

École polytechnique de Louvain

Use of Electrofuels in Homogeneous Charge Compression Ignition Engines

Numerical Study of Oxy-combustion Potential

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Abstract

The present master's thesis is a continuation of previous works on the HCCI technology conducted at UCLouvain. The latest focused on the use of electrofuels in HCCI engines for the electricity restitution phase of Power to Fuel to Power cycles. Research on fuel blending and water direct injection were thus previously performed.

In this thesis, the numerical investigation on the use of pure oxygen as oxidiser, i.e. oxy-combustion, in HCCI engines fuelled by methane is conducted. The comparison between conventional air combustion and oxy-combustion is emphasised and the use of carbon dioxide to reduce the oxy-combustion brutality is investigated.

The objectives of this work are multiple. First of all, the context in which HCCI oxy-combustion could be used is set. Fundamental concepts of HCCI engine operation and control are explained and the potential of HCCI oxy-combustion is detailed based on a review of the few scientific papers on the subject. A description of the engine test bench followed by the modifications required to perform oxy-combustion are presented.

A 0D numerical model is then used to determine the required intake thermodynamic conditions to have a proper auto-ignition timing for both combustion types. Different fuel contents and charge compositions are simulated. Afterwards, 3D axisymmetric simulations are performed to precisely predict the combustion behaviour in terms of timings and pressure rise rates.

Using the 3D simulation results, we define the optimal auto-ignition timing to maximise the engine load and indicated efficiency for different equivalence ratio contained in our research engine operating range. The impact of various parameters is discussed and the comparison is made between air and oxy-combustion. Ringing occurs at lower fuel content for pure oxy-combustion due to the more brutal and rapid combustion. In our research engine, with the optimal combustion timing, the limit is reached at FuelMEP ≈ 9 [bar] for an IMEPg of 3.7 [bar].

The addition of CO₂ in the intake charge has been proven to allow an increase of more than 40% in engine load by extending the combustion duration thus allowing the use of higher fuel contents.

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Nomenclature

Abbreviations

COV_{IMEP}	Coefficient Of Variation in IMEP
NO_x	Nitrogen Oxides
AHRR	Apparent Heat Release Rate
BESS	Battery Energy Storage Systems
BMEP	Break Mean Effective Pressure
CA05	Crank Angle where 5% of the combustion heat has been released
CA10	Crank Angle where 10% of the combustion heat has been released
CA50	Crank Angle where 50% of the combustion heat has been released
CA90	Crank Angle where 90% of the combustion heat has been released
CAD	Crank Angle Degree
CAES	Compressed Air Energy Storage
CCGT	Combined Cycle Gas Turbine
CFD	Computational Fluid Dynamics
CHP	Combined Heat and Power
CI	Compression Ignition
CPU	Central Processing Unit
DAC	Dynamic Adaptive Chemistry
DOC	Duration Of Combustion, in this thesis $DOC = CA90 - CA10$
EGR	Exhaust Gas Recirculation
EVC	Exhaust Valve Closing

EVO	Exhaust Valve Opening
FMEP	Friction losses Mean Effective Pressure
FuelMEP	Fuel Mean Effective Pressure
GHG	Greenhouse Gas
HCCI	Homogeneous Charge Compression Ignition
HRR	Heat Release Rate
ICE	Internal Combustion Engines
IEA	International Energy Agency
IMEP	Indicated Mean Effective Pressure
IMMC	Institute of Mechanics, Materials and Civil Engineering
ISAT	In Situ Adaptive Tabulation
IVC	Intake Valve Closing
IVO	Intake Valve Opening
LHV	Lower Heating Value
LNT	Lean NO _x Trap
LTC	Low Temperature Combustion
MEP	Mean Effective Pressure
MFC	Mass Flow Controller
MPRR	Maximum Pressure Rise Rate
NG	Natural Gas
ODE	Ordinary Differential Equation
P&ID	Piping and Instrumentation Diagram
PHES	Pumped Hydro-Electric Storage
PID	Proportional–Integral–Derivative (controller)
PMEP	Pumping losses Mean Effective Pressure
PtG	Power to Gas
RAS	Reynolds-Averaged Simulation

RES	Renewable Energy Sources
RI	Ringing Intensity
RPM	Rotation Per Minute
SCR	Selective Catalytic Reduction
SI	Spark Ignition
SOC	Start Of Combustion, in this thesis SOC = CA10
TDAC	Tabulation of Dynamic Adaptive Chemistry
TDC	Top Dead Centre
UHC	Unburned Hydrocarbons
WDI	Water Direct Injection

Symbols

η_c	Combustion efficiency
η_b	Brake efficiency
η_{indg}	Gross indicated efficiency
η_{indn}	Net indicated efficiency
η_{mec}	Mechanical efficiency
η_{ti}	Thermodynamic efficiency
γ	Ratio of specific heat, $\gamma=c_p/c_v$
ω	Engine angular velocity [CAD/s]
ϕ	Equivalence ratio (fuel-air)
σ	Standard deviation
τ_{eff}	Effective compression ratio
τ	Geometric compression ratio
θ	Crankshaft angular position, CAD
c_p	Constant pressure specific heat capacity
c_v	Constant volume specific heat capacity
MW _e	Megawatt Electrical

S_p	Piston mean speed
$T_{BDC}(CA10=TDC)$	Required BDC temperature to obtain $CA10 = TDC$
V_d	Engine displacement
V_{BDC}	Bottom dead centre volume
V_{TDC}	Top dead centre volume
B	Bore
Co	Courant Number
h	Newton convective heat transfer coefficient
L	Connecting rod length
m	Mass
N	Engine rotational speed
n	Number of moles
Q	Heat energy
R	Universal constant of ideal gas
r	Crank radius
S	Stroke
SP	Swirl Profile
SR	Swirl Ratio
U	Internal energy
W	Work

Introduction

The decarbonisation of the energy production sector is a key step to limit climate change and its dreadful effects on the environment. The energy transition towards renewable sources is an important challenge that our society needs to face. However, it is associated with an increasing need for electrical storage and restitution systems to overcome renewables intermittent production. Power to Gas is a promising long-term storage solution that converts hydrogen produced by electricity surplus into methane via the electrolysis of water. For power outputs lower than 3 MW_e, *Homogeneous Charge Compression Ignition* (HCCI) engines are the most efficient option of energy restitution using stored methane.

The HCCI combustion is an ingenious way of combining the high overall efficiency of compression ignition engines and the low soot and NO_x emissions of spark ignition engines. The charge that enters the cylinder is already premixed and its auto-ignition is caused by the in-cylinder compression. The combustion timing is only controlled by chemical kinetics and thus represents a major challenge for the technology. As the charge ignites almost instantaneously, low fuel contents are used to avoid brutal pressure rise rates. However, this leads to a relatively low power density.

This work builds upon a series of PhD and master's thesis on the HCCI combustion technology conducted at UCLouvain in recent years. The main goal of this thesis is to investigate the feasibility and potential benefits of using pure oxygen as the oxidiser, i.e. removing nitrogen from the system, for the combustion of methane in a HCCI engine. HCCI oxy-combustion has barely been studied by internal combustion engine research groups. Indeed, an oxygen-rich mixture is bound to increase the already problematic pressure rise rates of HCCI engines. Nevertheless, we sought to investigate its potential. To carry out this task, a 0D numerical model has been used and a 3D axisymmetric model has been developed.

The first chapter of the present work introduces the underlying context of this master's thesis and summarises the fundamental concept required for the comprehension of HCCI engine operations. To the best of our knowledge, at the time of writing this thesis, only one scientific paper was available on HCCI oxy-combustion. It is presented and discussed in the first chapter. In the second one, the UCLouvain HCCI setup is presented along with the modifications required for an oxy-combustion experimental campaign. The heat release rate computation is then detailed. The third chapter details the calibration and use of a 0D model to determine the intake conditions leading to an optimal combustion timing for different mixture compositions. Finally, the fourth and last chapter describes the design and calibration of a 3D axisymmetric numerical model. Simulated air and oxy-combustion behaviours are presented and compared in terms of high load limits. Then, the use of synthetic EGR to reduce the MPRR in oxy-combustion is investigated.

Chapter 1

General Context

This chapter introduces the context of this master's thesis. First, the incoming challenges of the energy transition are presented along with the potential of Power to Power processes for long-term energy storage and restitution. The second section outlines the fundamental concepts required for the comprehension of HCCI engine operation and control. Finally, the objectives of this work are presented and the potential and feasibility of methane HCCI oxy-combustion are theoretically investigated.

1.1 Power to Gas in the Energy Transition

In recent years, attention to climate change and energy dependency has increased. Driven by concerns for the environment and the human health, international agencies call for urgent action from all actors: governments, industry, research entities and citizens.

In the European Union, clean energy directives impose a 27% renewable supply on final energy consumption by 2030 and a 40% decrease in *GreenHouse Gas* (GHG) emissions against the 1990 levels [1]. The EU 2050 Roadmap aims for a global reduction of GHG of 80% from the 1990 levels and a specific decrease of 99% in the power generation sector to balance with less flexible sectors such as agriculture [2]. According to the *International Energy Agency* (IEA), new policies are not able to cope with the increasing world population and quality of living. IEA states that to stay within the 2[°C] pathway our energy-related greenhouse gas emissions must fall to zero by 2065.

The decarbonisation of the energy production sector is a key step for GHG emission reduction. However, this energy transition towards high penetration of renewables in the present energy mix leaves important challenges to overcome. *Renewable energy sources* (RES) such as wind and solar are, by definition, intermittent and irregular. They do not fit the real-time electricity demand because they depend mainly on the weather. The integration of a large number of renewable sources in the present grid will create an increasing demand for short and long-term energy storage solutions to absorb excess during peaks and provide power during troughs. These complex smart grids are a necessity for the system evolution towards a fully renewable generation to match production along with consumption and to ensure a continuous supply of electricity.

In the case of four possible energy transition scenarios for Belgium, Limpens and al. showed that short-term (daily) energy storage is required from 35-40 % of RES production share. Long-term storage, on the other hand, requires at least 75-85 % of RES production share (depending on the scenarios) [3].

Energy storage options to assist in load balancing include flywheels, *Battery Energy Storage Systems* (BESS), *Compressed-Air Energy Storage* (CAES), *Pumped Hydroelectric Storage* (PHES) and *Power to Gas* (PtG). These technologies are complementary and should form synergies to enable high RES penetration in future smart grids. Figure 1.1 summarises the storage capacity and time scale of the above-mentioned technologies.

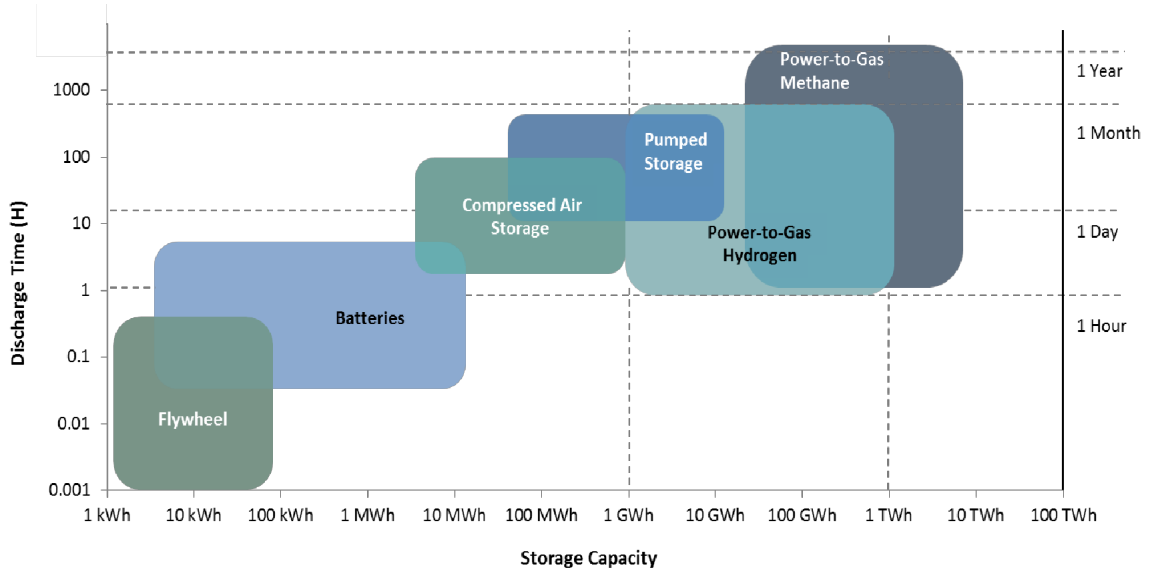
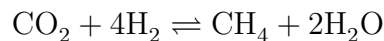


FIGURE 1.1: Energy storage technologies comparison, discharge time vs storage capacity [4].

Flywheels and BESS are only usable for short-term energy storage, from seconds to some hours. The main disadvantage of BESS, except for redox flow batteries, is that their energy-to-power ratio is fixed, leading to excessive installed power capacity.

CAES and PHES are usable for mid-term energy storage, up to some days. However, they are geographically dependent. CAES needs caves while PHES requires a significant difference in height. PHES is the only mature technology but its storage capacity in Europe is one order of magnitude lower than the required storage in the scenario of a fully renewable electricity network.

Power to Gas allows high capacity and long-term energy storage, up to months. It is attractive for seasonal storage thanks to its low storage cost. The PtG technology converts electricity surplus into hydrogen via water electrolysis. Hydrogen can then be transformed into other electrofuels suitable to use in an *Internal Combustion Engine* (ICE) such as hydrogen, methane, ammonia or methanol to improve storage properties. In this work, the gas of interest is methane produced from hydrogen and carbon dioxide with the Sabatier reaction:



This methanation process widens the range of applications of PtG as methane can be stored and distributed in the existing natural gas grid without any required treatment.

Gas to Power process includes *Combined Cycle Gas Turbines* (CCGT), Fuel Cells and ICE to convert back the stored methane to electricity. These processes imply a transformation efficiency ranging from 60% for CCGT and Fuel Cells to 30-50% depending on the size and the type of ICE.

The main handicap of Power to Power processes is their low overall efficiency due to the successive conversion losses. First, the electrolysis takes place with an efficiency of 70-75%. The methanation process then follows with an efficiency of roughly 80%. Finally, the restitution of electricity from the methane occurs with the efficiencies given above.

In his PhD thesis, M. Pochet [5] studied the minimisation of the conversion losses during the restitution phase of a Power to Power process. The study is focusing on a decentralised *Combined Heat and Power* (CHP) unit that has the potential of achieving 95% global efficiency. This is made possible by making use of the generated heat losses associated with the production of electricity. As the electrical power output goal of this unit was fixed between 0.3 and 3 [MW_e], the natural choice was an internal combustion engine. Among all the ICE types, the *Homogeneous Charge Compression Ignition* (HCCI) engine has been selected for its high overall efficiency (Diesel-like) and its ability to run on multiple fuels, helping to bring resilience to the cogeneration unit. Moreover, the low-pollutant emissions characterising the HCCI combustion is an undeniable asset.

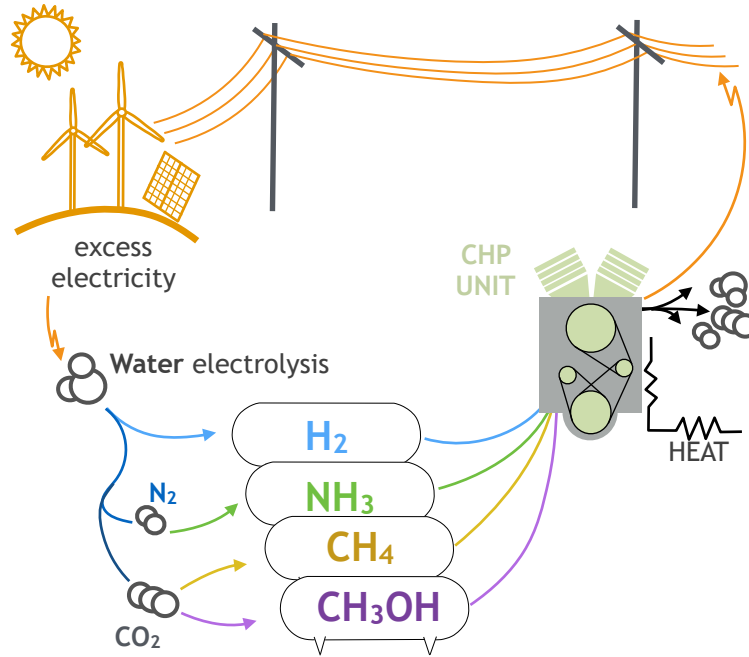


FIGURE 1.2: Full Power to Power system described in [5]

Following on from M.Pochet work, this thesis focuses on the numerical characterisation of methane HCCI air and oxy-combustion in the context of Power to Power process.

1.2 Fundamentals of the HCCI Engine

The HCCI outline made in this section is partly inspired by the previous master's thesis conducted at UCLouvain between 2016 and 2019 [6], [7], [8] and [9].

The *Homogeneous Charge Compression Ignition* (HCCI) engine is an ingenious way to combine the advantages of the two traditional engine types: the low NO_x and soot emissions of *Spark Ignition* (SI) engines and the high overall efficiency of *Compression Ignition* (CI) engines.

SI engines, commonly called gasoline or Otto engines, work with a homogeneous air-fuel mixture and ignite it via a spark plug. The combustion results in a propagating flame front expanding from the spark. CI engines, also referred to as diesel engines, only compress fresh air to begin with. The fuel is then injected before the *Top Dead Centre* (TDC) and auto-ignites quickly due to the high in-cylinder temperature conditions. Unfortunately, the in-homogeneity of the charge leads to soot creation. Lean conditions in CI engines prevent the use of the effective three-way catalytic converter and thus lead to higher net NO_x emissions. However, the lean global mixture along with a higher compression ratio provides better overall efficiency, reducing fuel consumption and CO_2 emissions.

As its name suggests, the HCCI combustion is characterised by a homogeneous air-fuel mixture, the mixing is done before the intake stroke. The mixture spontaneously auto-ignites when the compression leads to the adequate thermodynamic conditions of pressure and temperature (depending on the mixture itself). Conversely to traditional combustion, HCCI combustion timing is not controlled by an electric spark or fuel injection timing. The ignition is only governed by chemical kinetics and it is one of the major challenges of the technology. The optimal auto-ignition timing, allowing extracting the maximum mechanical work, is around the TDC.

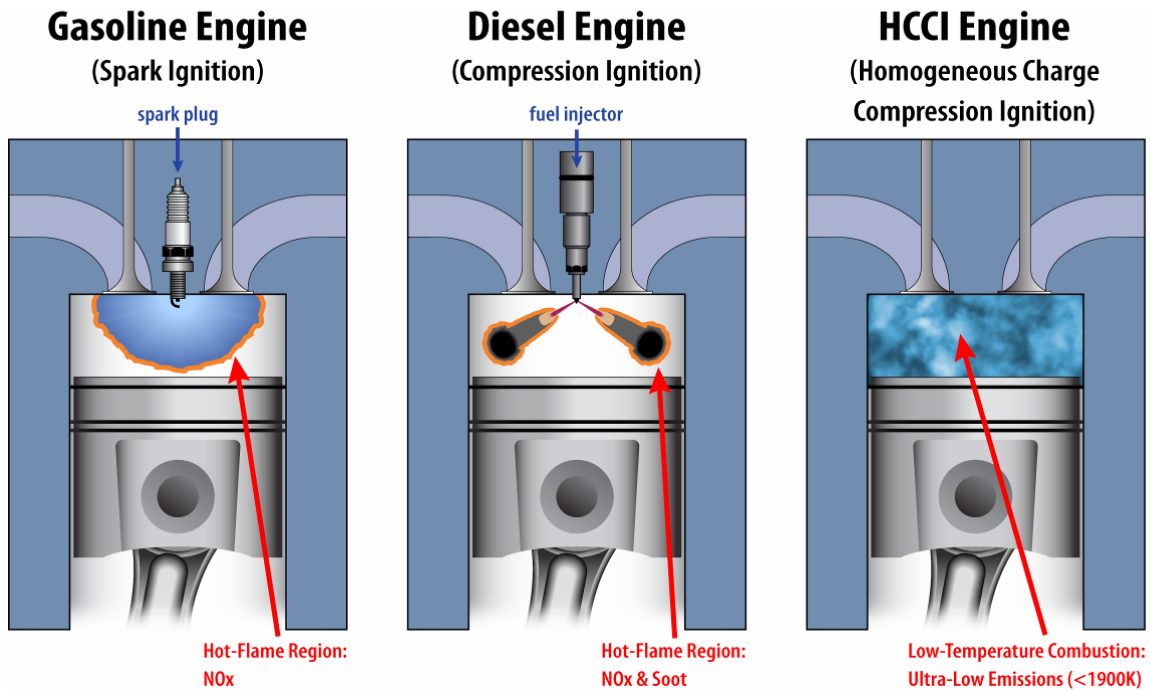


FIGURE 1.3: Schematic comparison between SI, CI and HCCI combustion ¹

¹<http://csyoo.unist.ac.kr/research/hcci-combustion/> last accessed on May 20, 2020

The challenge of combustion timing control is severe for ever-changing loads and rotational speed situations. Higher loads require higher fuel contents that influence the auto-ignition behaviour of the charge. Speed variations also have an impact on combustion timing. Therefore, simultaneously regulating all the parameters that influence the auto-ignition timing of the charge to keep optimum timing is proven to be a complex task. This situation limits the adoption of pure HCCI engines in the transport industry.

Consequently, the HCCI combustion strategy is more appropriated for stationary conditions with slow evolution of load requirements. The UCLouvain HCCI research engine is connected to a three-phase generator which is set at a constant rotational speed of 1500 [RPM]. Combustion timing control is thus only a challenge for suitable initial condition determination depending on the fuel and load request.

Given the homogeneous intake charge, temperature and pressure can be considered uniform in the cylinder as a first approximation. Indeed, a thermal gradient exists close to the cylinder wall due to heat transfer but this gradient is localised. The whole mixture auto-ignites almost simultaneously and the combustion duration is very short, up to 6 times shorter than for SI-CI combustion [5]. Besides, the combustion is not slowed down by flame propagation or diffusion process. To soften the combustion intensity, charge dilution and lean mixtures are used.

