficiency in Figure 4.30). This certainly warrants further exploration in future work, aiming to better classify the HCCI engine among its competitors and optimize the engine's input conditions to achieve the highest possible total efficiency.

Conclusion

The following final study work numerically investigated the influence of oxygen enrichment on the operating conditions, as well as the resulting performance of a methane-fueled HCCI engine.

The first chapter provides a general introduction to the current energy context by addressing the need to transition towards efficient storage solutions, particularly power-to-fuel storage. Different technologies suitable for this specific storage method are then compared to give an overall idea of their efficiency.

The second chapter provides a theoretical overview of key concepts of the HCCI engine, highlighting notions such as ignition timing, intake charge, mean effective pressures, and the limited operating range that characterizes the specific conditions under which the HCCI engine can operate optimally. Then, the oxygen enrichment strategy is discussed in detail, followed by a pre-evaluation of its influence on required intake parameters and its capability to address the low power density issue of the HCCI engine.

In the third chapter of this study, particular attention is given to the comprehensive development of a detailed single-zone Ordinary Differential (OD) model, outlining the mathematical and thermodynamic concepts essential for simulating the behavior of the HCCI engine. Despite the main limitation of this model in terms of instantaneous combustion, which affects the reliability of simulated pressure rise rates, meticulous calibration was performed using numerous experimental data specifically collected in the context of oxygen enrichment analysis for methane combustion. This calibration aimed to predict the start of combustion, a crucial step in estimating the required operating conditions to avoid the phenomenon of knocking.

The final chapter of this study begins with the development of a statistical correlation between the Maximum Pressure Rise Rate (MPRR) and the parameters that influence it, namely ignition timing and injected fuel quantity. Since the model calibration is solely based on combustion timing, the engine's performance in terms of output power and efficiency is quantitatively analyzed to provide an overall understanding of the parameters. However, this calibration accurately predicts the usable input conditions for the engine in order to enhance its input power density.

The oxygen enrichment strategy is then thoroughly investigated by manipulating intake temperatures, oxygen levels, and fuel injection quantities into the engine. Specifically, increasing the oxygen concentration in the oxidizer up to 100% reduces the minimum temperature required for ignition by 74 K, thereby allowing for an increased fuel density of 11.82% compared to combustion with air.

The output power is then roughly estimated while still respecting the maximum load range imposed by the engine's MPRR. Despite the unreliable values, increasing oxygen concentrations shows an improvement in output power density, resulting in higher mechanical efficiency and therefore brake efficiency.

Given the numerous assumptions made during the development of this model, an uncertainty analysis highlights the lack of robustness in approximating certain parameters, notably the temperature at the beginning of the simulation (T_{bdc}). The work concludes with a brief comparison of overall efficiencies with different technologies presented in earlier chapters, aiming to provide a perspective on the performance of the studied HCCI engine.

The strategy of oxygen enrichment proves to be a promising approach to improve the performance and efficiency of HCCI engines, offering an ideally suited solution for "power to gas" storage. However, to fully assess the impact of this technology, it would be pertinent to quantify the economic benefits resulting from the improved energy efficiency of the HCCI engine, taking into account the costs associated with replacing nitrogen molecules with pure oxygen. A thorough economic analysis would allow to evaluate the profitability of this oxygen enrichment strategy and determine its viability compared to competing technologies. A comparative economic analysis with the different technologies presented in the last section of the results would be essential to truly assess the contribution of this technology compared to existing solutions. This investigation would consider factors such as initial costs, operational costs, resource availability, and environmental impacts, in order to better evaluate the relevance and attractiveness of the HCCI engine in a global economic context.

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Energy storage technologies characteristics

EES Technology	Power density (W/l)	Specific power (W/ kg)	Energy density (W h/l)	Specific energy (W h/kg)	Capital Costs		Technology maturity
					Power (\$/kW)	Energy (\$/kW h)	
PHS	–	–	0.5–1.5	0.5–1.5	600–2000 (100–300)	5–100	Mature
CAES	–	–	0.5–1.5	0.5–1.5	1000	N/A	Demonstration
	–	–	3–12	30–60	400–800	2–50	Commercial
	–	–	3–12	30–60	700–100	40–80	R&D – Demonstration
	–	–	3–12	30–60	500–1000	10–100	Pre-commercial
	–	–	3–12	30–60	750–2000	40–200	Pre-commercial
Flywheel	1000–2000	400–1500	20–80	5–100	250–350	1000–5000	Commercial
LAES	–	–	50	~ 210	900–2000	260–530	Demonstration – Pre-commercial
PTES	–	–	~ 110–170	~ 50–140	~ 600	~ 60	R&D – Pre-commercial
Conv. Batteries	10–700	75–415	50–90	20–50	300–500	200–400	Mature
	75–700	100–300	60–150	40–75	500–1500	800–1500	Commercial – Mature
	500–3000	200–1500	140–300	45–80	600–1800	960–1800	Commercial
	1300–10,000	130–2000	200–500	70–250	1200–4000	600–2500	Commercial
HT Batteries	120–160	150–230	150–250	100–240	1000–3000	300–500	Commercial
	220–300	150–200	150–180	85–140	~ 400–1800	~ 500–1000	Commercial
Flow Batteries	0.5–2	166	16–33	10–35	600–1500	150–1000	Commercial
	1–25	45	30–60	30–85	700–2500	150–1000	Pre-commercial
	–	–	16–60	10–50	330–2500	120–1000	Demonstration
	100,000	500–5000	10–30	2.5–50	100–360	300–2000	Demonstration – Pre-commercial
Supercapacitors	–	–	–	–	–	–	–
SMES	1000–4000	500–2000	0.2–2.5	0.5–5	200–350	1000–10,000	Demonstration – Pre-commercial
PG+Storage +GrP	–	–	500–3000	–	1900–6300	1–10	R&D – Pre-commercial
	–	–	2000–7200	–	3500–5000	1–10	R&D – Demonstration