Homogeneous charge compression ignition engines can operate with multiple types of fuels, as long as internal and intake characteristics are adapted accordingly to ensure auto-ignition (compression ratio, intake temperature and pressure, fuel content, etc.). Granted that fuels are admitted under gaseous phase, Christensen et al. have demonstrated that almost any liquid fuel can be used in a HCCI engine, from high cetane number (heptane) to high octane number (iso-octane) fuels [10]. HCCI combustion researches conducted at UCLouvain have studied and used a large panel of gaseous fuels ranging from biomass syngas, methane, hydrogen, methanol and ammonia as well as various blends of these gases.

The piston alternates between the bottom dead centre and the top dead centre following a reciprocating movement driven by the crankshaft-connecting rod mechanism. The cylinder displacement volume V_d is defined by the difference between the maximum cylinder volume, V_{BDC} , and the minimum cylinder volume V_{TDC} . The in-cylinder compression is characterised by the geometrical compression ratio: $\tau = \frac{V_{BDC}}{V_{TDC}}$.

The equivalence ratio ϕ is defined as the actual fuel-to-oxidiser ratio over the stoichiometric fuel-to-oxidiser ratio:

$$\phi = \frac{m_{fuel}/m_{ox}}{(m_{fuel}/m_{ox})_{st}} = \frac{n_{fuel}/n_{ox}}{(n_{fuel}/n_{ox})_{st}}$$

These ratios can be expressed in terms of mass or mole and the oxidiser for conventional combustion is air. By definition, a mixture is stoichiometric when $\phi = 1$. The mixture is said rich when it presents a fuel excess ($\phi \geq 1$) and lean when it presents an oxidiser excess ($\phi \leq 1$).

Efficiencies and MEP

Efficiencies of ICE are quite far off the ideal isochoric heat addition Beau de Rochas cycle (see Equation (1.11)). A substantial part of the fuel energy is lost during each step of the conversion process from the chemical content of the fuel to the usable work at the crankshaft.

To quantify the amount of energy available at each of these steps and therefore define corresponding efficiencies regardless of the engine size, we can use the *Mean Effective Pressure*

(MEP) values expressed in [bar]. Those MEP values are energy quantities normalised by engine displacement (V_d).

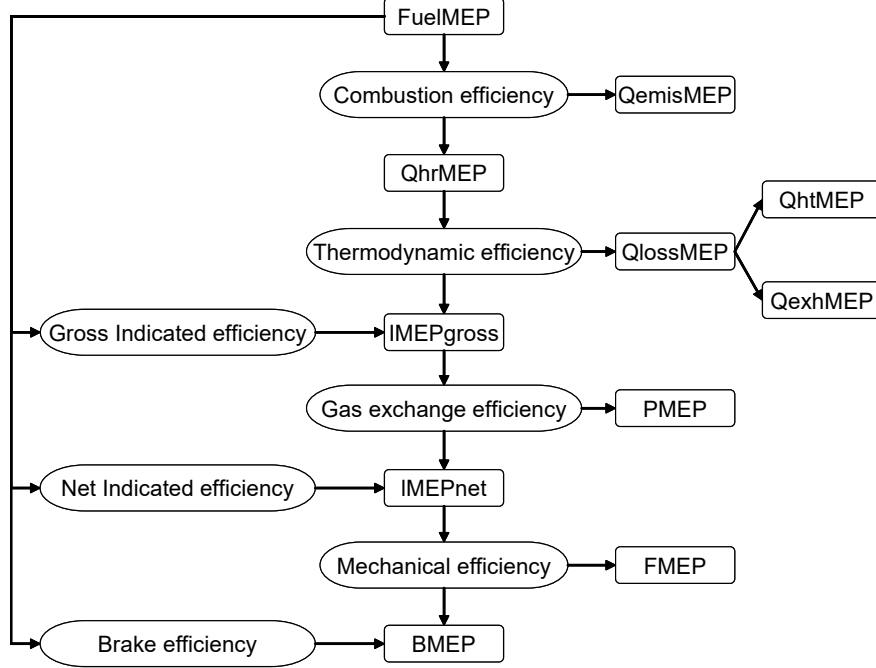


FIGURE 1.4: Energy conversion chart expressed in MEP from fuel chemical energy (FuelMEP) to brake mechanical work at the crankshaft (BMEP).[11]

The first MEP quantity used is the FuelMEP in Equation (1.1), characterising the energy content of the fuel in the cylinder. It depends on the fuel mass (m_{fuel}) and its *Lower Heating Value* (LHV).

$$\text{FuelMEP} = \frac{m_{fuel} \cdot \text{LHV}}{V_d} \quad (1.1)$$

The majority of the fuel is then burned and the heat released by the combustion can be expressed with QhrMEP. The intrinsic enthalpy of unburned compounds and incomplete combustion products is lost at the exhaust. This loss can be quantified by QemisMEP.

The combustion efficiency η_c can, therefore, be defined in Equation (1.2).

$$\eta_c = \frac{\text{QhrMEP}}{\text{FuelMEP}} \quad (1.2)$$

An increase of the charge intake temperature or equivalence ratio allow higher combustion temperature leading to higher combustion efficiencies.

However, the heat released by the combustion is not converted entirely into work on the piston. A certain quantity of energy is also lost through wall heat transfer and at the exhaust. Those two losses are quantified by QhtMEP and QexhMEP respectively.

Considering those losses, we can define the gross indicated MEP, IMEP_g .

The thermodynamic efficiency is the ratio between the cyclic work on the piston and the heat released:

$$\eta_{ti} = \frac{\text{IMEP}_g}{\text{QhrMEP}} = 1 - \frac{\text{QhtMEP}}{\text{QhrMEP}} - \frac{\text{QexhMEP}}{\text{QhrMEP}} \quad (1.3)$$

The gross indicated efficiency η_{indg} is also defined as:

$$\eta_{indg} = \eta_{ti} \cdot \eta_c = \frac{\text{IMEP}_g}{\text{FuelMEP}} \quad (1.4)$$

To take into account the pumping work during the breathing phase, PMEP is defined. It encompasses the head losses during the intake stroke and the pressure increase during the exhaust stroke that, together, represent the pumping work. It is approximated as follows:

$$\text{PMEP} = P_{out} - P_{in} \quad (1.5)$$

Where P_{out} and P_{in} are the mean in-cylinder pressures during the exhaust and intake stroke. Including those pumping losses into the gross indicated efficiency, we can define the net indicated MEP, IMEP_n and the net indicated efficiency, η_{indn} .

$$\text{IMEP}_n = \text{IMEP}_g - \text{PMEP} = \frac{-\oint p \cdot dV}{V_d} \quad (1.6)$$

$$\eta_{indn} = \frac{\text{IMEP}_n}{\text{FuelMEP}} \quad (1.7)$$

Then, we can consider the friction losses inside the engine with FMEP. Subtracting this value to the IMEP_n gives the brake MEP, BMEP. This quantifies the mechanical work available at the crankshaft of the engine:

$$\text{BMEP} = \text{IMEP}_n - \text{FMEP} \quad (1.8)$$

Using this last MEP, we can describe the mechanical efficiency, η_{mec} :

$$\eta_{mec} = \frac{\text{BMEP}}{\text{IMEP}_n} = 1 - \frac{\text{FMEP}}{\text{IMEP}_n} \quad (1.9)$$

Considering all the above-mentioned losses, we can eventually express the brake efficiency, η_b , which expresses the conversion of fuel chemical energy into work on the crankshaft:

$$\eta_b = \frac{\text{BMEP}}{\text{FuelMEP}} \quad (1.10)$$

Increasing fuel content is beneficial to the BMEP and η_b . Indeed, the produced work increases which reduces the relative importance of the friction losses. The only constraint on increasing the equivalence ratio is the increasingly brutal combustion.

The BMEP and the brake efficiency also rise with lower intake temperature. The in-cylinder temperature reduction leads to lower wall heat losses and denser charge. For a fixed equivalence ratio, the higher charge density allows burning more fuel.

1.2.1 High Efficiency

In HCCI engines, the combustion process is triggered by fuel auto-ignition, as in CI engines, leading to highly efficient combustion ($\eta_{comb} \approx 0.90 - 0.95$). The short combustion duration has a positive impact on the efficiency because it leans towards the ideal isochoric combustion (Beau de Rochas cycle). Lean conditions protect the engine from knocking. To reach auto-ignition conditions at TDC, HCCI engines must use high compression ratios, especially when used with high octane number fuels such as methane.

Approximating the HCCI cycle by the Beau de Rochas model of constant volume heat addition, we can have a qualitative idea of its efficiency:

$$\eta_{th} = 1 - \frac{1}{\tau^{\gamma-1}} \quad (1.11)$$

This model considers isentropic compression and expansion with a compression ratio τ [12]. HCCI high compression ratio, combined with a higher ratio of specific heat ($\gamma = \frac{C_p}{C_v}$), due to lean mixtures [13], have the benefit of a higher efficiency (as reported in Figure 1.5).

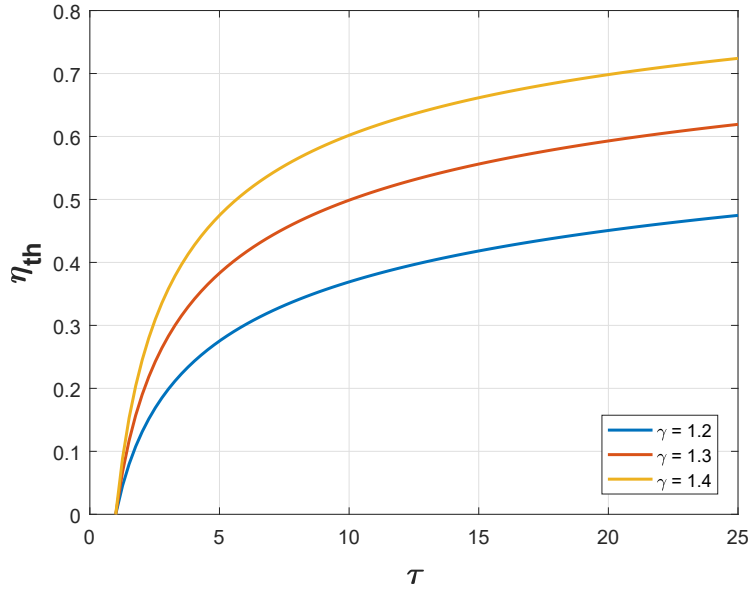


FIGURE 1.5: Influence of τ and γ on Beau de Rochas theoretical efficiency: η_{th}

Furthermore, the highly diluted air-fuel mixture reduces heat transfer losses and allows a throttle-less operation, cutting down pumping losses.

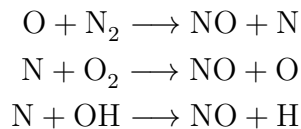
Research-lab light-duty HCCI engines currently reach overall brake efficiency of 43-45% [5].

1.2.2 Low Pollutant Emissions

This section is partially based on the excellent course of engine emission control given by Prof. Federico Millo at Politecnico di Torino [14].

Low equivalence ratios and homogeneous air-fuel mixtures lead to *Low Temperature Combustion* (LTC) in HCCI engines. This type of combustion is characterised by a flameless combustion and extremely low levels of NO_x and soot emissions (see Figure 1.3).

The main formation mechanism of *Nitrogen Oxides* (NO_x) in internal combustion engines is the thermal mechanism, also known as the extended Zeldovich mechanism:



The first reaction has extremely high activation energy, resulting in sensitivity to in-cylinder temperature. The NO_x emissions are thus almost insignificant at temperatures below 1700 [K] but a significant increase is observed above 2000 [K]. In addition to high temperatures, Zeldovich mechanism requires oxygen availability and time for these chemical reactions to complete.

In SI engines, the homogeneous and stoichiometric air-fuel mix burns by flame propagation. The formation temperature threshold is reached in the burned gas region but poor oxygen availability limits the NO_x emissions. For CI engines, nitrogen oxides form on the lean side of the diffusion flame and in hot post-combustion gases. The higher oxygen availability, due to the globally lean mixture used ($\phi \leq 0.6$), leads to higher NO_x emissions.

Soot is composed of elemental carbon particles that agglomerate and adsorb other species. They form under extremely rich local conditions ($\phi \geq 2$) during the premix burn phase of CI combustion and progressively grow in size during the combustion. If the temperature is sufficient ($T \geq 650$ [°C]), produced soot is partially burned out at the diffusion flame due to OH-radical attacks in an oxidising atmosphere. On the other hand, SI engines use a homogeneous stoichiometric charge preventing soot production.

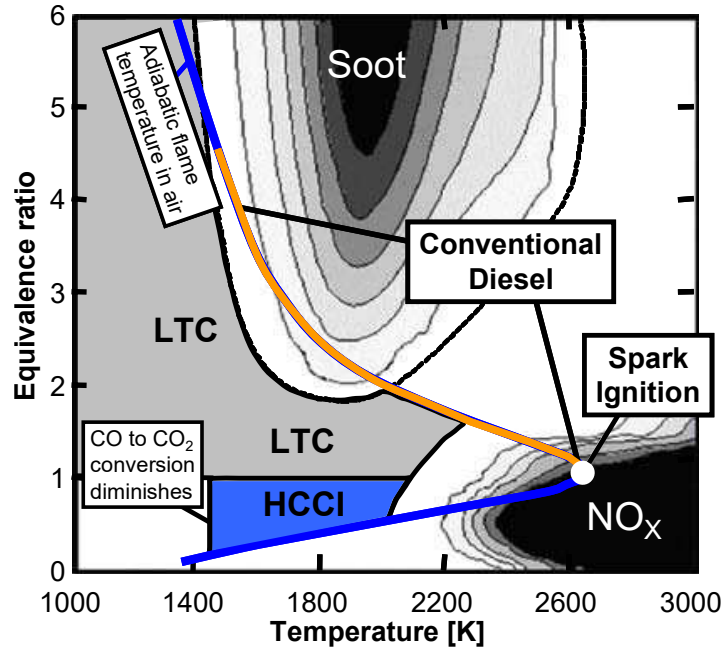


FIGURE 1.6: Kamimoto-Bae diagram of soot and NO formation regions for conventional diesel (CI), LTC diesel, SI and HCCI engines [15]

Kamimoto and Bae illustrated the soot and NO forming region on a temperature/equivalence ratio plot for emission control [16]. In Figure 1.6, we observe that conventional diesel engines emit soot and nitrogen oxides while SI engines only emit NO_x . For low-temperature combustion, and especially HCCI combustion, none of the pollutant formation conditions are met, explaining insignificant emissions. This allows HCCI engines to meet actual stringent emission regulations in terms of NO_x without costly, lean conditions, after-treatment systems used for CI engines such as *Lean NO_x Trap* (LNT) or *Selective Catalytic Reduction* (SCR).

However, HCCI combustion is not flawless. LTC strategies can quench near the cylinder walls resulting in an incomplete combustion inducing carbon monoxides and *Unburned Hydrocarbons*

(UHC) emissions. Methane having 21 times the impact of CO₂ on the greenhouse effect [14], this drawback is significant for natural gas HCCI engines.

CO emission is strongly dependent on the temperature and the oxidation reaction of CO to CO₂ (Equation (1.12)) is the slowest in the oxidation chain. HCCI in-cylinder temperature being typically between 1400 and 1900[K], CO may not totally be oxidised in CO₂. CO conversion diminishes with temperature (Figure 1.6), it is, therefore, more critical for ultra-lean mixtures.



These incomplete combustion products can be treated easily by relatively cheap oxidation catalyst with a conversion efficiency in excess of 90%. Yet, this results in a pure loss of combustion efficiency. Indeed, the intrinsic enthalpy of UHC and CO are lost causing a decrease of the global combustion efficiency to 90-95% compared to almost 100% in CI engines.

1.2.3 Combustion Timing Control

The complexity of HCCI combustion is due to the difficulty of controlling the combustion phasing. The chemical kinetics that governs the auto-ignition of the homogeneous mixture depends on several parameters such as charge pressure and temperature, fuel type, equivalence ratio, wall temperature, residual gas fraction, engine compression ratio, rotational speed, etc. In order to ensure proper combustion timing, these parameters have to be controlled.

Amneus et al. indicate that the charge temperature is the main factor influencing chemical kinetics and that other factors such as the pressure and air-fuel ratio have less impact [17]. Indeed, an increase of 0.6% in intake temperature has the same impact on the auto-ignition timing advance than a 10% richer air-fuel ratio or also an 11% increase of the intake pressure.

The spontaneous combustion occurs when the mixture auto-ignition temperature is surpassed during a longer time than the charge ignition delay. The compression phase increases progressively the charge temperature. Chemical reactions then gradually release heat and reactive radicals, leading to chain branching reactions and auto-ignition of the charge.

Intake charge heating is used to control the ignition timing. The required intake temperature depends on the engine operating conditions and geometrical parameters. The charge composition is also one of the key parameters influencing this temperature. Indeed, high octane number fuels need a higher temperature to auto-ignite and this ignition occurs sooner for higher fuel content. To help the mixture reach its auto-ignition temperature, a higher engine compression ratio should be used. Unfortunately, it is not always sufficient to attain the necessary temperature at the end of the compression stroke, especially with ignition resistant fuels. The intake charge needs to be preheated, even though higher intake temperatures further reduce the power density by decreasing the in-cylinder charge density. This phenomenon is the main drawback of intake heating.

Wang et al. [18] have shown that an increase of the intake temperature advances the *Start of Combustion* (SOC) and reduces the *Duration of Combustion* (DOC) as well as increases the in-cylinder pressure and the *Heat Release Rate* (HRR). Figure 1.7 confirms that high intake temperatures are required for high octane (auto-ignition resistant) fuel combustion such as natural gas. Given that natural gas is also composed of lower octane number hydrocarbons than pure methane, therefore advancing the auto-ignition, pure methane combustion requires even higher intake temperatures.

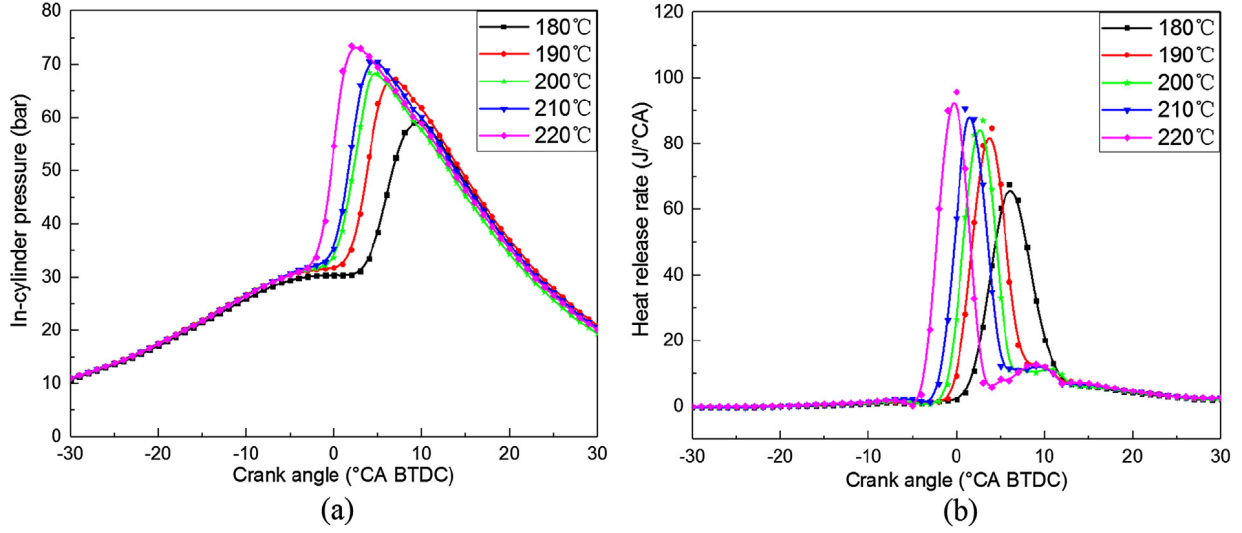


FIGURE 1.7: Impact of T_{in} on in-cylinder pressure (a) and HRR (b). Experiment results with a naturally-aspirated HCCI engine with $CR = 19.5$, $\phi = 0.42$ and NG (89% of CH_4) [18]

The impact of the air-fuel ratio on the start of combustion is usually modest. However, for natural gas HCCI engine, its impact is non-negligible. The reaction rate depends on the mixture fuel content: a rich blend auto-ignites more rapidly than a lean mixture, i.e. at a lower in-cylinder temperature. In the lean mixture region, an increased equivalence ratio (ϕ) has an ignition-promoting effect causing a decrease of the ignition delay. In a running engine, this effect can partly be explained by an increase of its thermal load resulting in a higher temperature at the start of compression for a fixed intake temperature. The SOC is thus advanced as the mixture becomes richer. On the other hand, the DOC is reduced leading to more brutal combustion.

The sensitivity of the SOC to ϕ is engine speed dependant. The equivalence ratio has a bigger impact at low engine speed and this impact decreases as the speed increases, where the intake temperature has a preponderant effect. In brief, the concentration and composition of the mixture alter the whole combustion process by affecting the reactivity of the mixture and its ignition delay.

1.2.4 Narrow Operating Range

Ring and misfire frontier results in a narrow operating range for HCCI combustion.

If this combustion happens too early during the compression stroke (large advance), the pressure and temperature rise rate will be excessive, leading to a thermal production of NO_x and destructive effects on the engine. If, on the contrary, the combustion happens too late during the expansion stroke, the in-cylinder temperature drop could cause bulk quenching and misfire. To extend this operating range while keeping an optimal combustion timing, we can modify it, namely retarding it at high loads and advancing it at low load conditions (Figure 1.8a).

HCCI operating range is commonly expressed in terms of MEP, which express the engine load. For stationary engines, the load is adjusted by the equivalence ratio and the intake temperature. High loads are reached with richer mixtures and lower intake temperatures while engine loads decrease for leaner mixtures and higher intake temperatures (Figure 1.8b). A. Gharehghani observed that the IMEP is mainly influenced by the equivalence ratio and only slightly by the

intake temperature in HCCI operation [19]. That observation was deduced from the almost horizontal iso-IMEP curves of Figure 1.8b.

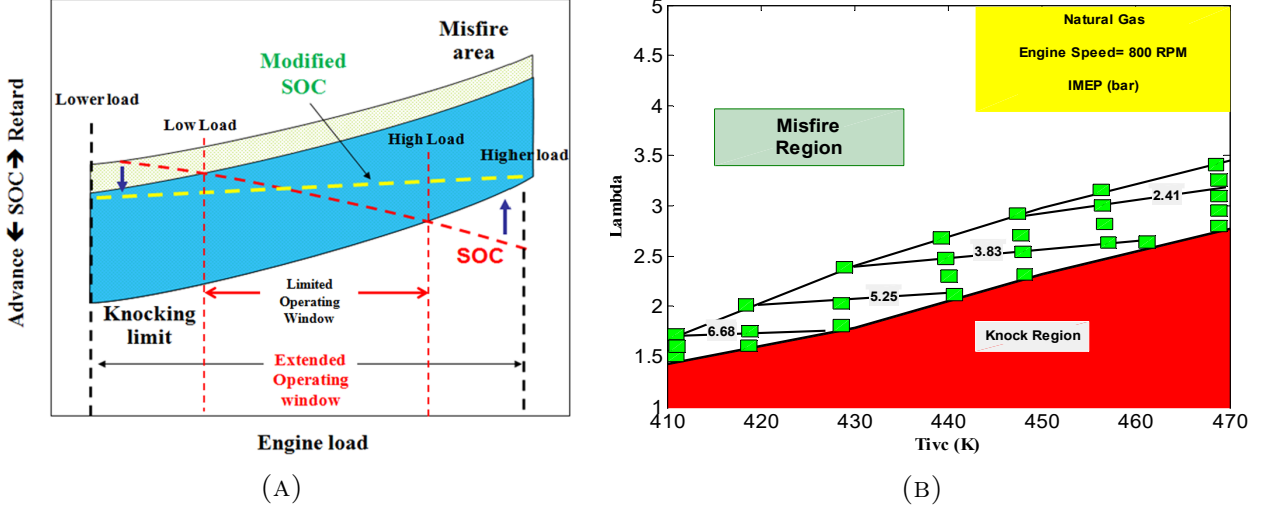


FIGURE 1.8: (A) Extended operating range of HCCI engine by combustion timing modifications. (B) Example of a stationary natural gas HCCI operating range [19].

The air-fuel equivalence ratio, λ , used as y-coordinate in Figure 1.8b is the exact inverse of the fuel-air equivalence ratio, ϕ , normally used in this work. Leaner mixtures are characterised by higher value of λ .

Low Load Limit

At low loads, partial oxidation and higher cycle-to-cycle variations limit the HCCI engine operating range. The SOC is too retarded to sustain combustion and there is a misfire.

The *Coefficient of Variation of IMEP* (COV_{IMEP}) is a measure of the cyclic variability. This factor, expressed in terms of percentages, is the ratio between the standard deviation of IMEP and the mean IMEP over a number of consecutive cycles:

$$COV_{IMEP} = \frac{\sigma_{IMEP}}{IMEP} \cdot 100 \quad (1.13)$$

This measure is obtained experimentally and the misfire limit is taken, depending on the application, as $COV_{IMEP} \leq 5 - 10\%$.

Fuels with lower octane numbers are suitable for low load operations (lower intake temperature and lean mixtures) and will increase the operating range in that region.

High Load Limit

Rapid combustion processes can generate pressure oscillations that result in increased engine noise and engine damage in the worst case.

The cylinder pressure oscillations from HCCI combustion are denoted as *ringing* and pressure wave intensity is characterised by [20]:

$$\text{Ringing Intensity} \approx \frac{1}{2\gamma} \frac{[\beta(\frac{dP}{dt})_{\max}]^2}{P_{\max}} \sqrt{\gamma RT_{\max}} \quad (1.14)$$

where $\gamma = \frac{C_p}{C_v}$ is the ratio of specific heat, β is a tuning parameter (0.05 for light duty HCCI), R is the ideal gas constant, $\left(\frac{dP}{dt}\right)_{\max}$ is the *Maximum Pressure Rise Rate* (MPRR), $P_{\max}$ is the peak cylinder pressure and $\sqrt{\gamma RT_{\max}}$ is the speed of sound.

The Ringing limit is taken as $RI \leq 5 - 6$ [MW/m] and can also be expressed in terms of MPRR limit. Depending on the fuel and air-fuel mixture, the limit on MPRR is 10-15 [bar/CAD] for a naturally aspirated HCCI. Fuels with high octane number, such as methane, expand the operating range to higher loads.

Lean mixtures are used to reduce the MPRR and prevent critical mechanical loadings on the engine block. The air-fuel dilution is the reason for HCCI low power density.

1.3 Oxygen Valorisation and Oxy-combustion

This master thesis aims to investigate the feasibility and the potential benefits of using pure oxygen instead of air as the oxidiser in a homogeneous charge compression ignition engine powered by methane.

The first benefit of this combustion is the simplified composition of the exhaust gases. As represented in the case of an ideal complete oxy-combustion of methane in Equation (1.15), at stoichiometry, the exhaust gases are only composed of carbon dioxide (CO_2) and water (H_2O).



Therefore, capture and storage of carbon dioxide are conceivable through exhaust water condensation, reducing carbon dioxide emissions in the atmosphere. This almost pure flow of carbon dioxide can be used to produce methane from hydrogen through the Sabatier reaction presented in Section 1.1. Integrated into a Power to Gas to Power system using renewable electricity sources, this can result in a net zero-emissions power storage and production cycle. The aforementioned carbon neutral cycle is represented schematically in Figure 1.9. Starting from renewable electricity producing hydrogen through electrolysis, the oxygen created as a by-product can be valorised as the oxidiser for the engine. This pure source of oxygen removes the main energy penalty encountered in oxy-combustion processes at the air separation unit, separating oxygen and nitrogen, which has a typical consumption of $190 \text{ [kWh/t}_{O_2}]$ [21].

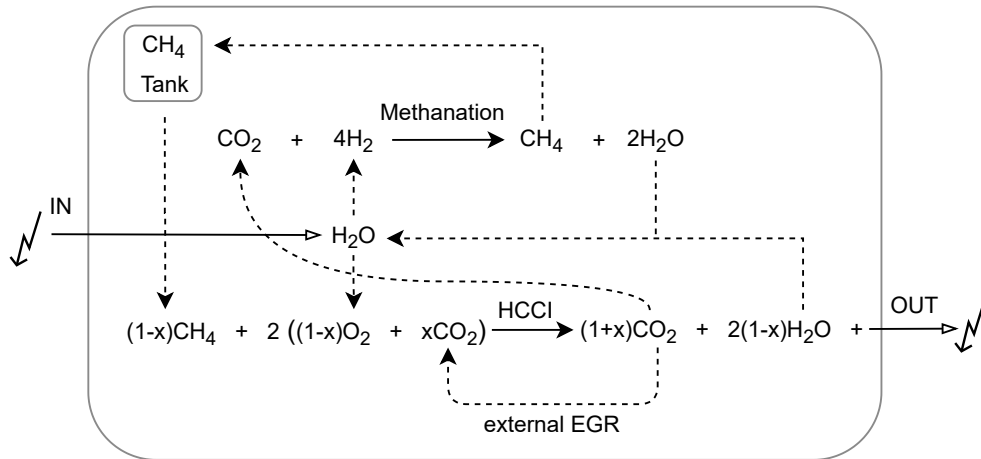


FIGURE 1.9: Oxy-combustion power-to-gas-to-power system with EGR, inspired from [5]

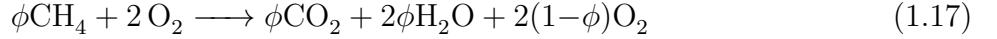
The second benefit of an oxy-combustion is the absence of nitrogen in the combustion. In fact, *nitrogen oxides* (NO_x) are produced in presence of oxygen and nitrogen at high temperature, as explained in Section 1.2.2. Those gases, namely nitric oxide (NO) and nitrogen dioxide (NO_2), contributes to the formation of smog and atmospheric rain, as well as affecting tropospheric ozone [22]. Their absence during the combustion can therefore drastically reduce the after-treatment cost of the exhaust gases. However, in the case of HCCI combustion, this advantage is minor as NO_x emissions are already low.

1.3.1 Oxy-combustion Equivalence Ratio Definition

The complete stoichiometric oxy-combustion reaction of methane is written in Equation (1.15). With that reaction, we define the methane oxy-combustion equivalence ratio as:

$$\phi_{oxy} = \frac{\text{fuel-to-oxidiser ratio}}{(\text{fuel-to-oxidiser ratio})_{st}} = \frac{\frac{n_{\text{CH}_4}}{n_{\text{O}_2}}}{\frac{1}{2}} \quad (1.16)$$

If we include the equivalence ratio in the methane oxy-combustion reaction of Equation (1.15), we get:



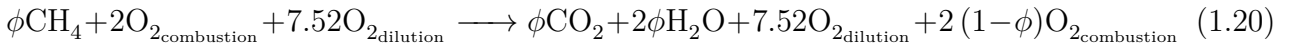
On the other hand, the methane air combustion, simplified by a mix of oxygen and nitrogen, is:



The equivalence ratio of this methane-air combustion is:

$$\phi_{air} = \frac{\text{fuel-to-oxidiser ratio}}{(\text{fuel-to-oxidiser ratio})_{st}} = \frac{\frac{n_{\text{CH}_4}}{n_{\text{air}}}}{\frac{1}{9.52}} \quad (1.19)$$

If we want to express the same molar fraction of methane between air combustion and oxy-combustion, we should distinguish between the oxygen used for dilution of the charge and the one used for the combustion:



Thus, to express the same quantity of methane between air (1.19) and oxy-combustion (1.16) equivalence ratio, a factor has to be used:

$$\phi_{oxy} = \frac{\phi_{air}}{4.76} \quad (1.21)$$

1.3.2 Expected Challenges

Even though oxygen and nitrogen are both diatomic molecules, the heat capacity of oxygen is slightly higher than nitrogen. Consequently, for a maintained fuel content, replacing nitrogen by oxygen should slightly delay the start of combustion. Nonetheless, the increase of mixture reactivity, linked to the increase of the oxygen content, reduces the ignition delay, consequently counteracting the first effect. Moreover, as oxygen is the oxidiser of the combustion, increasing its availability in the combustion chamber while keeping the same amount of fuel will accelerate the fuel oxidation, thus shortening the combustion duration.

Kang et al. have experimented with n-heptane oxy-combustion in HCCI conditions [23], all the figures presented in this section are from their work. To our knowledge, it is the only oxy-combustion comparative study in a HCCI engine up to date. However, n-heptane is a very different fuel from methane, the figures are not to be considered valid in our case and should only be seen as qualitative results. N-heptane is a large paraffinic fuel that exhibits a low-temperature reaction (first rise in the HRR curve). This two-stage combustion is a characteristic of complex fuels. Being a compact and auto-ignition resistant fuel, methane has, on the contrary, single-stage combustion.

The heat release rate curves for a conventional air-combustion (21% O_2) and an oxy-combustion (100% O_2) illustrated in Figure 1.10 present the previously discussed effects. Indeed, the two combustion start approximately at the same time (CA10 at 344.5 [CAD] for the air-combustion and at 345 [CAD] for the oxy-combustion). The HRR curve of the air combustion spreads over a larger crank angle range. The oxy-combustion duration is thus shorter. The two other curves should not be compared, as their energetic content is lower, depicting the use of EGR.

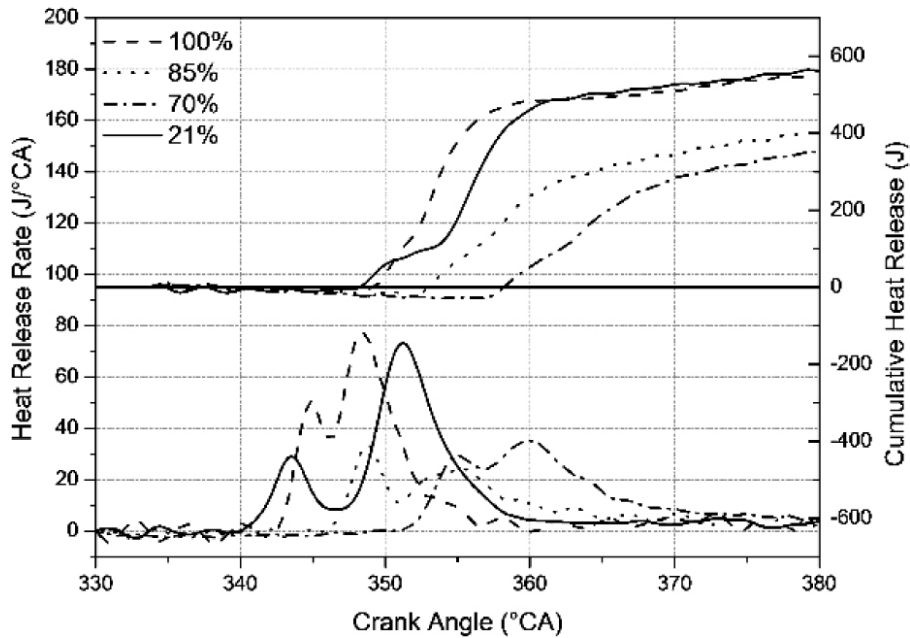


FIGURE 1.10: Heat release rate and cumulative heat release under air (21% O_2), pure oxygen (100% O_2) and a mix of oxygen and carbon dioxide (85% O_2 & 15% CO_2 or 70% O_2 & 30% CO_2) [23].

It appears that the cumulative heat release curves are time-shifted by 5 [CAD] for an unknown reason in Figure 1.10. Based on the CA10 values of Figure 1.11 and on the author's observation that the combustion occurs mainly before the TDC, the heat release rate curve is considered correct.

As Li et al. have shown numerically [24], an increase in the O_2 fraction from 21 to 30% increases drastically the mixture reactivity. This poses both advantages and disadvantages in the case of HCCI methane oxy-combustion.

The main benefit is the possible increase in power density through a reduced required intake temperature to get a start of combustion near the top dead centre. A numerical approximation of the reduced intake temperature is discussed in Section 3.4.2.

Unfortunately, increased reactivity of the mixture constitutes the real challenge of this thesis. The intense combustion observed in HCCI engines, due to the homogeneity of the charge, coupled to the intensified heat release of oxy-combustion, as a result of the increased oxidiser content, limits the admissible fuel loading. The Ringing phenomenon has to be avoided by keeping the MPRR below the threshold discussed in Section 1.2.4.

Therefore, pure oxygen-fuel mixtures should only be used at low equivalence ratios if no damping system is used. Improving power density calls for the use of systems to slow down the combustion such as *Exhaust Gas Recirculation* (EGR) and *Water Direct Injection* (WDI).

Exhaust Gas Recirculation

Introduced in the 1970s to reduce NO_x emission on diesel engines, the EGR uses a fraction of the exhaust gas to be re-injected into the intake manifold. Those non-reactive exhaust gases act as a diluent in the air-fuel mixture, reducing the combustion temperature and NO_x formation. The reduction of oxygen availability slows down the kinetics, thus the combustion rate, and postpones the start of combustion. These effects have been demonstrated experimentally for an oxy-combustion by Kang et al.[23].

The EGR used throughout this thesis is a simplified representation only made up of a pure flow of carbon dioxide instead of real exhaust gases composed of CO_2 , H_2O and unburned species.

The complete oxy-combustion of methane with exhaust gas recirculation is represented in Equation (1.22).



Where x is the volume proportion of CO_2 , from 0 to $1-\phi$, with respect to O_2 . Moreover, as the molar fraction of CH_4 at the intake remains constant, the volume proportion of CO_2 should also not exceed $1 - \frac{2}{9.52} \approx 0.79$. This condition ensures to keep the same equivalence ratio for the combustion between the different EGR rates because only the whole proportion of excess O_2 used for dilution is replaced by CO_2 at this EGR rate.

N_2 and CO_2 are both inert gases in the chamber, they inhibit the combustion process. Removing the nitrogen to perform an oxy-combustion should lead to more abrupt combustion. The usage of CO_2 can greatly counteract this effect. CO_2 being a triatomic molecule, its heat capacity is much larger than N_2 . Lower proportions than typical nitrogen concentration in the air are thus used.

Compared to pure oxygen conditions, the heat capacity in the combustion chamber with EGR is therefore increased which causes a lower bulk pressure and temperature during the compression stroke. The decreased temperature in the cylinder also postpones the peak combustion pressure, as observed in Figure 1.11.

Figure 1.11 also presents the combustion duration under air and O_2 - CO_2 mixtures. As expected, the shorter combustion under pure O_2 compared to air combustion is observed as well as the combustion inhibition properties of CO_2 , prolonging the combustion duration.

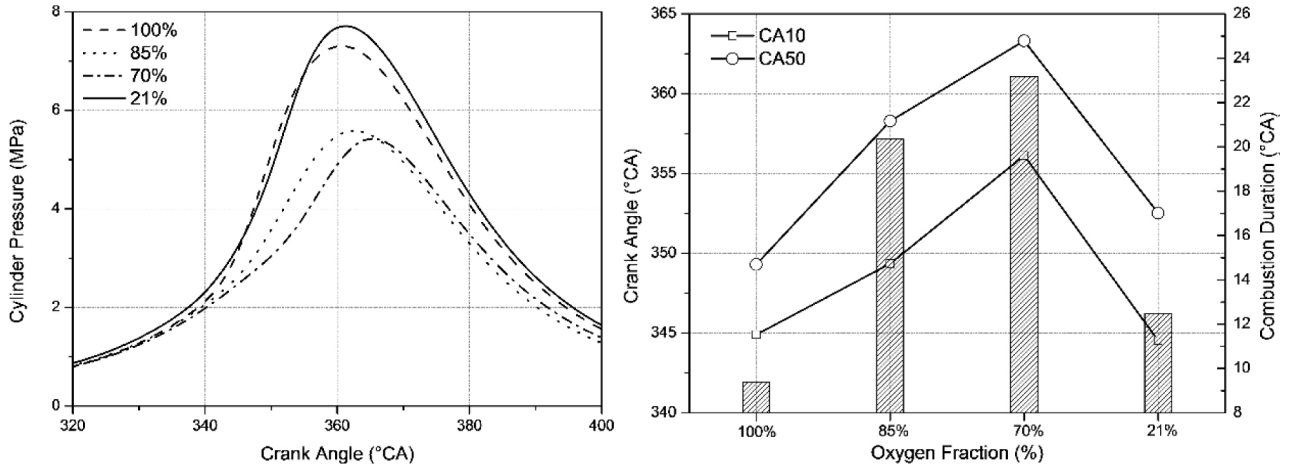


FIGURE 1.11: Pressure and combustion duration under air (21% O_2), pure oxygen (100% O_2) and a mix of oxygen and carbon dioxide (85% O_2 & 15% CO_2 or 70% O_2 & 30% CO_2) [23].

In the context of oxy-combustion, the combustion damping ability of EGR is of prime importance. It allows increasing the fuel content in the mixture by reducing the maximum pressure rise rate. However, the maximum usable CO_2 fraction is also limited by the coefficient of variation in IMEP (COV_{IMEP}). This standardised measure of dispersion helps to quantify the occurrence of misfires, as explained in Section 1.2.4.

For n-heptane experiment, under pure oxygen or air content, the COV_{IMEP} remains under 5% but with 30% of CO_2 , this value exceeds 10%, which is unstable for an ICE application. The COV_{IMEP} value depends on a myriad of parameters but a decrease of combustion stability is to be expected with EGR.

As shown in Figure 1.12, the IMEP difference between pure oxygen and air intake is very small. The IMEP is greatly reduced with increasing EGR rates. This outcome highlights the impact of EGR on the indicated efficiency. Nevertheless, higher fuel contents are allowed with EGR, counteracting this decrease.

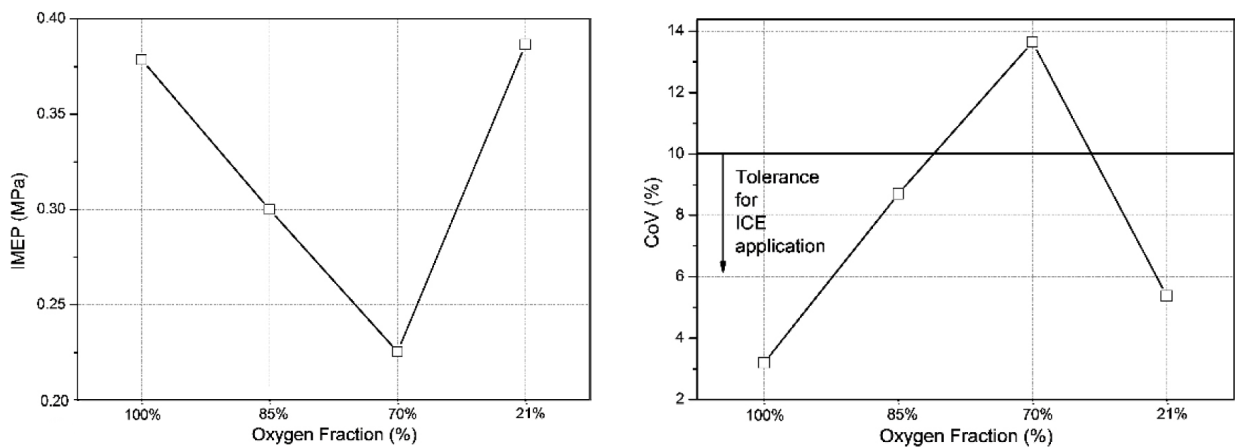


FIGURE 1.12: IMEP and COV_{IMEP} under air (21% O_2), pure oxygen (100% O_2) and a mix of oxygen and carbon dioxide (85% O_2 & 15% CO_2 or 70% O_2 & 30% CO_2), adapted from [23].

Water Direct Injection

In order to reduce the combustion brutality, namely the pressure rise rate, the combustion duration has to be extended. Water direct injection is an alternative way to prolong the combustion by increasing the thermal stratification of the charge. The local evaporation of injected water spray can create thermal gradients inside the cylinder. In such a way, a wider temperature distribution is obtained in the combustion chamber, causing the charge to auto-ignite locally at different moments. The combustion duration is therefore expanded. As the water spray is injected during the late part of the compression stroke, WDI does not require a considerable increase in the intake temperature to maintain the optimum combustion timing, unlike EGR. This conclusion allows for better cycle-to-cycle combustion control and improved system thermal efficiency.

Colette and Gatin investigated the impact of WDI on hydrogen HCCI combustion in their master's thesis [9]. They have demonstrated experimentally that WDI raised the ringing limit, allowing for higher fuel contents and load increases. Rising concurrently the injected water mass and the equivalence ratio, they reached a net IMEP of 4.3 [bar] at $\phi=0.5$.