Table .11: Energy storage technologies characteristics

Water electrolysis technologies

	Alkaline	AEM	PEM	Solid Oxide
Anode reaction	$2\text{OH}^- \rightarrow \text{H}_2\text{O} + \frac{1}{2} \text{O}_2 + 2\text{e}^-$	$2\text{OH}^- \rightarrow \text{H}_2\text{O} + \frac{1}{2} \text{O}_2 + 2\text{e}^-$	$\text{H}_2\text{O} \rightarrow 2\text{H}^+ + \frac{1}{2} \text{O}_2 + 2\text{e}^-$	$\text{O}^{2-} \rightarrow \frac{1}{2} \text{O}_2 + 2\text{e}^-$
Cathode Reaction	$2 \text{H}_2\text{O} + 2\text{e}^- \rightarrow \text{H}_2 + 2\text{OH}^-$	$2 \text{H}_2\text{O} + 2\text{e}^- \rightarrow \text{H}_2 + 2\text{OH}^-$	$2\text{H}^+ + 2\text{e}^- \rightarrow \text{H}_2$	$\text{H}_2\text{O} + 2\text{e}^- \rightarrow \text{H}_2 + \text{O}^{2-}$
Overall cell	$\text{H}_2\text{O} \rightarrow \text{H}_2 + \frac{1}{2} \text{O}_2$	$\text{H}_2\text{O} \rightarrow \text{H}_2 + \frac{1}{2} \text{O}_2$	$2\text{H}_2\text{O} \rightarrow \text{H}_2 + \frac{1}{2} \text{O}_2$	$\text{H}_2\text{O} \rightarrow \text{H}_2 + \frac{1}{2} \text{O}_2$
Electrolyte	KOH/NaOH (5M)	DVB polymer support with 1 M KOH/NaOH	Solid polymer electrolyte (PFSA)	Yttria stabilized Zirconia (YSZ)
Separator	Asbestos/Zirfon/Ni	Fumatech,	Nafion [®]	Solid electrolyte YSZ
Electrode/Catalyst (Hydrogen side)	Nickel coated perforated stainless steel	Nickel	Iridium oxide	Ni/YSZ
Electrode/Catalyst (Oxygen side)	Nickel coated perforated stainless steel	Nickel or NiFeCo alloys	Platinum carbon	Perovskites (LSCF, LSM) (La,Sr,Co,Fe) (La,Sr,Mn)
Gas Diffusion layer	Nickel mesh	Nickel foam/carbon cloth	Titanium mesh/carbon cloth	Nickel mesh/foam
Bipolar Plates	Stainless steel/Nickel coated stainless steel	Stainless steel/Nickel coated stainless steel	Platinum/Gold-coated Titanium or Titanium	Cobalt coated stainless steel
Nominal current density	0.2–0.8 A/cm ²	0.2–2 A/cm ²	1–2 A/cm ²	0.3–1 A/cm ²
Voltage range (limits)	1.4–3 V	1.4–2.0 V	1.4–2.5 V	1.0–1.5 V
Operating temperature	70–90 °C	40–60 °C	50–80 °C	700–850 °C
Cell pressure	<30 bar	<35 bar	<70 bar	1 bar
H ₂ purity	99.5–99.9998%	99.9–99.9999%	99.9–99.9999%	99.9%
Efficiency	50%–78%	57%–59%	50%–83%	89% (laboratory)
Lifetime (stack)	60 000 h	> 30 000 h	50 000–80 000 h	20 000 h
Development status	Mature	R & D	Commercialized	R & D
Electrode area	10 000–30 000 cm ²	<300 cm ²	1500 cm ²	200 cm ²
Capital costs (stack) minimum 1 MW	USD 270/kW	Unknown	USD 400/kW	> USD 2000/kW
Capital costs (stack) minimum 10 MW	USD 500–1000/kW	Unknown	USD 700–1400/kW	Unknown

Table .12: Technical characteristics of typical water electrolysis technologies [44]

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