Considering HCCI oxy-combustion, water direct injection could help reduce the destructive ringing caused by the charge high reactivity. Kang et al. studied the effect of WDI on HCCI cycle performance to avoid the ringing detected under pure O_2 content[23].

As illustrated in Figure 1.13, using adapted WDI strategy, the mild knock has been suppressed. Besides, Kang detected no deterioration on engine performances as the injection of water did not influence significantly the in-cylinder pressure trace compared to the dry cycle.

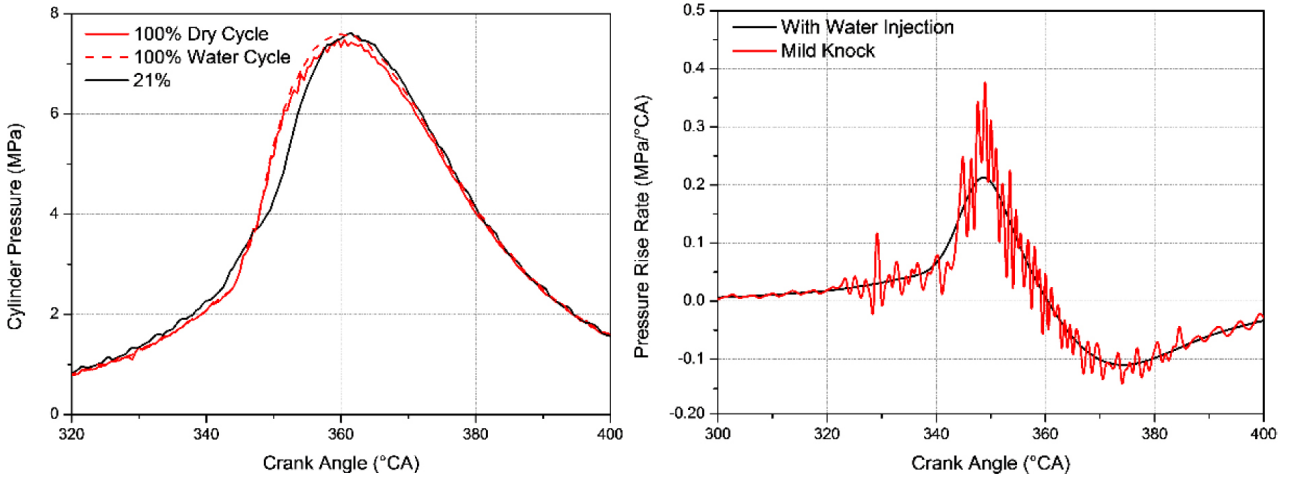


FIGURE 1.13: Comparison of cylinder pressure evolution and pressure rise rate with and without WDI, adapted from [23]

However, WDI is extremely challenging to model because it requires multi-zone numerical simulations [25]. It will thus not be instigated in our work as it is out of the scope of this thesis. Nevertheless, WDI potential and the possible synergies with EGR provides an interesting outlook for future experimental investigations.

Chapter 2

Experimental Setup

In this Chapter, the UCLouvain HCCI research engine setup is described briefly. The previous modifications are discussed whereas the ones needed to run an oxy-combustion experimental campaign are explained. Even though this thesis ended up containing mostly numerical investigations, the specifications of the engine are required to faithfully represent the combustion chamber. Finally, the procedure to estimate the heat release rate and the wall heat losses is explained.

2.1 Engine Specifications

The engine of the UCLouvain HCCI test bench is the Yanmar L100V. Originally, this engine was a four-stroke CI engine designed for stationary industrial use. Its simple configuration, being an air-cooled single-cylinder, offered the perfect base for modifications.

The actual engine specifications are listed in Table 2.1 and the original ones are available in Appendix A.2.

UCLouvain HCCI research engine	
Engine type	Air-cooled Four-stroke Single-cylinder
Displacement volume, V_d	436 [cm ³]
Geometric compression ratio, τ	23.0 : 1
Effective compression ratio, τ_{eff}	21.65 : 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 closure, IVC	-127 [CAD]
Exhaust valve opening, EVO	127 [CAD]

TABLE 2.1: HCCI engine specifications

A WEG three-phase induction motor/generator (W22 IE2, 55 kW) is coupled to the Yanmar engine. This electric machine is used as a motor during the engine start-up phase and then as a generator inducing a brake torque all along the stabilised operation. For this purpose, a Mitsubishi four-quadrant frequency variator (FR-A741-55k) is used to impose a constant rotational speed of 1500 RPM.

The Yanmar L100V was firstly converted to a HCCI engine by S.Bhaduri in the framework of his PhD thesis [26]. To study syngas HCCI combustion, a modified low turbulence shallow bowl piston was used, reducing the compression ratio to 12. The flat cylinder head was machined to include a piezoelectric pressure transducer and the diesel injector was replaced by a spark plug whose only purpose is to seal the cylinder head. The apparent engine cooling fan was equipped with a variable opening cover to control the cylinder walls temperature manually. The Syngas being simulated as a complex mixture of pure gases, six *Mass Flow Controllers* (MFC) were installed at the intake side of the test bench.

M.Pochet later modified the engine compression ratio for his research work on ammonia-hydrogen blends HCCI combustion [5]. The piston bowl has been filled by welding to reach an effective compression ratio of 21.9:1, reducing the required intake temperature of the auto-ignition resistant ammonia. The result is a flat piston crown giving a combustion chamber shaped like a perfect cylinder together with the flat cylinder head. Simple combustion chambers are well suited because except for the thermal stratification, HCCI combustion is essentially independent of turbulence [17]. Moreover, a flat piston minimises crevices volume and thus unburned fuel for a given stroke-to-bore ratio and compression ratio. The intake system has also been adapted for ammonia-hydrogen blends along with simulated EGR. Following successive experiments with ammonia combustion, a small hole was created leading to a decrease of the effective engine compression ratio to 21.65:1.

Finally, A.Gatin and T.Colette have modified the cylinder head to host an injector to study the effect of *Water Direct Injection* (WDI) [9]. This has been done on a second Yanmar L100V cylinder head, the test bench can thus be used with or without the WDI system.

2.2 Test Bench Modifications

The IMMC laboratory of UCLouvain has recently been updated with the addition of a protective room enclosing the three most critical engine test benches. This room is called a *casemate* in French and protects against toxic gases, noise pollution and risks of mechanical parts breakage. To allow the construction work, the HCCI test bench has been dismantled and stored in pieces. One objective of our work was to coordinate the reinstallation and modifications of the test bench. For that purpose, we realised a risk analysis and a preliminary operating manual.

The operating principle and nearly all the components of the actualised test bench are identical to what is presented in previous works. In this section, we will only focus on the modifications required to perform oxy-combustion experiments safely.

An overview of the test bench described in this section is presented in Figure 2.1

The *Piping and Instrumentation Diagram* (P&ID) shown in Appendix A.3 represents all the elements constituting the bench and offers a more detailed view of the experimental setup.

The engine intake charge is a mixture of pure gases stored in gas cylinders, except the air that is coming from the compressed air network of the IMMC laboratory.

The compression ratio selection in M.Pochet thesis was motivated by the desire of having a multi-fuel capable HCCI engine test bench. The geometric compression ratio of 23:1 is a compromise between a high τ value needed for auto-ignition resistant fuels, such as methane or ammonia, and lower τ value to prevent hydrogen combustion from ringing. Considering the test bench maximal intake preheating temperature ($T_{in,max} = 240[^\circ C]$), a pure ammonia HCCI combustion was not possible. Besides, an increase in intake temperature reduces significantly the IMEP due to the decrease of the charge density. Furthermore, high intake temperatures increase heat losses and might lead to TDC temperatures exceeding the LTC zone threshold, therefore promoting thermal-NO_x production.

To reduce the required intake temperature for pure methane combustion and increase the IMEP and thus η_{ind} , we have considered further increasing the engine compression ratio. This change would also allow for higher EGR rates decreasing the critical MPRR associated with oxy-combustion. Indeed, the more EGR rate used, the higher the required intake temperature, therefore leading to the maximum intake temperature the bench can provide. However, due to the Yanmar L100V low stroke-to-bore ratio ($S/B = 0.87$), a higher compression ratio would induce a shorter clearance between the valves and the piston. To avoid contact between the piston and the exhaust valve, the minimum clearance is 3.2 mm. The geometric compression ratio of 23:1 gives a clearance of 3.5 mm and is thus the maximal compression ratio attainable [5]. Other approaches to reduce the necessary intake temperature such as fuel blending will be investigated in Section 3.4.4.

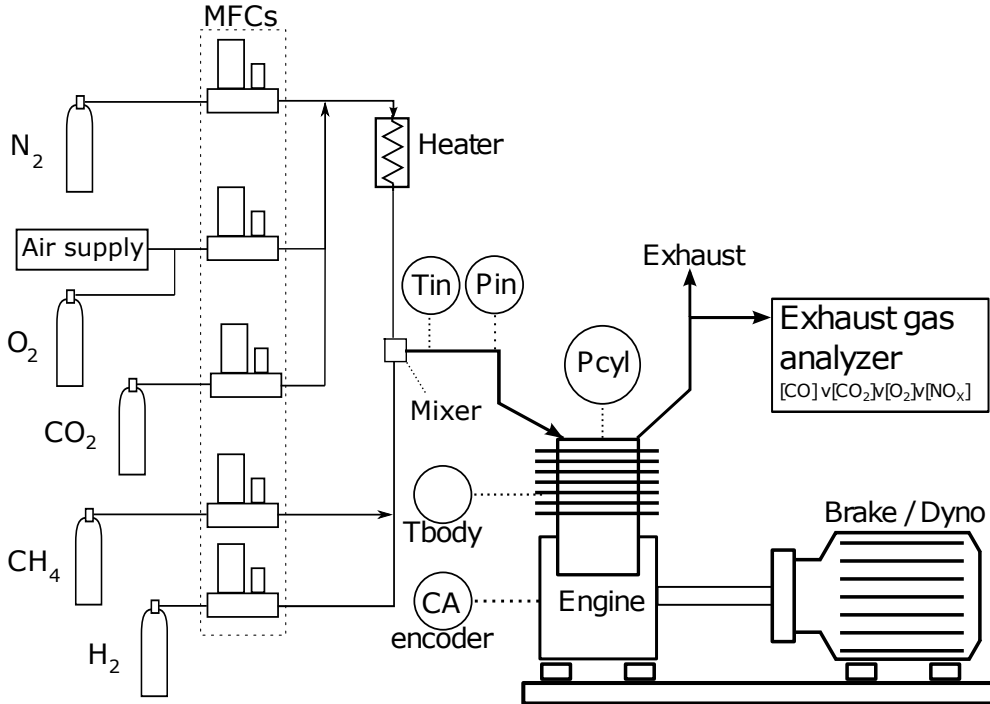


FIGURE 2.1: Scheme of the HCCI test bench adapted from [26]

The main modification required on the test bench compared to last year's thesis [9] and M.Pochet's PhD thesis [5] is the intake system. Indeed, the fuels and required mass flows being different, the fuel and oxidiser control system had to be modified as shown in Figure 2.1. To run conventional air-combustion and oxy-combustion experiments, we need air as well as a pure

oxygen intake source. A carbon dioxide admission has been added to simulate dry EGR while a nitrogen source is used as an inert gas to purge the system.

In future works, nitrogen could also be used together with pure oxygen to study HCCI combustion with oxygen-rich oxidiser blends. Eventually, on the fuels part of the intake system, a methane admission has been added and the hydrogen one has been conserved.

To accurately select the mixture composition, all species mass flows are controlled by Brooks SLA585X Mass Flow Controller. The measuring part of a thermal MFC is composed of a laminar flow element from which a fraction of the flow is bypassed to a thermal mass flow sensor. The sensor consists of a heater surrounded by two temperature probes. The gas stream is warmed up and the mass flow is computed from the difference of temperature measured by the upstream and downstream probes knowing the gas specific heat. With no flow, the temperature difference will be zero and this difference is directly proportional to the mass flow. The measured flow is compared to the required value by a microprocessor and a PID controller actuates an electromagnetic valve accordingly. A detailed view of the internal elements of a thermal MFC is presented in Figure 2.2. These instruments measure and control the mass flow accurately at high frequency. They can provide steady and extremely accurate required flow.

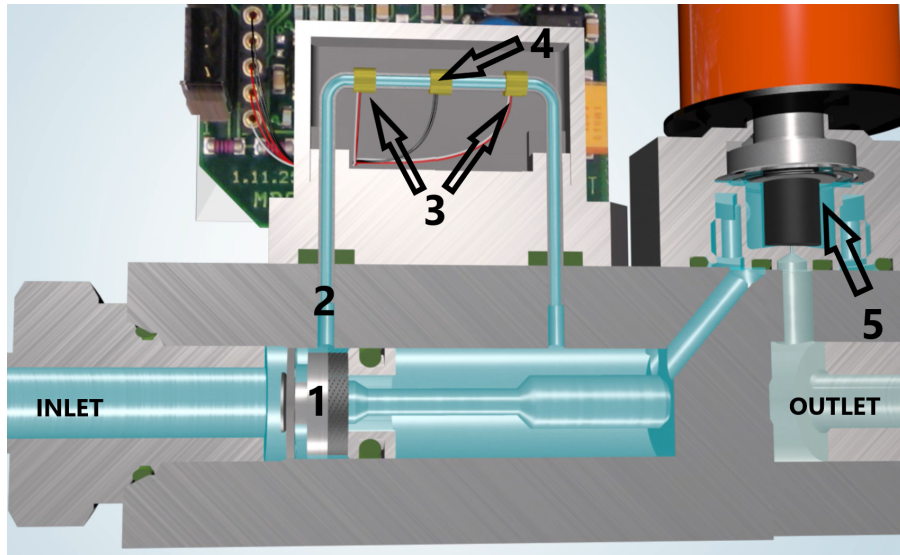


FIGURE 2.2: cross-sectional view of a thermal MFC: (1) Laminar flow element, (2) flow by-pass, (3) temperature probes, (4) heater, (5) electromagnetic valve ¹

These MFCs are commonly built and calibrated for use with nitrogen on a certain mass flow range. However, the laminar flow element allows modelling the instrument for any other gas using this simple formula:

$$\text{New mass flow} = \text{Actual mass flow} \times \frac{\text{new gas factor}}{\text{actual gas factor}} \quad (2.1)$$

The gas factors are given by the MFC manufacturer (see Appendix A.1). Nitrogen being the reference gas, it has a gas factor of 1.

¹<https://www.bronkhorst.com/en-us/service-support/technologies/thermal-mass-flow-sensor-for-gases-bypass-principle/>

Provided that its mass flow range is adequate and that its seal material is compatible, a MFC can be converted to work with a different gas. We defined the maximum required mass flow of every species considering limiting cases using the 0D model described in Chapter 3. Luckily, a compatible MFC for every gas has been found in the stock of the IMMC laboratory.

The MFC used for the compressed air can be used for the pure oxygen intake. The experimental campaign to compare the two types of combustion should thus be separated into two parts, firstly air-combustion and then oxy-combustion. Before the oxy-combustion experiments, the MFC and the entire pipe network must be dry-cleaned of any greases to avoid undesired combustion. Indeed, pure oxygen can violently oxidise organic matter including grease residues.

Additional security modifications are required due to the high reactivity of oxygen-rich mixtures. In an effort to reduce the volume between the engine admission and the two intake line check valves, the 10 litres surge drum has to be bypassed. Its role was to ensure a uniform temperature and good mixing of the fuel-oxidiser blend. However, a gas/gas mixer already ensures the homogeneous blend and the bypass highly reduces the severity of a potential explosion in the intake pipe. To further reduce this risk, a smaller, temperature resistant, safety valve is fitted in the intake pipe to prevent it from exploding. This safety valve is set at 2 [barg] to evacuate the gases in the event of a sudden pressure rise caused by ignition of the intake mixture.

Originally, a dilution cone was fitted to the exhaust line after the exhaust analyser. The objective of this piece was to dilute the exhaust gases using the Venturi effect to reduce the probability of exhaust post-combustion. However, the IMMC lab technicians criticised its use because of exhaust leaks during long-duration experiments. Consequently, the cone should be deleted for the exhaust to flow directly in the smoke extraction system through a flexible pipe. The extraction system puts the exhaust in depression thanks to its draught. If necessary, dilution can be obtained by an opening in the extraction pipe upstream of the HCCI test bench. That way, the exhaust system is airtight and secure.

We also noticed that the variable opening cover of the engine cooling fan comported a risk of serious wounds. Indeed, it is manually operated while the engine runs to adjust the wall temperature. A protective mesh should be put over the cooling air intake to avoid hand contact with rotating cooling blades. Additionally, the strict respect of the ATEX (Explosive Atmosphere) zones around potential leakage areas (such as a gas bottle connector, safety valves, etc.) is mandatory.

All the preventive measures to restrain accidents probabilities are detailed in the risk analysis documents. The main risk analysis chart, written in French due to legislation, is available in Appendix A.4.

2.3 Heat Release Computation

In this section, the procedure to derive the heat release rate from the in-cylinder pressure trace is explained. Between the *Intake Valve Closing* (IVC) and the *Exhaust Valve Opening* (EVO), the cylinder can be considered as a closed system by neglecting the flow through crevices and piston rings. The first law of thermodynamics for a closed system can thus be written for that crank angle window as:

$$\Delta U = Q + W \quad (2.2)$$

With ΔU the variation of internal energy, Q and W the heat energy and the work received by the charge from its environment respectively. The combustion heat is included in the term Q .

Differentiating this first law with respect to the crank angle θ , we get:

$$nc_v \frac{dT}{d\theta} = \frac{dQ}{d\theta} - p \frac{dV}{d\theta} \quad (2.3)$$

The perfect gas equation $pV = nRT$ can be written in its differential form with respect to θ :

$$p \frac{dV}{d\theta} + V \frac{dp}{d\theta} = nR \frac{dT}{d\theta} \quad (2.4)$$

Injecting Equation (2.4) into Equation (2.3), the *Apparent Heat Release Rate* (AHRR) equation can be derived:

$$\frac{dQ}{d\theta} = p \frac{dV}{d\theta} + \frac{c_v}{R} \left(p \frac{dV}{d\theta} + V \frac{dp}{d\theta} \right) \quad (2.5)$$

$$= \left(1 + \frac{c_v}{R} \right) p \frac{dV}{d\theta} + \frac{c_v}{R} V \frac{dp}{d\theta} \quad (2.6)$$

Knowing the ratio of specific heat $\gamma = \frac{c_p}{c_v}$ and Mayer's relation $R = c_p - c_v$:

$$\frac{dQ}{d\theta} = \frac{\gamma}{\gamma - 1} p \frac{dV}{d\theta} + \frac{1}{\gamma - 1} V \frac{dp}{d\theta} \quad (2.7)$$

In the AHRR equation, Q is the total heat exchange between the charge and the environment. From now on, we will call it Q_{net} . This Q_{net} is composed of two terms: the heat released during the combustion (Q_{gross}) and the heat lost through the cylinder walls (Q_{loss}):

$$Q_{net} = Q_{gross} - Q_{loss} \quad (2.8)$$

The AHRR can thus be rewritten isolating the combustion heat release to finally obtain the *Heat Release Rate* (HRR or RoHR for *Rate of Heat Release*) equation:

$$\frac{dQ_{gross}}{d\theta} = \frac{\gamma}{\gamma - 1} p \frac{dV}{d\theta} + \frac{1}{\gamma - 1} V \frac{dp}{d\theta} + \frac{dQ_{loss}}{d\theta} \quad (2.9)$$

The cumulative heat release is the result of the integration of Equation (2.9) over the combustion crank window (from -10 [CAD] to 10 [CAD] aTDC in Figure 2.3). This value indicates the total heat released from the combustion as a function of the angular position of the crankshaft θ .

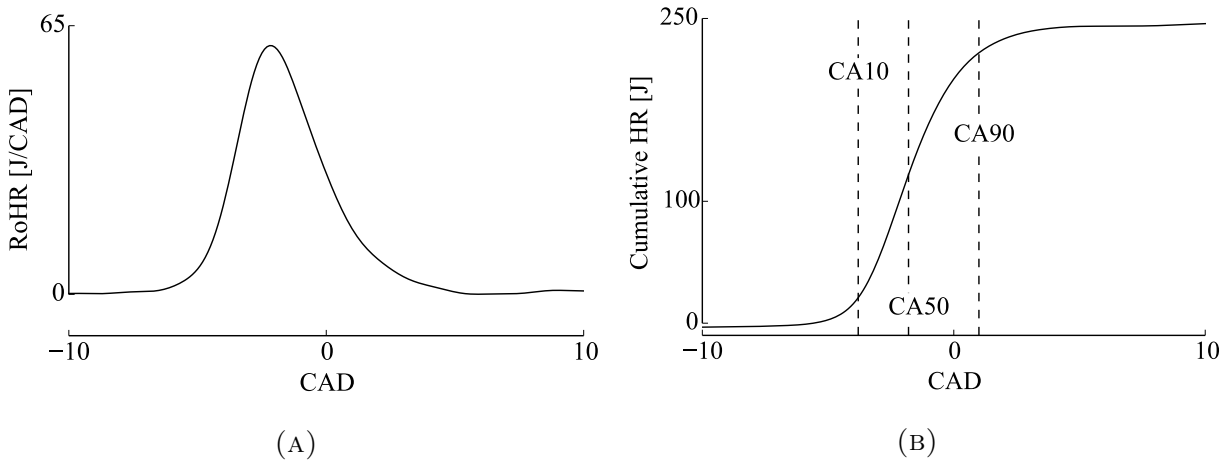


FIGURE 2.3: A typical HCCI combustion HRR (A) and its cumulative $Q_{gross}(\theta)$ (B) [26]

The CA_X parameters, commonly used to describe combustion events in ICE, correspond to the angular position at which $x\%$ of the total heat has been released by the charge combustion, i.e. at which $x\%$ of the fuel has been burned. The heat released at CA_X is:

$$Q_X = \frac{x}{100}(Q_{gross\ max} - Q_{gross\ min}) \quad (2.10)$$

In this thesis, the SOC will be characterised by CA10, the combustion midpoint by CA50 and the DOC by $CA90 - CA10$.

2.3.1 Geometrical Parameters

By convention, the crank angle degree θ is set as zero at the compression TDC. For a four-stroke cycle, the CAD window ranges from -180[CAD] to 540[CAD] with -180 [CAD] indicating the start of the compression stroke, i.e. piston at BDC.

The knowledge of the intake valve closing and exhaust valve opening also is of prime importance. Indeed, the cylinder is a closed system between these two valve timings, the total mass can be considered constant. The delayed IVC together with blow-by and immeasurable volume imperfections (piston ring crevices, valve-seat and piston crown deflection, etc.) result in a reduced in-cylinder effective compression. This real compression is characterised by the engine effective compression ratio which is by definition smaller than the geometrical one. The τ_{eff} is found during experimental data post-processing and an effective IVC can be computed leading to the definition $\tau_{eff} = \frac{V_{IVCeff}}{V_{TDCeff}}$. For the UCLouvain engine, the effective IVC has been proved to be at -152 [CAD] for a simplified intake pressure of 1[bar] [5]. This value is used in the 0D model but, to improve the accuracy of the results with the 3D model, the effective IVC has been determined to be at -146 [CAD] for an intake pressure of 1.025[bar].

Other valve timings such as *Intake Valve Opening* (IVO) and *Exhaust Valve Closing* (EVC) are also marked down in Figure 2.4.

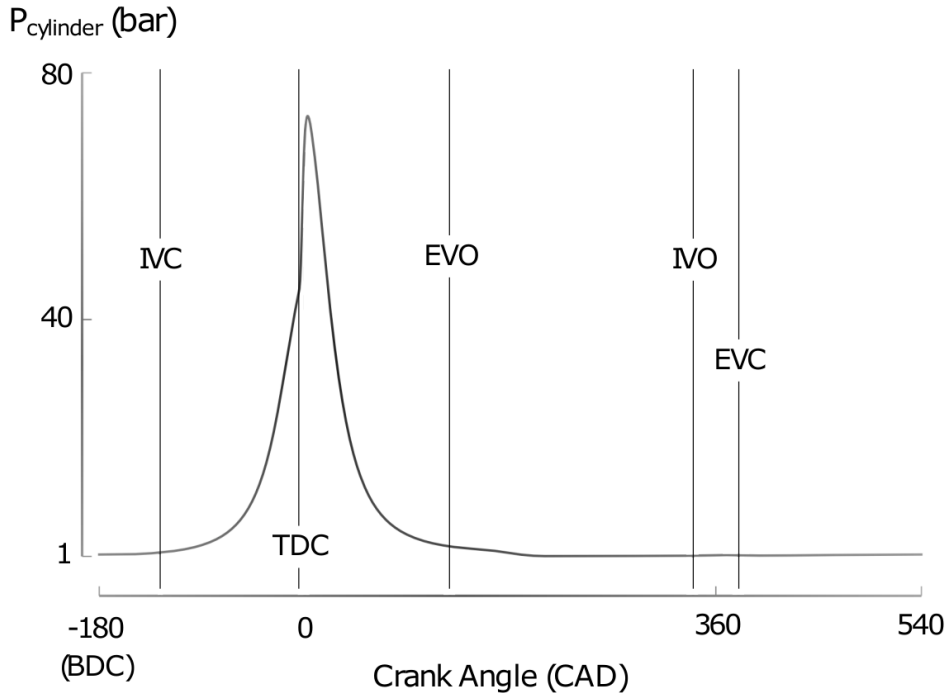


FIGURE 2.4: A typical HCCI in-cylinder pressure curve as a function of the CAD [5]

The computation of the heat release rate from the in-cylinder pressure requires the instantaneous cylinder volume and its derivative. These values can be derived from the crank-slider mechanism of the engine (without wrist pin offset):

$$V(\theta) = \frac{V_d}{\tau - 1} + \frac{V_d}{2} \left(\frac{L}{r} + 1 - \cos(\theta) - \sqrt{\left(\frac{L}{r}\right)^2 - \sin^2(\theta)} \right) \quad (2.11)$$

$$\frac{dV}{d\theta} = \frac{V_d \sin \theta}{2} \left(1 + \frac{\cos \theta}{\sqrt{\left(\frac{L}{r}\right)^2 - \sin^2 \theta}} \right) \quad (2.12)$$

Using the engine geometrical parameters such as L, the length of the connecting rod and r, the crankshaft radius.

2.3.2 Heat Losses Estimation

The wall heat losses have to be determined to compute the HRR. These heat losses impact HCCI ignition timing and burning rate so it is critical to evaluate them accurately. In the literature, the heat transfers from the bulk gas to the combustion chamber walls are generally assumed as purely convective. Particles cause radiating heat transfer, so this hypothesis is only valid for low soot emissions combustion, which is the case of HCCI combustion. The wall heat flux can be estimated using Newton's law of convective heat transfer:

$$\frac{dQ_{\text{loss}}}{dt} = h \cdot A \cdot (T - T_{\text{wall}}) \quad [W] \quad (2.13)$$

$$\frac{dQ_{\text{loss}}}{d\theta} = h \cdot A \cdot (T - T_{\text{wall}}) \cdot \frac{1}{\omega} \quad [J/CAD] \quad (2.14)$$

The term A is the total mixture-wall exchange surface in [m²]. It is composed of the piston and cylinder head constant areas plus the liner lateral area that varies with the angular position of the crankshaft. Thereby, we assume a uniform temperature over the combustion chamber walls, although the exhaust valves and piston are hotter in reality. The multiple assumptions are absorbed by the definition of an apparent heat transfer coefficient. This method has been used in the 0D model described in Chapter 3 but not the 3D axisymmetric model, as an approximation of the wall heat losses was not required.

T and T_{wall} are the charge and combustion chamber wall temperatures in [K] respectively and ω is the angular velocity of the engine considered in [CAD/s].

The last term to determine is Newton convective heat transfer coefficient h in $\left[\frac{W}{m^2 K}\right]$. The determination of precise correlations for this coefficient is very challenging and constitutes a research field on its own. All model correlations are derived from convective heat transfer correlations for simple geometries. Models commonly used to describe the heat transfer coefficient in SI and CI engines like Woschni, Annand and Hohenberg have been compared by Soyhan et al. [27]. Without any modification to their original correlation except for the scaling factors, the validity study concludes that Hohenberg correlation gives the best agreement with the HCCI experimental data.

$$h_{\text{Hohenberg}} = \alpha_{\text{scaling}} V^{-0.06} p^{0.8} T^{-0.4} (S_p + 1.4)^{0.8} \quad (2.15)$$

With V the cylinder volume in [m³] used to define a characteristic length, p the in-cylinder pressure in [bar], T the charge temperature in [K] and S_p the mean piston speed in [m/s]

determined by $S_p = 2 \cdot \text{Stroke} \cdot \text{RPM}/60$. All of these parameters are instantaneous except the mean piston speed.

The value of the correlation scaling factor is 130 for SI and CI engine. To obtain more satisfactory results, α_{scaling} requires a recalibration based on experimental data for every working point (engine geometry and speed, temperatures, energetic content, fuel, etc.).

Later studies by Broekaert et al. compared the above-mentioned models including also the Chang model (based on Woschni) and the Hensel model (based on Annand) developed especially to suit HCCI operations [28, 29]. These studies have demonstrated that none of the discussed models predict accurately the heat transfer without calibration of their scaling factor. After calibration, non-Woschni-based models can predict the heat flux for one engine operating point. However, they all over-evaluate the heat flux during the expansion phase, leading to an overestimation of the total heat losses. Currently, available models capture the effect of the compression ratio and engine speed on the wall heat transfer but not the inlet temperature and fuel type or mass. This requires them to be recalibrated for each operating point to satisfactorily predict the heat flux. Broekaert et al. concluded by saying: "*existing models lack some parameters that have a significant influence on the heat transfer during HCCI combustion*".

Considering its ease of use and relatively good performances, the calibrated Hohenberg correlation is used in this thesis to describe the convection coefficient, similarly to what was done in M.Pochet PhD thesis [5].

Chapter 3

0D Numerical Simulations

To determine the right intake conditions for different mixtures, a HCCI single-zone model was used. The main goal of this model is to accurately predict the auto-ignition timing (CA10) of a chosen fuel-oxidiser mix for selected pressure and temperature intake conditions.

Indeed, the initial goal of our thesis was the experimental characterisation of methane and methane-hydrogen blends combustion and oxy-combustion, aiming to observe the potential of pure oxygen combustion. As preliminary calculations, we needed to determine accurately a suitable set of intake conditions such as equivalence ratio, intake temperature as well as EGR rate to obtain an auto-ignition near the TDC within the engine operating range.

Considering the number of configurations to assess, the *0-Dimensional* (0D) approach was selected on account of its simplicity leading to short computational time. Moreover, a single-zone model suits the HCCI combustion given the quasi-simultaneous auto-ignition of the homogeneous charge. The absence of high-temperature gradient due to flame propagation or diffusion phenomena along with the fact that fluid dynamic effects, i.e. turbulence, have a low impact on HCCI auto-ignition also play in favour of our model.

The 0D model used originates from M.Pochet PhD thesis [5] and runs using the open-source, C++ based, OpenFOAM-3.0.1 toolbox. OpenFOAM has a built-in CHEMKIN package solving the chemical kinetics using detailed combustion mechanisms. With the thermodynamic conditions (temperature and pressure) and the local mixture composition as inputs, CHEMKIN computes the consumption/production of every chemical species involved in the combustion mechanism based on the reaction rate coefficients. The package thus allows computing the combustion heat release $Q_{\text{gross}}(t)$ and the species molar evolution $n_i(t)$ at each time step.

The chemical kinetic mechanism selected to model methane and hydrogen combustion in this present work is AramcoMech 1.3 [30]. It provides kinetic, thermochemical and transport properties in the Chemkin format for C1-C4 based hydrocarbons and oxygenated fuels. It has been validated against experimental measurements over a wide range of conditions. And notably for HCCI-like fuel-air ignition in a shock tube and rapid compression machine: low equivalence ratio ($0.06 \leq \phi \leq 1$), high pressure ($30 \leq p \leq 260$ [bar]) and low temperature ($833 \leq T \leq 2500$ [K]). However it has not been validated for oxygen-rich mixture that characterises oxy-combustion. Furthermore, the mechanism contains reactions explicitly defined for inert gases which act as third body colliders. A very small concentration of argon (≈ 1 ppb) should be added to the studied mixture [30].

3.1 Model Derivation

The model base principle is to compute the thermodynamic evolution of the charge for different intake temperatures. Starting from the intake conditions specified by the user such as the temperature, the pressure as well as the molar fractions of the different species, the model computes the evolution inside the engine over a defined simulation CAD interval. Once all the conditions have been computed, the starting temperature is increased by 1 Kelvin and a new combustion is computed. This iterative process continues until one of the two threshold conditions is reached. Either the computed CA50 happens before -1.5[CAD] or the difference between the actual and first iteration temperature is greater than 100[K].

This single-zone model considers the whole combustion chamber as one cell volume, V , thus with uniform pressure and temperature fields. The piston motion is imposed in OpenFOAM taking into account all the geometrical parameters of the YANMAR experimental HCCI engine. The rotational speed is fixed at 1500 RPM as our interest lies in stationary electricity generation. From this piston motion, the instantaneous cylinder volume, $V(t)$, can be computed at each time step from Equation (2.11), knowing the corresponding crank angle.

The model is based on the first law of thermodynamics for a closed system (Equation (2.2)). The single-zone model assumes a closed system throughout the simulation and does not consider residual gases inside the cylinder.

To obtain Equation (3.1), resolved at each time step by the chemistry solver of OpenFOAM, the fuel-oxidiser mixture is assumed as an ideal gas and the net heat release is separated in two parts: $Q_{\text{net}} = Q_{\text{gross}} - Q_{\text{loss}}$.

$$dU = n c_v dT = \partial Q_{\text{gross}} - \partial Q_{\text{loss}} - p dV \quad (3.1)$$

As previously mentioned, the built-in chemistry solver reads the provided chemical reaction mechanism files and computes Q_{gross} as well as the evolution of the moles of each species trapped in the cylinder $n_i(t)$. This algorithm is made at each time step from the instantaneous thermodynamic conditions.

The wall heat losses, Q_{loss} , are approximated using Newton's convective heat transfer law, as in Section 2.3:

$$\partial Q_{\text{loss}} = h A (T - T_{\text{wall}}) dT \quad (3.2)$$

With the coefficient of convective heat transfer, h in $\left[\frac{W}{m^2 K}\right]$, computed using a calibrated Hohenberg correlation, as in Equation (2.15). The wall temperature, T_{wall} , is set at 380 [K] in agreement with the body temperature measured by A.Gatin and T.Colette during their experimental runs on the HCCI test bench [9]. Whereas $P_{\text{start}}=P_{\text{in}}$ is fixed at 1 [bar] for all the 0D simulations as the test bench is naturally aspirated.

The mixture specific heat capacity at constant pressure, c_p , is obtained at each time step using a weighted average of the species-specific heat capacities from the JANAF polynomial correlations: $c_p(T) = c_{p,i}(T) \times n_i(t)/n(t)$.

The temperature increment is computed at each time step from the internal energy increment as $dT = dU/(n c_v)$. From that and $T(t-1)$ we can derive $T(t)$. The pressure is then obtained from the ideal gas law.

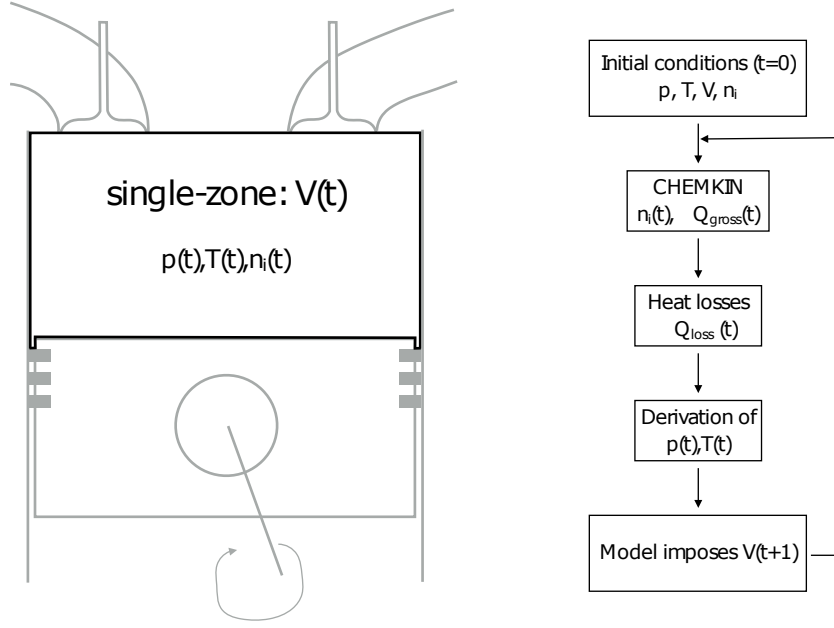


FIGURE 3.1: Schematics of the 0-Dimensional model algorithm [5]

As illustrated in Figure 3.1, the initial conditions defined at $t = 0$ are necessary to start the model algorithm. The accuracy of the model results is largely impacted by the determination of these initial conditions.

Additionally, to better simulate the pressure evolution during the compression stroke, we used the effective compression ratio because it represents the real cylinder compression. For this purpose, the 0D model uses a modified TDC volume $V_{TDC,model} = V_d/(\tau_{eff} - 1)$ being larger than the geometrical one. The modelled cylinder volume varies between V_{BDC} and $V_{TDC,model}$.

3.2 Model Limitations

In a single-zone 0-Dimensional model, the in-cylinder pressure and temperature are scalars representing the whole mixture. The thermodynamic conditions are considered uniform over the whole cylinder volume.

Therefore, the principal default of the single-zone model is its inability to estimate the DOC. Once the auto-ignition requirements are reached inside the combustion chamber, the modelled combustion is almost instantaneous. Based on a chemical kinetics model, the combustion of a perfectly uniform charge would lead to excessively quick combustion linked to an abrupt pressure rise rate because the purely kinetic delay is negligible. As a result, the 0D model overestimates the maximum pressure rise rate (MPRR). Therefore, the high load limit of the HCCI operating range (Section 1.2.4) cannot be defined accurately using this simplified model. For relatively high equivalence ratio simulations ($\phi_{air} \geq 0.3$), the 0-Dimensional model gives us MPRR values in the order of 1000 [bar/CAD]. These unrealistic values mean that the simulated combustion is quicker than the model time step. Reducing too much the model time step is not a good approach as it increases greatly the computational time. Moreover, using such nonphysical pressure rise rates, the combustion damping effect of EGR cannot be well represented.

To correctly predict combustion duration and pressure rise rates, we should consider the temperature inhomogeneities inside the combustion chamber. Actually, the combustion is not as instantaneous as it could be expected. Recent progress in combustion imaging allows us a better understanding of HCCI auto-ignition and combustion. Researchers of the Sandia National Laboratories have used *Planar Laser-Induced Fluorescence* (PLIF) imaging with an optically accessible HCCI research engine. They observed that, towards the end of the compression stroke, colder regions begin to appear through the charge. This natural thermal stratification is coming from wall heat losses combined with turbulent convective transport (engine-dependent) and hot residual gases. This temperature non-uniformity causes the combustion to spread out in time, as parts of the mixture auto-ignite at different times. This reduction of combustion rate goes with a reduction of the MPRR, allowing to stay below the Ringing limit.

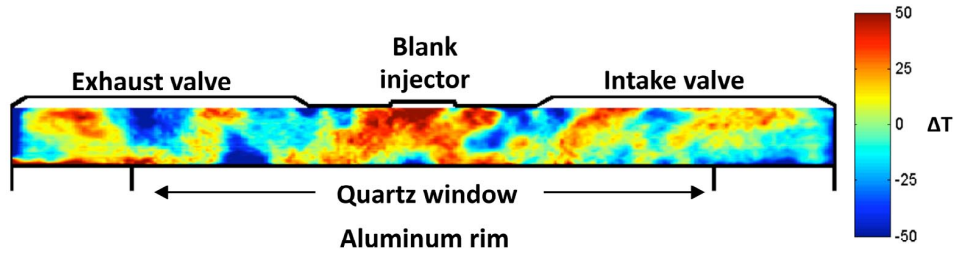


FIGURE 3.2: Thermal map of a HCCI combustion at TDC obtained by PLIF imaging ¹

Finally, an anomaly was identified near the end of the analysis of this chapter's simulation results. The computation of the total intake moles present in the cylinder should be performed at the start of each combustion simulation using the law of perfect gases. It depends on the intake pressure, temperature and volume of the combustion chamber. Once the cycle at the first starting temperature, specified by the user, is ended, the code increases iteratively the intake temperature by one kelvin. However, this iterative increase in temperature is not taken into account in the computation of the total intake moles. Therefore, the code does not consider the decrease of the charge density when the iterative intake gas temperature is increased. Hence, the decrease in volumetric efficiency is not taken into account. For the same initial molar composition of the charge, starting the 0D model at a higher temperature reduces the in-cylinder fuel content, thus the modelled auto-ignition is slightly delayed.

To highlight this inconsistency, simulations were performed duplicating the same simulation parameters excepted this first iteration temperature. Using the calibration based on the fitting of the combustion timing presented in Section 3.3.1, methane oxy-combustion results were studied at an equivalence ratio of 0.063. The difference observed in total intake moles and, subsequently, in FuelMEP depending on the first iterative temperature is represented in Table 3.1.

First iteration temperature [°C]	126.85	136.85	146.85
Total intake moles	0.0137	0.0134	0.0131
FuelMEP [bar]	7.72	7.53	7.35

TABLE 3.1: Influence of the first iteration temperature on the total intake moles and FuelMEP

¹<https://crf.sandia.gov/characterizing-the-development-of-thermal-stratification-in-hcci-engines/>

As the main focus of this chapter is to determine combustion timing, Figure 3.3 illustrates the total intake moles influence on the combustion timing for the above-mentioned conditions. At the same T_{BDC} iterated, a difference of approximately 0.4[CAD] is observed for the CA10 between the simulations that started at 126.85[°C] and 136.85[°C] or 136.85[°C] and 146.85[°C]. This small difference, combined with limited time constraints, convinced us to keep the generated results.

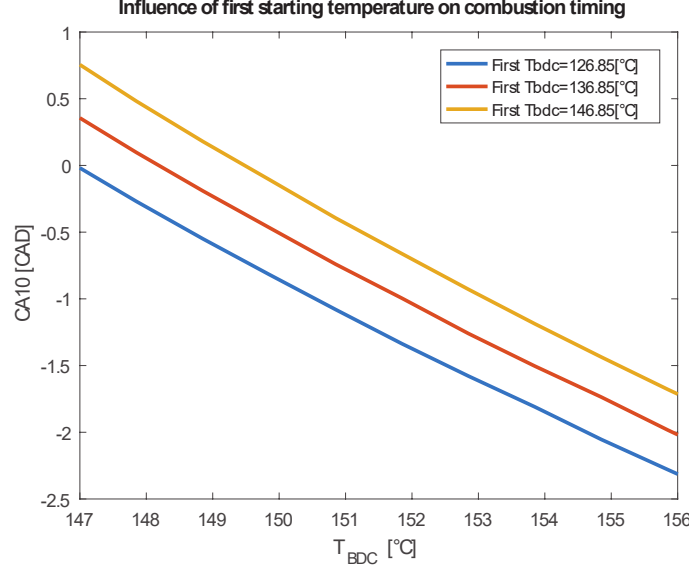


FIGURE 3.3: Influence of the first iteration temperature on the combustion timing

In the following represented simulation results, the same first iteration temperature is used for each curve on the same graph. The total number of moles therefore stays the same for each curve. The only exception is at Section 3.4.2 where the air and oxy-combustion are compared. Indeed, the air combustion simulations started at a temperature 19[K] higher than with oxy-combustion. As those air conditions required higher intake temperatures for a similar timing, the comparison can be considered slightly more accurate.

To ease the comparison between all the simulations in this section, the energetic content in [J/Nl] has been used instead of the FuelMEP. It is defined as:

$$\text{Energetic content} = \frac{m_{\text{fuel}_{\text{in}}} \cdot \text{LHV}_{\text{fuel}}}{\text{Normal equivalent volume of the charge}} \quad (3.3)$$

This definition can also be used in the case of fuel blends by simply adding the contribution of each fuel species in the numerator of the above formula.

The normal equivalent volume of the charge in [Nl] is computed with:

$$\text{Normal equivalent volume} = \frac{n_{\text{tot intake}} \cdot R \cdot T_n}{P_n} \cdot 1000 = \frac{n_{\text{tot intake}} \cdot 8.314 \cdot 293.15}{101325} \cdot 1000 \quad (3.4)$$

Because this definition divides the complete energetic content by the total number of moles computed at the intake, it does not highlight the aforementioned difference in total moles.

3.3 Model Calibration

The calibration of the 0D-model is based on the experimental hydrogen-air combustion results of last year's thesis [9] which are detailed in Table 3.2.

P_{in} [bar]	T_{in} [° C]	T_{body} [° C]	ϕ	CA05 [° CAD]	$IMEP_{net}$ [bar]	MPRR [bar/CAD]
1.0	80.5	103.8	0.20	-1.07	2.00	8.5
1.0	80.2	104.5	0.20	-2.25	2.00	11.3

TABLE 3.2: Hydrogen-air combustion: Experimental results from Collette and Gatin [9].

As presented in Section 3.1, the inputs of the model are the intake gas molar fractions, the pressure and temperature at the start of the simulation, the Hohenberg scaling factor (see Section 2.3.2) as well as the engine geometrical parameters and starting CAD.

Unfortunately, this 0D-model is not able to accurately estimate the intake conditions for the desired combustion timing while approximating the heat losses with the same scaling factor. Consequently, the results of two different scaling factors will be represented. Actually, the use of a small scaling factor underestimates the heat losses but leads to a realistic combustion timing for the given intake conditions. This effect is detailed in Section 3.3.1. On the other hand, using a scaling factor with a higher value provides an improved approximation of the heat losses that better fits the pressure curve but, unfortunately, the required intake temperature can no longer be computed. This calibration is detailed in Section 3.3.2.

Furthermore, all the results presented in this chapter only provide a prediction of the behaviour because to accurately predict the timing or pressure evolution, the Hohenberg scaling factor should be adapted for each thermodynamic condition and fuel concentration on the basis of experimental results.

3.3.1 Combustion Timing Fitting

To fit the experimental intake conditions leading to the desired combustion timing for a set mixture, the simulation should firstly start at *Bottom Dead Centre* (BDC), even though in reality the cylinder becomes a closed system only from IVC (-127 CAD). Starting the simulation at IVC is prone to errors given the difficulty to choose values of P_{IVC} and T_{IVC} when intake conditions are given as a constraint. Furthermore, P_{IVC} and T_{IVC} are influenced by the engine geometry and operating conditions. The simulation therefore starts at BDC so that the total number of moles inside the cylinder is slightly over-estimated. Although, due to the crank-slider motion of the piston, the difference is negligible compared to a simulation that started at the effective IVC. However, the intake temperature is very different from the BDC temperature because of wall heat transfer, gas dynamic effects and mixing with trapped residual gases.

To approximate the corresponding intake temperature from the BDC one, correlations were experimentally developed by Pochet [5]. Fortunately, a correlation has been developed for the studied conditions, namely hydrogen-air combustion on the UCLouvain single-cylinder HCCI engine at an equivalence ratio of 0.2 for intake temperatures between 53 and 115 [°C], in Equation (3.5).

$$T_{BDC} = 0.548 \cdot T_{in} + 49.835[°C] \quad (3.5)$$

As explained in Section 3.2, the 0D model considers the bulk of gas as one scalar, the modelled wall heat losses thus decrease uniformly the charge temperature. In a real compression, heat transfer affected areas are located close to the combustion chamber walls, with a thermal gradient contained in a thin boundary layer. As methane and hydrogen are simple single-stage ignition fuels, their auto-ignition will arise in the highest temperature region. This region being the core zone, to describe the core temperature evolution, the 0D model has to underestimate the heat losses during the compression stroke so that it correctly predicts HCCI ignition timing.

However, the combination of lower modelled heat losses through a low convective coefficient and virtual IVC at -180 [CAD] leads to an overestimation of the temperature and pressure evolution. Indeed, the start of the simulation is at BDC whereas the model considers a closed cylinder throughout the simulation. A different scaling factor and starting CAD should, therefore, be used to match experimental pressure data.

As an exception, the start of combustion is taken as CA05, similarly to the convention used for the results of last year master's thesis. The scaling factor to retrieve the same CA05 in reproduced thermodynamic conditions of Table 3.2 was found to be 50 and the results are presented in Table 3.3.

	Results 1		Results 2	
	Experimental	Model	Experimental	Model
T_{BDC} [° C]	93.9*	91.9	93.8*	96.9
T_{in} [° C]	80.5	76.7*	80.2	85.8*
CA05 [° CAD]	-1.07	-1.01	-2.25	-2.32

TABLE 3.3: Results of the model to fit the experimental intake temperature giving the appropriate timing.

*: Obtained from correlation (3.5)

As expected, a scaling factor of 50 largely underestimates the heat losses, as presented in Figure 3.4a

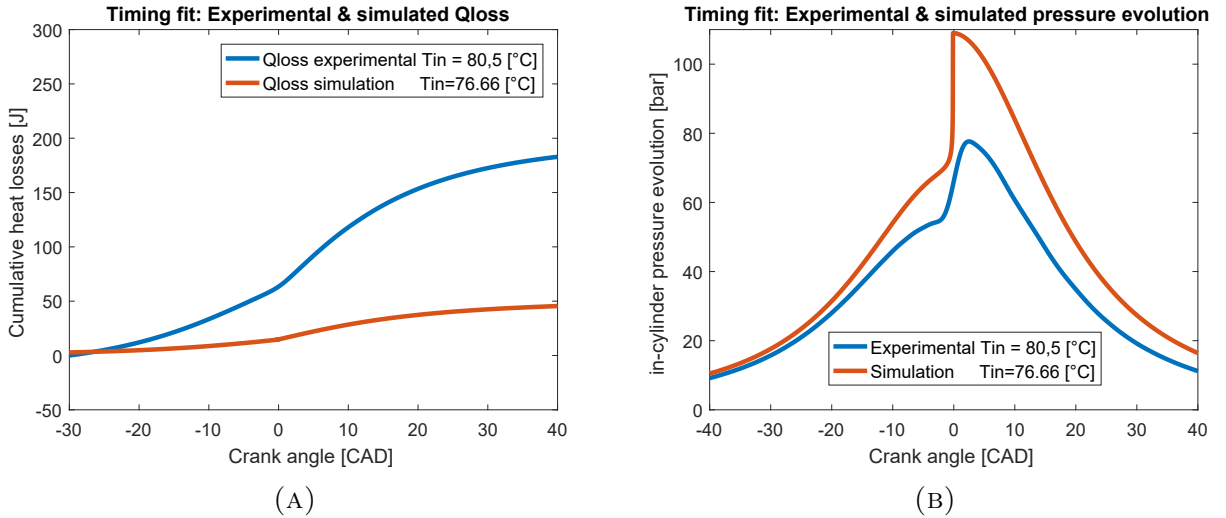


FIGURE 3.4: (A) Wall heat losses and (B) pressure evolution for the fitting of the combustion timing: comparison between experimental results and simulation

As the heat losses are underestimated, the simulated pressure curve, presented in Figure 3.4b, overestimates the pressure evolution during the compression stroke compared to experimental results.

3.3.2 Pressure Curve Fitting

To fit the pressure curve, the starting CAD of our simulation should firstly be changed. As our HCCI research engine has a particularly late IVC at -127 [CAD], this engine loses a substantial amount of compression pressure compared to more conventional valve closure timings which are roughly at -150 [CAD]. As mentioned in Section 3.1, the 0D model considers a closed system since the start of the simulation. Therefore, the simulation has to start at the effective IVC of our HCCI engine mentioned in Section 2.3.1, namely -152 [CAD], to better fit the measured experimental pressure curve. The temperature specified at the start of the simulation is thus no longer T_{BDC} and no correlations can be used to approximate the intake temperature.

Secondly, as wall heat losses cause a significant decrease in the temperature and pressure evolution, the scaling factor has to better represent those losses. Consequently, a higher scaling factor of 200 has been selected. This higher scaling factor also induces a lower gross heat release because the simulated pressure and temperature are lower.

The comparison between experimental and simulated results for wall heat losses and gross cumulative heat release is represented in Figure 3.5.

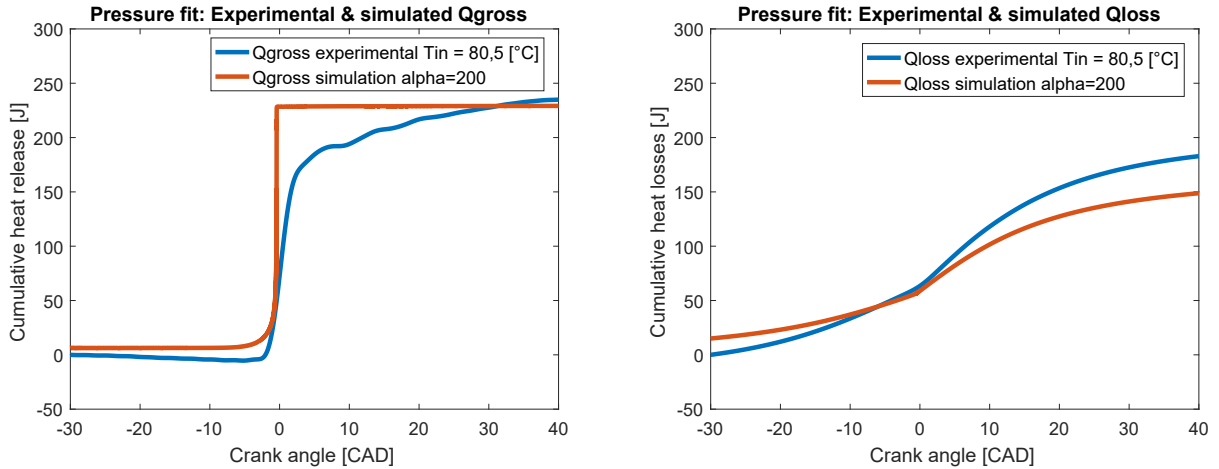


FIGURE 3.5: Gross cumulative heat release and wall heat losses for the fitting of the pressure curve: comparison between experimental results and simulation

The pressure curve is eventually represented in Figure 3.6. The fitting of the pressure during the compression stroke is more realistic than the one shown in the previous section. However, due to the fact that the bulk of gas is considered as one volume with uniform temperature and pressure, the pressure rise rate observed during combustion is still overestimated.

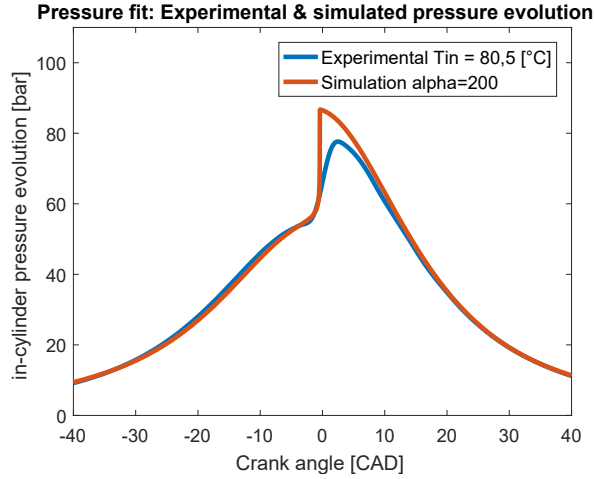


FIGURE 3.6: Pressure evolution for the fitting of the pressure curve: comparison between experimental results and simulation

3.4 Simulation Results

The main objective of this 0D simulation is the approximation of the required intake parameters, mainly the intake temperature required for a start of combustion near the TDC with a given fuel-oxidiser mixture.

Using the calibration based on the combustion timing of hydrogen-air mixtures seen in Section 3.3.1, a first approximation of the required BDC parameters can then be estimated. The intake temperature is subsequently approximated with correlations based on experimental results, as used in the calibration of the combustion timing. However, those correlations are not only dependent on the engine used but also on the operating conditions such as equivalence ratio, cylinder wall temperature, etc. Unfortunately, no correlations for the UCLouvain experimental setup have been developed for methane combustion.

The next paragraphs therefore detail the available correlations.

The first correlation found is the one from F.Contino et al.[31]. It is based on a HCCI engine test bench of UOrléans with significantly different engine geometrical parameters such as an effective compression ratio of 14.15:1, an IVC at 157 [CAD] and a cooling temperature of 90[°C]. Based on the method of M. Sjöberg and J.E. Dec [32], this correlation was developed for valeric biofuels (i.e. Methyl, Ethyl, Propyl, Butyl and Pentyl) at an equivalence ratio of 0.3. Considered valid between 40 and 200 [°C] with an estimated overall error of 10%, it is expressed in Equation (3.6).

$$T_{BDC} = 0.652 \cdot T_{in} + 138[K] \quad (3.6)$$

Using experimental results, M.Pochet deduced correlations for the UCLouvain single-cylinder HCCI test bench at a wall temperature of 106 [°C] [5]. The correlation (3.5) seen in Section 3.3.1 is adapted for hydrogen-air combustion at an equivalence ratio of 0.2 for intake temperatures between 53 and 115 [°C]. A second correlation, expressed in Equation (3.7), has been established with experimental results of ammonia-hydrogen blends at an equivalence ratio of 0.35 for intake temperatures between 49 and 233[°C].

$$T_{BDC} = 0.657 \cdot T_{in} + 57.917[°C] \quad (3.7)$$

The first hydrogen correlation in Equation (3.5) has a temperature range that ends at a too low temperature of 115[°C]. On the other hand, although the correlation (3.6) of F.Contino et al. has a well-suited temperature range, the engine geometrical parameters are too different to use it. Therefore, as the engine geometrical parameters and the temperature range of the NH₃-H₂ correlation in Equation (3.7) are better suited for our experiments, it is represented on a second scale of the x-axis on the temperature simulation results.

However, one should note that this last correlation only gives a qualitative idea of the intake temperature because the fuel used is different and no correlation for methane combustion or oxy-combustion could be elaborated from experimental results. The simulated BDC temperatures should be preferred for a more accurate comparison. Moreover, as pointed in Section 3.3, the Hohenberg scaling factor should be adjusted for each engine operating point because it is not only dependent on the engine geometrical parameters but also on the fuel composition, temperature and equivalence ratio as well as eventual EGR rate. Therefore, in addition to the 0D model limitations discussed in Section 3.2, the results presented in this section are not to be considered quantitatively exact.

3.4.1 Methane Combustion

The present subsection seeks to numerically study the combustion characteristics of methane with air in our HCCI test bench.

To that end, using the combustion timing calibration, an analysis of the influence of the BDC and intake temperature as well as the equivalence ratio on the start of combustion (CA10) is illustrated in Figure 3.7. As expected, the auto-ignition timing is mainly controlled through the charge temperature, with higher temperatures enabling quicker ignition. Surprisingly, a rise in the equivalence ratio from 0.25 to 0.4 led to an increase in the required BDC temperatures of 2[°C]. Although this temperature increase does not corroborate with our expectations (discussed in Section 1.2.3), the negative influence is limited.

Methane is a single-stage ignition fuel, thus the first radicals obtained after the ignition delay trigger the whole combustion process from branching to termination reactions. A small rise in fuel content (from $\phi=0.25$ to 0.4) does not increase dramatically the mixture reactivity but the overall blend heat capacity is modified, leading to a slightly later combustion timing. However, in running engines, the increase in the equivalence ratio causes a higher thermal load because of a more intense heat release. This results in higher in-cylinder temperatures at the start of the compression stroke for identical BDC temperatures, and ultimately, to an earlier auto-ignition. The 0-Dimensional model does not take into account this increase in engine thermal load as we only simulate one cycle. Hence, the model results are somewhat misleading. The required BDC temperature for a start of combustion near the TDC, named $T_{BDC}(CA10 = TDC)$ in the following of this thesis, is expected to be reduced for increasing fuel contents even though our model does not depict this phenomenon.

We should bear in mind that the sensitivity of the SOC to ϕ is engine speed dependant. The equivalence ratio has a bigger impact at low engine speed and this impact decreases as the speed increases.

Temperature & equivalence ratio influence on combustion timing

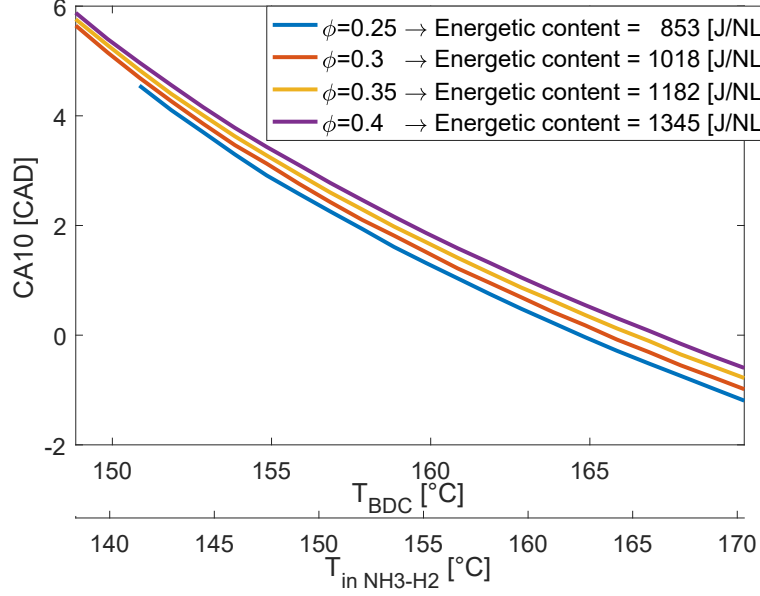
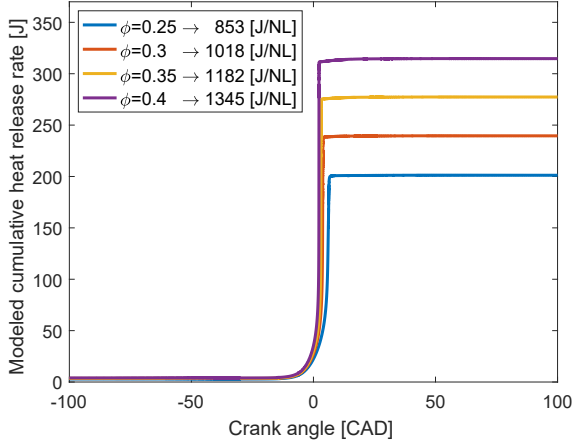


FIGURE 3.7: CH4-Air combustion: T_{bdc} and ϕ influence on combustion timing (First $T_{\text{iter}}=146.85[^\circ\text{C}]$)

Modifying the calibration used to better fit the pressure evolution, the influence of the energetic content on the gross cumulative heat release can be represented in Figure 3.8a as well as its influence on the pressure evolution in Figure 3.8b. Supposing that the maximum pressure is still overestimated, the IMEP is also overestimated. Using the pressure evolution at an energetic content of 853[J/NL], the IMEP has been estimated at 0.99[bar]. This fuel content is therefore too weak for our application.

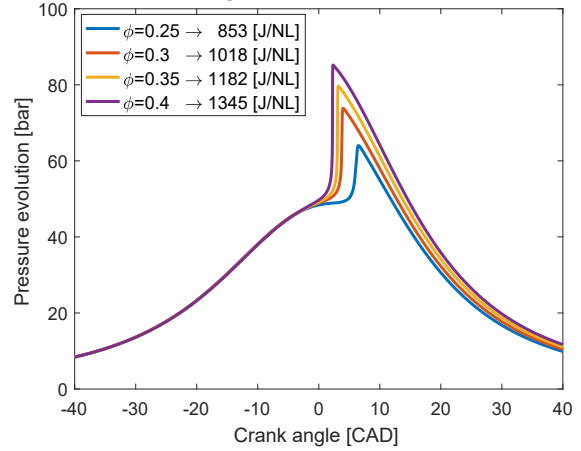
Increasing the equivalence ratio also increases the IMEP. The only limit on increasing fuel content will be the apparition of ringing as the MPRR and the maximum in-cylinder pressure will increase with ϕ , as explained in Section 1.2.

Influence of energetic content on model cumulative heat release



(A)

Influence of energetic content on pressure evolution



(B)

FIGURE 3.8: CH4-Air combustion: energetic content influence on (A) gross cumulative heat release and (B) pressure evolution

3.4.2 Methane Air and Oxy-combustion Comparison

The purpose of this subsection is to investigate some of the claims made in Section 1.3 regarding the divergence between air and oxy-combustion. Firstly, applying the calibration adapted to the combustion timing, the influence of the BDC temperature for methane-air combustion and oxy-combustion at the same energetic content of 1182[J/Nl] is represented in Figure 3.9. A reduction of 20[°C] in T_{BDC} (CA10 = TDC) is noticed for the oxy-combustion. This is beneficial as lower intake temperatures lead to higher charge density and thus to a higher volumetric efficiency of the engine for a set equivalence ratio. This significant reduction of required temperature provides additional support to the potential of oxy-combustion. This advantage is observable over the optimal combustion timing range, the difference goes from 15[°C] (for late timing, i.e. CA10 at 6 [CAD]) to 21[°C] (for early timing, i.e. CA10 at -2 [CAD]). Moreover, we might want to have a later timing in oxy-combustion compared to a conventional air-combustion to limit the MPRR, which further reduces the required BDC temperature.

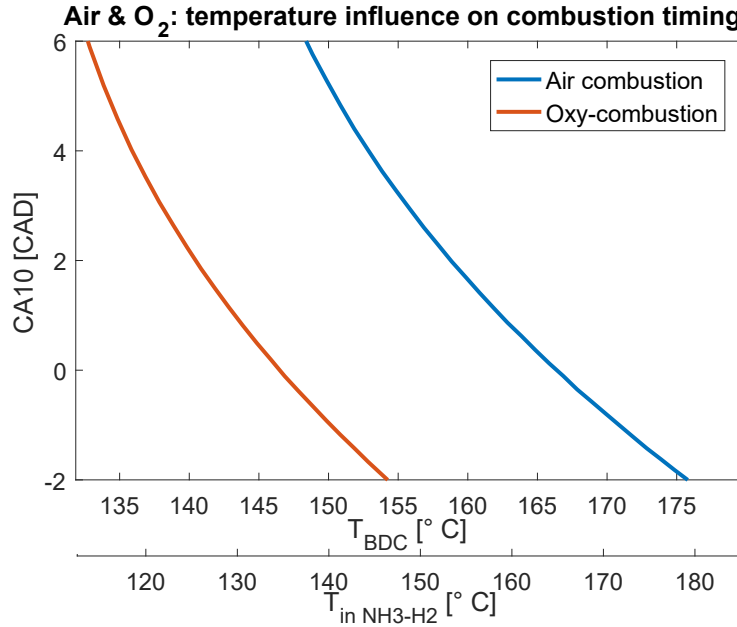


FIGURE 3.9: Comparison of the influence of T_{BDC} on combustion timing between methane-air and oxy-combustion at the same energetic content of 1182[J/Nl]

Then, using the pressure calibration, Figure 3.10 presents the pressure evolution of methane combustion and oxy-combustion at the same energetic content of 1182[J/Nl] and with starting conditions that lead to a SOC (CA10) at the TDC. The oxy-combustion reaction reaches higher pressure at the same ignition timing compared to methane air combustion. Although the combustion speed is largely overestimated in 0D simulations, this observation would indicate that, at the same energetic content, higher MPRR and maximum pressure are reached in oxy-combustion. Those phenomena are explained by the increased reactivity in behalf of higher oxidiser availability and absence of nitrogen, which would otherwise act as a heat buffer. We expect to meet the Ringing limit for lower values of energetic content in oxy-combustion, which is an important drawback as the HCCI engine has already quite a narrow operating range. Accordingly, the oxy-combustion of methane in HCCI engines would require the use of EGR or WDI to moderate the speed of the combustion, as stated in Section 1.3.2.

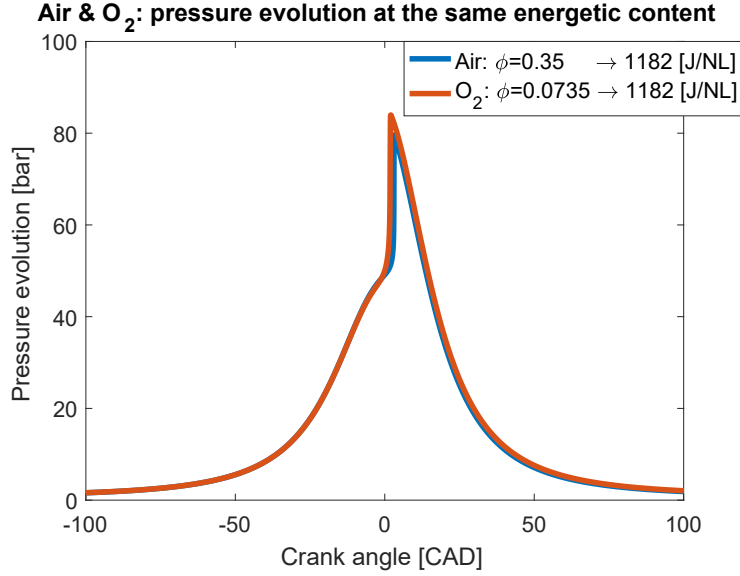


FIGURE 3.10: Comparison between methane-air and oxy-combustion pressure evolution at the same energetic content of 1182[J/Nl]

Unfortunately, due to the limitation mentioned at the end of Section 3.3, the pressure comparison is not the most accurate. As the starting temperature of the methane air and oxy-combustion simulations are different, the total number of moles in the cylinder are different and so the FuelMEP is 9% lower in air combustion. A better comparison of methane air and oxy-combustion pressure evolution is presented in the next chapter.

3.4.3 Methane Oxy-combustion

This subsection approximates the required intake conditions for an optimal methane oxy-combustion.

To this extent, the same procedure used in the two previous sections is applied. The calibration of the combustion timing is firstly utilised and the intake temperature is represented using the ammonia-hydrogen blend correlation specified in Section 3.4.

However, extreme caution must be exercised with those intake temperatures as the correlation validity is not proven with methane-oxygen mixtures. Conservatively, as oxy-combustion is supposed to have higher reactivity, lower intake temperatures must be firstly used on the test bench and increased gradually until the user gets a satisfying combustion timing.

Figure 3.11 exhibits the influence of T_{BDC} , equivalence ratios and, to a lesser extent, T_{in} on the start of combustion. Similarly as for methane air-combustion, the auto-ignition timing is mainly controlled through the charge temperature. A rise in the charge intake temperature leads to an advanced start of combustion. In opposition to the behaviour observed for methane air combustion, an equivalence ratio increase advances slightly the auto-ignition timing. Taking into account the claims of Section 3.4.1, we might expect a higher influence of equivalence ratio on combustion timing in oxy-combustion for corresponding energetic contents. To confirm these expectations, experiments should be conducted.

Temperature & equivalence ratio influence on combustion timing

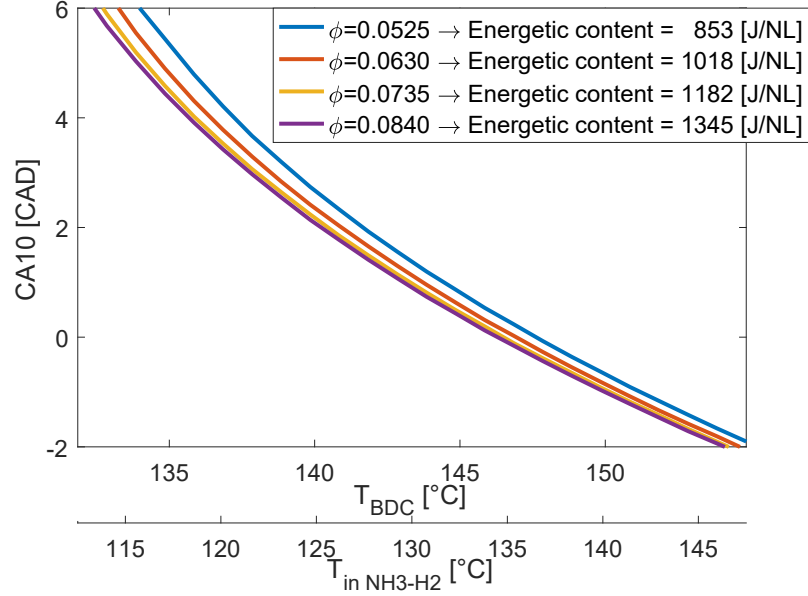
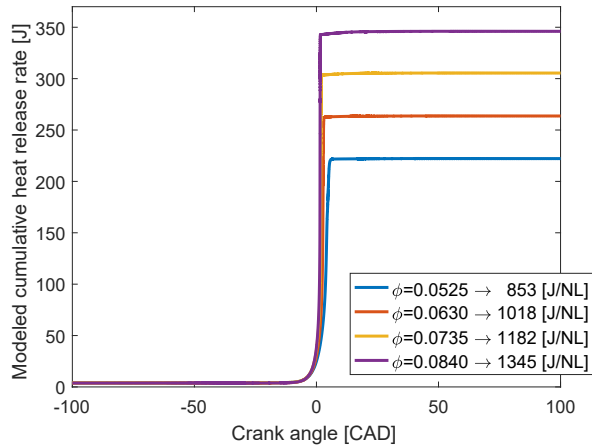


FIGURE 3.11: Methane oxy-combustion: T_{bdc} and ϕ influence on combustion timing (First $T_{\text{iter}}=126.85[^\circ\text{C}]$)

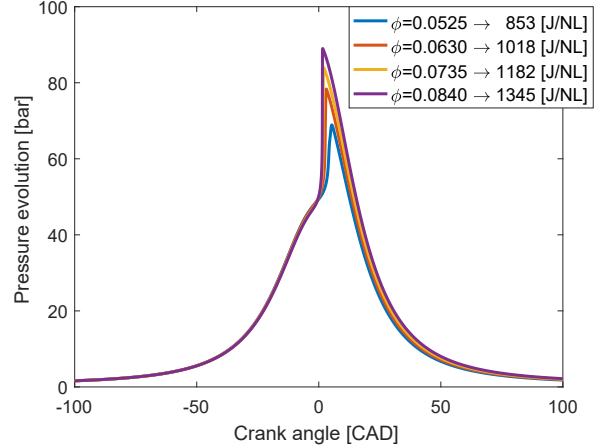
Secondly, the pressure-fitting calibration allows to represent the energetic content influence on gross cumulative heat release in Figure 3.12a and on the pressure evolution in Figure 3.12b. As anticipated, the significant increase in the total gross heat release and pressure evolution noticed when the energetic content increase matches the behaviour of methane air combustion. Higher MPRR and maximum pressure are unfortunately expected and observed when the reactivity of the mixture is increased.

Influence of energetic content on model cumulative heat release



(A)

Influence of energetic content on pressure evolution



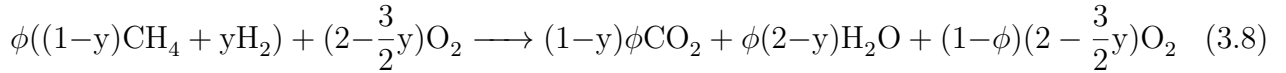
(B)

FIGURE 3.12: Methane oxy-combustion: Influence of energetic content on (A) gross cumulative heat release and (B) pressure evolution

3.4.4 Hydrogen-Methane Blends Oxy-combustion

To further reduce the intake temperature required to induce the combustion near the TDC, fuel blending is an interesting path to investigate. To promote the auto-ignition of methane, a fuel with a low ignition temperature is needed. Hydrogen is characterised by a low ignition energy and a high reactivity. As methane can be produced from hydrogen, methane-hydrogen combustion is conceivable in the studied power to power system.

The complete oxy-combustion reaction of methane-hydrogen blends is represented in Equation (3.8).



Where y is the molar proportion of H_2 in the $\text{CH}_4\text{-H}_2$ blend at an equivalence ratio of ϕ .

Hydrogen has an auto-ignition temperature range between 500 and 585[°C] while methane only auto-ignites from 586[°C]. To some degree, this observation can be explained by the compactness of the molecule and the molecule bond strength [5]. Therefore, the addition of hydrogen helps the mixture to ignite at a lower temperature.

Given the lower activation energy of hydrogen, it reacts with a lower energy input, i.e. heat induced by compression of the charge. Hydrogen reacts first and releases H, O and OH radicals that promote the oxidation of methane. The heat released by the first steps of hydrogen oxidation also influences the kinetics of the reaction. An experimental study for premixed laminar methane/air flames with and without hydrogen addition has been conducted by Hu et al. [33]. In this study, they concluded that hydrogen addition leads to a significant increase of H and OH radicals. The peak heat release rate of methane-hydrogen blends increased with higher hydrogen fractions. Additionally, this peak value appears at a relatively lower temperature, which denoted that hydrogen additions can promote reaction speed and lower reaction temperature. They also concluded that the reaction $\text{OH} + \text{H}_2 \rightleftharpoons \text{H} + \text{H}_2\text{O}$ (R84), which uses the created OH radicals, is one of the most governing reactions to the early part of heat release.

However, careful attention must be paid when one uses hydrogen in a HCCI engine. Hydrogen is a fuel with higher kinetic reactivity than methane. The laminar burning velocity of hydrogen of 3.51[m/s] compared to 0.38[m/s] for methane also explains this higher kinetic reactivity [5]. As discussed in Section 1.2.4, rapid combustion processes can result in ringing phenomena that increase engine noise and can result in permanent engine damage. Given the higher reactivity of oxy-combustion due to higher oxidiser availability, the use of hydrogen must remain moderate in such engine.

Zhang et al. [34] studied the characteristics of methane/hydrogen blends in a shock tube at conditions similar to HCCI combustion, namely temperatures in the range of 900-1750[K] and equivalence ratios of 0.5. They characterised three ignition regimes, namely methane chemistry dominating ignition ($x \leq 40\%$), combined chemistry of methane and hydrogen ignition ($x = 60\%$) and hydrogen chemistry dominating ignition ($x \geq 80\%$). As the fuel of interest of this master's thesis is methane, hydrogen volume fraction greater than 40% will not be studied.

One must note that the energetic content (see Equation (3.3)) will slightly increase with the hydrogen fraction. Therefore, the influence of the hydrogen volume fraction in the fuel on the energetic content of air combustion and oxy-combustion is represented in Table 3.4.

H ₂ % vol	0	5	10	15	20	25	30	35	40
energetic content [J/Nl]	1018	1020	1022	1024	1026	1028	1030	1033	1036

TABLE 3.4: Influence of H₂% vol in the fuel on air and oxy-combustion energetic content

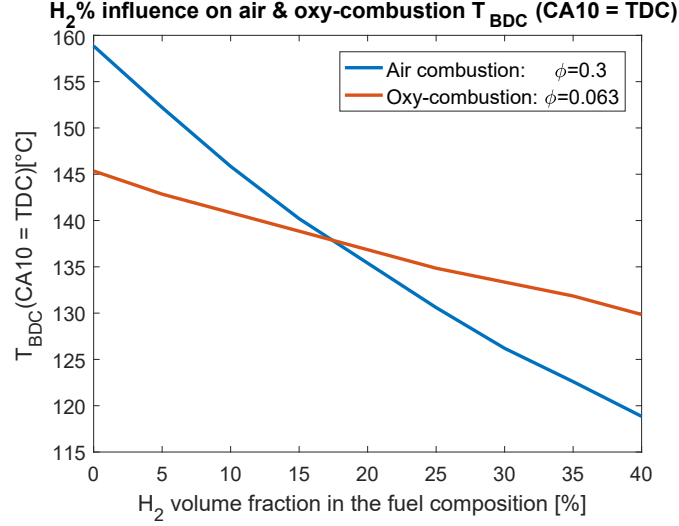


FIGURE 3.13: Methane air and oxy-combustion: Influence of hydrogen volume fraction on $T_{BDC}(CA10 = TDC)$

Figure 3.13 compares the influence of hydrogen fraction on $T_{BDC}(CA10 = TDC)$ between methane air combustion and oxy-combustion. The reduction of modelled required BDC temperature appears to be substantially greater in air combustion than in oxy-combustion. However, one should remember that the chemical mechanism used was not validated for pure oxy-combustion conditions. Therefore, the above-mentioned results should also be considered only qualitatively.

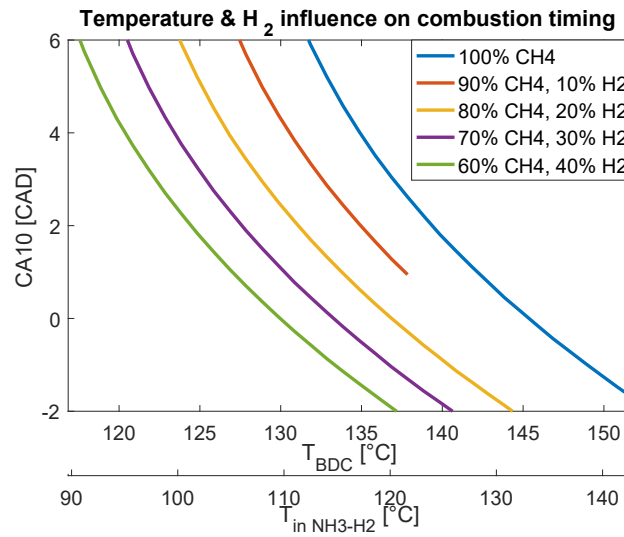


FIGURE 3.14: Methane oxy-combustion at $\phi = 0.063$: Hydrogen mix and T_{bdc} influence on combustion timing (First $T_{iter}=114.85[°C]$)

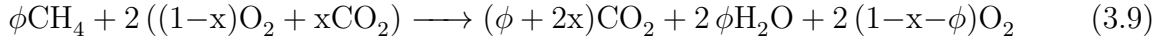
The simulation results represented in Figure 3.14 illustrate the influence of the hydrogen fraction and T_{BDC} on a broader range of oxy-combustion timing. A decrease in $T_{\text{BDC}}(\text{CA10} = \text{TDC})$ of $15[^\circ\text{C}]$ is observed from a pure methane to a 60/40% methane-hydrogen oxy-combustion. However, for unknown reasons, the simulation at 10% hydrogen molar fraction encounters an error and would not compute for temperatures higher than $137.85[^\circ\text{C}]$.

The observed decrease in required charge temperature for methane-hydrogen blends is lower than what was expected on the basis of the results obtained for air-combustion by M.Pochet [5]. The potential increase in IMEP_g is restrained by the charge reactivity increase owing to hydrogen addition. HCCI oxy-combustion being already limited due to the rapid combustion process leading to high pressure rise rates, hydrogen addition is considered detrimental. The concept of fuel blending will thus not be further explored in this work.

3.4.5 EGR Impact

Oxy-combustion in HCCI engines will experience higher pressure rise rates limiting the engine power density. To study its damping effect on the combustion, a carbon dioxide source has been implemented on the blueprints of the test bench. The 0D model is used to determine the impact of CO_2 addition at the intake on the required BDC temperature.

As a reminder, to keep the same amount of fuel throughout the simulations, the chemical Equation (3.9) is used to specify the synthetic EGR.



The EGR rate used is thus x , the molar proportion of carbon dioxide with respect to oxygen, ranging from 0 to $1 - \frac{2}{9.52}$. Indeed, as mentioned in Section 1.3.2, this molar proportion should not exceed $1 - \frac{2}{9.52} \approx 0.79$ to avoid affecting the O_2 used for the combustion to keep the same equivalence ratio throughout the different EGR rates.

The influence of this EGR on $T_{\text{BDC}}(\text{CA10} = \text{TDC})$ is represented in Figure 3.15. Those results were computed for a methane oxy-combustion with an equivalence ratio of 0.084 that correspond to the highest fuel content used in this chapter. The required BDC temperature seems proportional to the carbon dioxide volume fraction in the mixture.

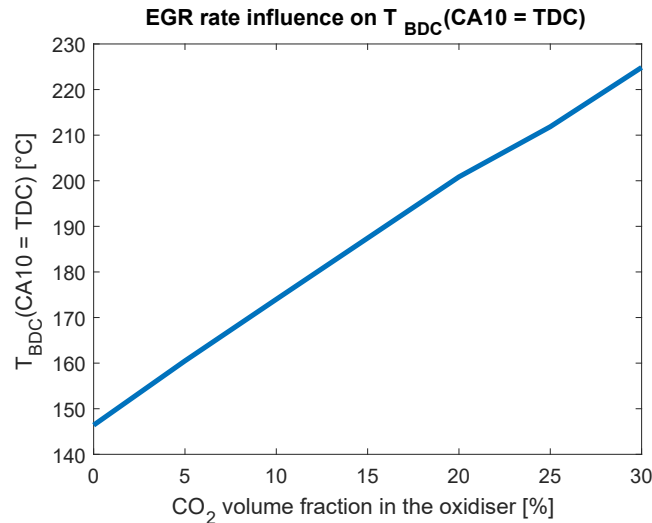


FIGURE 3.15: Influence of CO_2 proportion on $T_{\text{BDC}}(\text{CA10} = \text{TDC})$ for $\phi = 0.084$

As expected, CO_2 inhibits the combustion process by absorbing part of the heat released. With increasing EGR rates comes the necessity of higher intake temperatures to get the same combustion timing. Indeed, when the EGR is greater than 7.5%, the required BDC temperature is more than $20[^\circ\text{C}]$ higher than in pure oxy-combustion. This increase is comparable to the difference observed between methane-air and oxy-combustion. Because carbon dioxide is a triatomic molecule, as explained in Section 1.3.2, its heat capacity is greater than nitrogen. Lower proportions of CO_2 compared to N_2 in the air will affect the combustion in the same manner. In our particular application where the EGR is a pure source of CO_2 coming from a tank, this increase is a concern. However, in a real-world application, this observation would be less critical as the EGR is already composed of hot exhaust gases that do not require heating and could even heat up the intake charge.

Figure 3.16 illustrates the influence of certain EGR rates for a broader range of combustion timing. The relative parallelism between the EGR rate curves from 0 to 20% is the reflection of the linear relation observed in Figure 3.15.

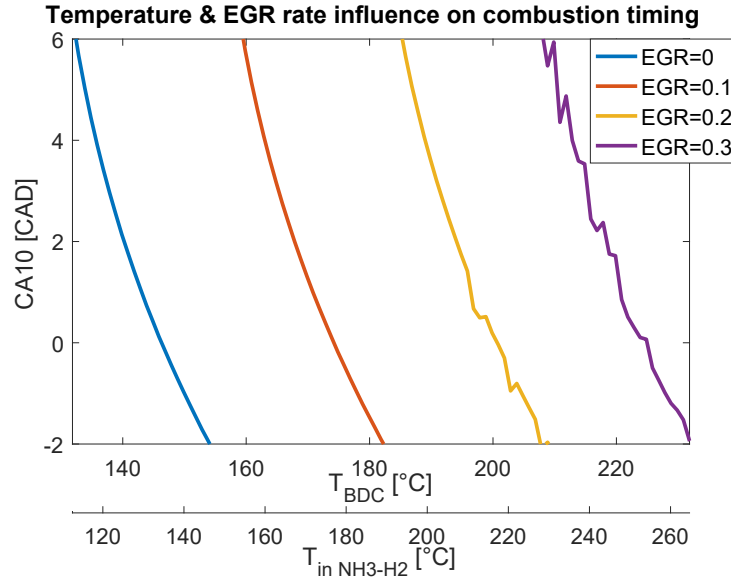


FIGURE 3.16: Methane oxy-combustion at $\phi = 0.084$: Influence of T_{BDC} and CO_2 proportion in the oxidiser on combustion timing (First $T_{\text{iter}}=126.85[^\circ\text{C}]$)

From EGR rates of 20%, inconsistencies between required starting temperatures increase and combustion timing are noticeable. Increasing the EGR rate to 30% further increases the tendency. Previous findings reported by Kang et al. [23] suggested that, at 30% EGR rate, with the same EGR definition as used in this work, the COV_{IMEP} is greater than 10%. This value is a threshold beyond which, the thermodynamic conditions are excessively unstable for an ICE application and may lead to severe misfire. The behaviour observed in our graph might lend support to this statement. Thus, to avoid combustion instabilities, the EGR rate should be kept below 30%.

Chapter 4

3D Axisymmetric Numerical Simulations

To simulate more precisely the HCCI combustion process, a three-dimensional axisymmetric CFD model has been developed. In the previous chapter, the limitations of 0D engine simulations were highlighted. Primarily its inability to depict the combustion duration and to predict precisely the combustion pressure trace. The main goal of this more refined model is to have a better evaluation of the MPRR, allowing us to find the high load limit. Given the highly reactive nature of HCCI oxy-combustion, we expect to be limited earlier in the fuel content compared to HCCI air-combustion. This chapter results in the determination of the mixture composition leading to the high load limit as well as the impact of simulated EGR on this limit.

A modelled thermal boundary layer along with turbulent engine flow allows a more accurate representation of the wall heat losses. This turbulent convective heat transfer leads to thermal stratification, ultimately triggering the charge auto-ignition at slightly different moments inside the cylinder. However, a full 3D simulation is necessary to completely represent this phenomenon. To save computational costs, the 3D model used is axisymmetric. The model aim is not to have a perfect estimation of real conditions but to give a better image of the global combustion behaviour and thus of the MPRR. Using the modelled combustion, the main concern of this chapter is the relative comparison between air and oxy-combustion.

This 3D axisymmetric model was developed using the free-to-use, open-source numerical simulation software OpenFOAM-7 (Open Field Operation and Manipulation). OpenFOAM has high physical modelling capabilities and can simulate a lot of physical problems such as turbulent fluid flows, chemical reactions, heat transfer and stress analysis. It is a C++ object-oriented library composed of modules creating miscellaneous precompiled utilities and solvers. Utilities are executable performing pre- or post-processing like mesh operations or data manipulation. Solvers are designed to solve a specific problem in computational continuum mechanics. OpenFOAM also includes a variety of chemical, combustion and thermophysical models as well as finite volume discretisation schemes and linear equation solvers [35].

To discover the implemented solvers scope, OpenFoam7 comes with numerous tutorial cases. These example cases can serve as a base to implement a more specific problem.

The typical structure of an OpenFOAM case is presented in Figure 4.1. The *case* directory contains, at minimum, three mandatory subdirectories: *system*, *constant* and *time*.

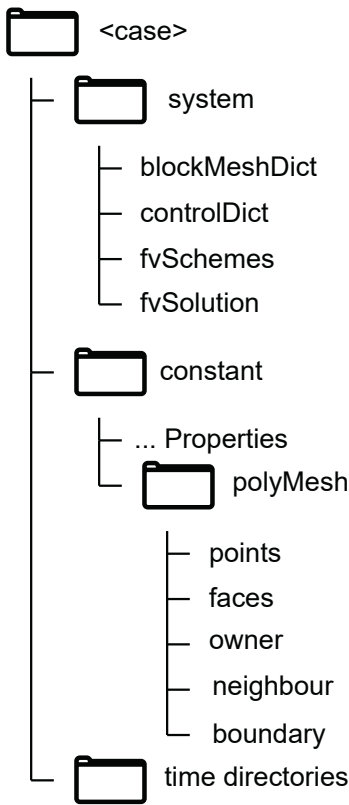


FIGURE 4.1: OpenFOAM case directory structure

The **system** directory contains at least three files setting the parameters associated with the solution procedure:

controlDict sets the main simulation run parameters such as start/end time, solver choice, time step adaptability, maximum Courant number, etc.

fvSchemes selects the finite volume discretisation schemes such as gradients and derivatives for the equation solvers.

fvSolutions contains the selection of equation solvers and their respective tolerances.

blockMeshDict is an additional file used to specify the mesh geometry, boundary patches and generation controls. This file is commonly used for complex meshes generation.

The **constant** directory contains files specifying the physical properties depending on the case (thermodynamic, combustion, chemistry, turbulence, etc.). It also includes a full description of the case mesh in the *PolyMesh* subdirectory generated by the blockMesh utility.

For engine simulations, the mesh is dynamic with an automatic motion of the piston. To correctly model this motion, the engine geometry parameters (e.g. bore, stroke, connecting-rod length, clearance) and revolution speed are specified in the *engineGeometry* file of the constant directory.

In the case of piston engine simulations, the **time** directories are represented by crank angle degrees rather than the actual simulation time. The starting time directory is created by the user to define the problem with its initial conditions for the boundaries and the internal fields of every computed variable (e.g. temperature, pressure, velocity, mass concentration of the chemical species). The parameters required by the turbulent solver, such as the turbulent kinetic energy (κ) and its dissipation rate (ϵ), the thermal diffusivity (α_t) as well as the turbulent viscosity (ν_t) are also specified in this directory. Then, during the simulation, computation results are written by OpenFOAM in new folders named according to the simulated CAD. The writing interval of those folders is specified in *controlDict*. At its conception, the writing interval angle was set to 5 [CAD] to limit the number of created files. This value was later changed to 0.1 [CAD] for the post-processing utilities in combination with the purgeWrite option to reduce the output file size.

Firstly, the *freePiston* tutorial case of the *ColdEngineFoam* solver was used to set the problem geometry and to study the motoring pressure evolution in our modelled HCCI single-cylinder engine. *ColdEngineFoam* is a solver for non-combustion flow in internal combustion engines including mesh motion for the moving piston and using a turbulent flow solver.

The test case was then adapted to run with the *EngineFoam* combustion solver for compressible, turbulent and reacting engine flow. The solver is implemented with the possibility to model a spray fuel injection aimed at CI engine simulation. However, as HCCI combustion is fully premixed, this option was disabled.

4.1 Case Definition

As mentioned, the mesh is dynamic and evolves with the simulation time according to the engine geometrical parameters. OpenFOAM is designed for fully *3-Dimensional* (3D) simulations but an axisymmetric mesh can be simulated by applying special wedge boundary conditions. These wedge conditions are only used when the mesh is one cell thick as one face maps back to the opposite face of the same cell, allowing computations in the third dimension. The three physical limits (piston, liner and cylinder head) are specified as walls with corresponding boundary conditions. The studied engine has a flat cylinder head and flat piston crown. Neglecting the crevice zone, the combustion chamber is assumed as a perfect cylinder and is represented in Figure 4.2. Because the model is 3D axisymmetric, the mesh is a 2° section of a cylinder with only one cell of thickness.

We performed a sensitivity analysis of the number of cells in the mesh on the simulation results to find the best trade-off between precision and computational time. Indeed, the chemistry ODE system has to be integrated for each cell at every time step. Doubling the number of cells in one direction, for example, would double the computational time.

The selected mesh is composed of 50 cells radially, 130 cells along the cylinder axis and one cell in thickness. To correctly model turbulent cylinder wall heat transfer, the mesh is progressively refined close to the walls. The multi-grading ability of the blockMesh utility has been used to obtain a cell expansion ratio of 0.25 on the last 20% of the mesh length, meaning that the cell length gradually decreases by a factor 4.

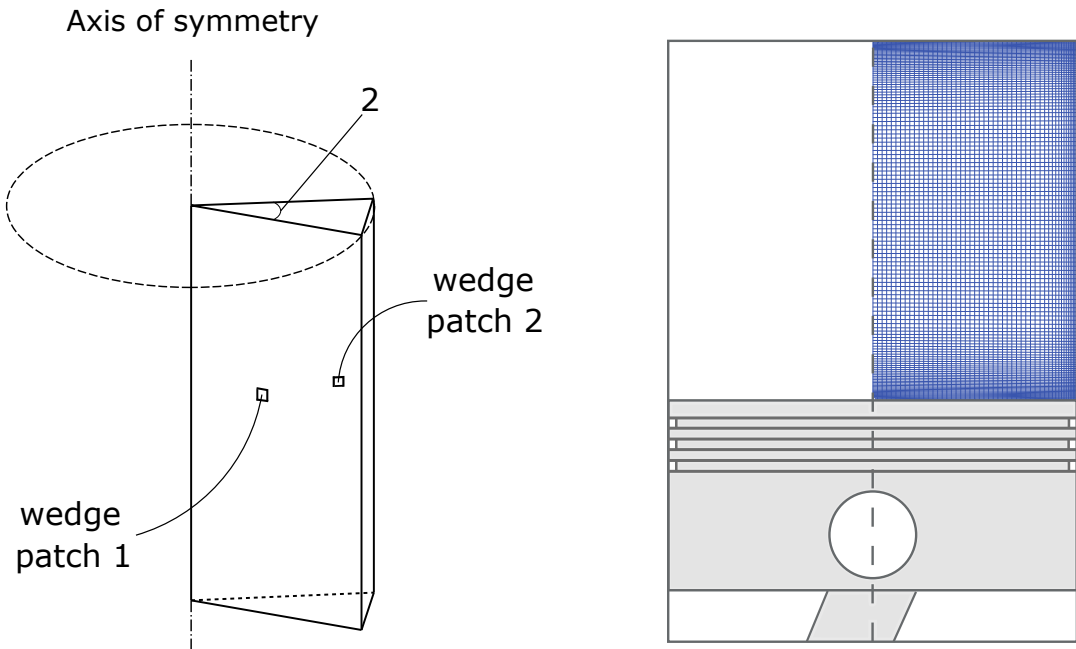


FIGURE 4.2: 3D and 2D representation of the wedge-type mesh used at -146[CAD]

Contrary to the 0-Dimensional model, the accuracy of the modelled TDC volume is important to depict heat transfer during the combustion and thus have a correct prediction of the MPFR. Hence, the geometrical compression ratio of the engine of 23:1 is used between BDC and TDC. To take into account the particularly late IVC of the engine and because the model assumes a closed system, the simulation is started later than -180 [CAD]. We have decided to use -146

[CAD] as the start of our simulations to model the effective engine compression of 21.65:1 between the simulation start and the TDC. The effective IVC used in the 0D model was -152 [CAD] with a starting pressure of 1 [bar]. Here, as we try to be as accurate as possible, we used the experimental intake pressure of 1.025 [bar] (cf. Section 4.3). For this different initial pressure condition, the effective IVC has been modified to better fit the engine effective compression.

The thermophysical models used for the in-cylinder charge are specified in a specific file of the constant directory. Combustion are simulated so that the charge is modelled as a reacting mixture with the different models required for chemical reaction and variable composition. The transport properties are based on Sutherland's law (Equation (4.1)), the dynamic viscosity (μ) is computed as a function of the temperature using the standard values of Sutherland coefficient ($A_s=1.67 \text{e-}6$) and temperature ($T_s=170.672$ [K]). From that, the thermal conductivity (κ) and thermal diffusivity (α), also used in internal enthalpy equations, are evaluated.

$$\mu = \frac{A_s \sqrt{T}}{1 + T_s/T} \quad (4.1)$$

The janaf method is used at each time step to evaluate the specific heat capacity at constant pressure (c_p) of the charge. The function giving c_p with respect to the current temperature (T) is the NASA polynomial [36] (Equation (4.2)) using NASA coefficients specified in the thermal data file of the chemical kinetics mechanism used:

$$c_p = R \left(a_4 T^4 + a_3 T^3 + a_2 T^2 + a_1 T + a_0 \right) \quad (4.2)$$

Additionally, the constants a_5 and a_6 are used to compute the enthalpy (Equation 4.3) and entropy (Equation 4.4) respectively:

$$H = RT \left(\frac{a_5}{T} + a_4 \frac{T^4}{5} + a_3 \frac{T^3}{4} + a_2 \frac{T^2}{3} + a_1 \frac{T}{2} + a_0 \right) \quad (4.3)$$

$$S = R \left(a_6 + a_4 \frac{T^4}{4} + a_3 \frac{T^3}{3} + a_2 \frac{T^2}{2} + a_1 T + a_0 \ln(T) \right) \quad (4.4)$$

All these coefficients are provided in the thermal file of the chemical mechanism for every species. Knowing the exact charge composition at each time step, the model computes these parameters using a weighted average. The perfect gas equation of state is used to derive other fluid properties. The energy form used for the energy equations is the sensible enthalpy. Sensible values are better suited to account for energy changes due to the reaction and the enthalpy is the norm used by the chemical kinetics package used.

The *Reynolds-Averaged Simulation* modelling (RAS) defines the in-cylinder turbulence with the standard k-epsilon turbulence sub-model for compressible flows. The initial internal turbulent kinetic energy (κ) and its dissipation rate (ϵ) are set to the standard values of $2.4\text{e-}5[\text{m}^2/\text{s}^2]$ and $5.7\text{e-}5[\text{m}^2/\text{s}^3]$ respectively. Pre-implemented wall functions are then used as boundary conditions.

HCCI combustion occurs in a homogeneous premixed charge so that the limiting factor is the chemical kinetics. Turbulence has a low impact on combustion. Therefore, a laminar combustion model is used with the option of the integrate reaction rate computation.

As stated previously, the starting point of our simulations is -146 [CAD]. Together with the endpoint of 30 [CAD], it is specified in the *controlDict* file of the test case. This endpoint is

selected to have the whole combustion range simulated but reduces the simulation time, as we are less interested in late expansion data.

The mesh refinement is essential to allow for a stable computational process and for the convergence of the solution. However, the simulation time step also is of prime importance. After a sensitivity analysis, a time step of 0.02 [CAD] has been determined as a trade-off between results accuracy and CPU time. The selected time step leads to a simulation maximum Courant number of $Co = 0.25$ for the calibration case (cf. Section 4.3). The Courant number is defined for one cell as:

$$Co = \frac{\partial t |U|}{\partial x} \quad (4.5)$$

Where ∂t is the time step, $|U|$ is the magnitude of the velocity field through the cell and ∂x is the cell size in the direction of the velocity [35]. CFD best practice is to keep this value under 0.3 for a stable and convergent simulation.

The finite volume discretisation schemes, linear equation solvers and tolerances (specified in fvSolutions and fvSchemes) were adapted from the *coldEngineFoam* tutorial ones with the experienced advice of Prof. Contino.

A complex chemical reaction mechanism is required for realistic computational fluid dynamics HCCI simulations. Indeed the combustion process starts by the auto-ignition of the premixed charge at high temperature and pressure. To this end, the built-in CHEMKIN chemical reading package is used on a detailed mechanism, similarly as in the 0D model. The chemical kinetics mechanism and the thermodynamic values used in this 3D axisymmetric model are still from AramcoMech 1.3. The mechanism contains 124 species and 765 reactions in total. However, solving the detailed system of equations describing the oxidation of the fuel on each of the 6500 mesh cells is bound to be time-consuming. Indeed, at each time step and in each cell, the chemistry ODE solver computes the temperature, pressure and species concentrations by integrating the chemical problem and the energy equations.

To reduce the computational cost, we implemented the *Tabulation of Dynamic Adaptive Chemistry* (TDAC) method to the chemistry solver [37]. TDAC is a coupling of two methods: the *Dynamic Adaptive Chemistry* (DAC) reduction scheme and the *In Situ Adaptive Tabulation* (ISAT) both allowing a computation time reduction. The DAC method reduces the chemical mechanism for local thermochemical conditions. It removes from the complete mechanism the species with computed influence lower than a user-defined reduction tolerance. This method hence reduces the impact of the mechanism size. A trade-off between mechanism precision and CPU cost had to be found. A tolerance value of 1e-4 was advised in [37] but we selected a more strict tolerance in the order of magnitude of 1e-5.

The ISAT algorithm stores the computationally demanding results already performed to reuse them. The thermochemical state is linearly approximated when the error is lower than the specified tabulation tolerance. The stiff ODE solver is thus not called at each time step on every cell, which decreases the impact of the total number of cells in the mesh. To represent accurately the pre-ignition reactions along with the first step of the combustion, a very small tabulation tolerance value is required. Initially, a tolerance of 3e-3 was used, leading to excessive pressure rise rates in the early phase of the combustion. Modelling the wall heat transfer requires a high number of cells, especially near the walls. This increases the level of in-homogeneities, hence a more severe tolerance is required. After a sensitivity analysis on our particular calibration case (cf. Section 4.3) the tabulation tolerance value of 3e-5 was selected.

4.2 Setup of Initial and Boundary Conditions

The initial chemical species concentrations are described in terms of mass fractions in files contained in the starting time directory. The concentration of the initial species is defined precisely to obtain the desired equivalence ratio in the different simulated cases. The other species contained in the chemical reaction mechanism are initialised at zero at the start of the simulation. The boundary conditions for the chemical species are defined as a zero gradient type.

The pressure boundary conditions are Von Neumann zero gradient conditions imposed on each wall. As the test bench is adapted for natural aspiration, the in-cylinder pressure at the start of the simulation (-146 [CAD]) will be close to 1 [bar]. To compare with an experimental result, the internal pressure field is set to 1.025 during the model calibration (see Section 4.3). For the sake of continuity, this initial pressure value is kept throughout the performed simulations.

To model cylinder wall heat transfer, Dirichlet boundary temperature conditions are imposed on the three walls of the axisymmetric mesh. The liner and cylinder head temperatures are fixed to 380 [K] according to previous experimental body temperature measurements. Conversely to the other surfaces, the piston is not directly cooled by the engine air-cooled system but mainly by the engine oil. Its temperature is thus fixed at a higher value of 430[K], which is a typical value found in the literature [35], [37]. However, these Dirichlet boundary conditions are an approximation. In reality, the wall temperature fluctuates spatially and temporally during the engine cycle. The internal charge temperature is set at a uniform value depending on the mixture composition to reach the auto-ignition close to the TDC. As a first approximation, the temperature values computed with the 0D model were used.

The charge velocity field is a vector along the three main directions (U_x, U_y, U_z) with x,y,z being respectively the radial, circumferential and axial directions. No-slip conditions are set at every solid boundary, stating that the fluid will have zero velocity relative to the boundary. A zero velocity is maintained throughout the simulation for cells bordering with the liner and the cylinder head. However, to maintain the fluid zero relative velocity during the piston motion, the axial velocity of the piston boundary cells will be set automatically to the piston velocity at each time step.

Originally, the internal velocity field of the in-cylinder charge was initialised to (0,0,0), but this initial condition was judged nonphysical at -146 [CAD] and did not allow to model the wall heat losses correctly. Indeed, engine intake flow and geometry combine usually to create a turbulent charge flow. Considering that the Yanmar L100V engine is, at conception, a CI direct-injection engine with a flat cylinder head and in-piston bowl, it is highly conceivable that the intake port was designed to create a swirl motion to optimise intake air and injected fuel mixing. The swirl flow macro-structure describes an organised rotation of the charge with respect to the cylinder axis, represented in Figure 4.3a. Swirl is created during the intake stroke by bringing the charge into the cylinder with an initial angular momentum, for example using a directed or helical intake ducts [38]. For homogeneous charge cases, mixing is not necessary. However, flow turbulence has an important impact on wall heat losses and thermal stratification. Hence, engine swirl has to be modelled to have an accurate simulation. Precise measurements of swirl are complex to obtain, they require a specific impulse swirl meter and no such experimental tests have been performed on our particular research engine.

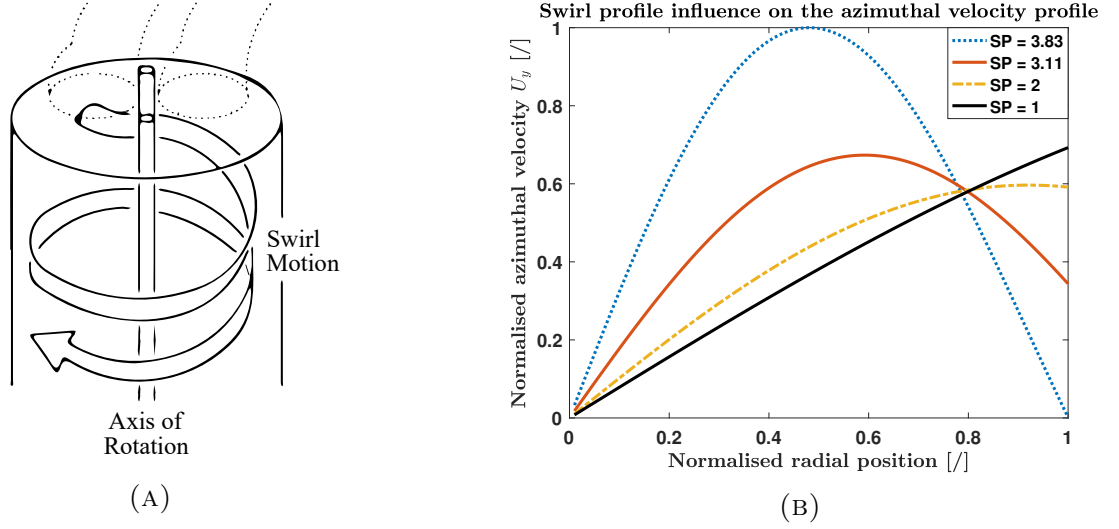


FIGURE 4.3: (A) Scheme of the engine swirl vortex (B) Azimuthal velocity U_y profile as function of the swirl profile

A swirling velocity field is initialised with the *engineSwirl* OpenFOAM pre-processing utility. This field is assumed perfectly centred around the stroke axis. The azimuthal velocity along the radial direction, $U_y(x)$, is defined by a complex Bessel function using three parameters: the swirl profile, swirl ratio and engine rotational speed. The swirl profile defines the global shape of the azimuthal velocity profile along the radial direction, as represented in Figure 4.3b. The Bessel function is defined to give the same angular momentum for the same swirl ratio. Higher values of the swirl profile correspond to higher initial slope of the azimuthal profile. The swirl profile of 3.11, suggested by Wahiduzzaman and Ferguson [39] for typical engine applications, was selected.

The swirl ratio scales the velocity of the flow field with the engine speed. It is defined as:

$$SR = \frac{\omega_s}{2\pi \cdot N} \quad (4.6)$$

where ω_s is the equivalent swirl velocity. It is defined as the angular velocity of a solid body rotating flow that has an equal angular momentum as the actual flow [38]. N is the engine rotational speed which is fixed at 1500 RPM in our case. The characterisation of the swirl ratio is done during the model calibration to fit the experimental pressure curve (cf. Section 4.3).

4.3 Model Calibration

To ensure physically correct and reliable simulation results, a model calibration based on experimental results is required. Unfortunately, methane-air combustion experiments have never been conducted on the UCLouvain HCCI test bench. Last year's hydrogen-air experiments are the closest results to our conditions. The main goal of this 3D axisymmetric model being to precisely describe the combustion pressure rise rate and duration, accurate results provided by M. Pochet were used.

The results supplied are from hydrogen-air combustion at an equivalence ratio of 0.2055 and an intake temperature of 352.5 [K]. They are post-processed with the TDC offset correction and

ready to be used. The file contained pressure data of 150 consecutive cycles of which the mean is represented further down this section in Figure 4.5. The measured average MPRR is 17.3 [bar/CAD] with a start of combustion at -3.5 [CAD] and a combustion duration of 1.8 [CAD].

The experimental measurements of the in-cylinder pressure are oscillating around 1.025 [bar] from the BDC to the effective IVC at -146 [CAD]. Measuring experimentally the pressure is challenging due to the quick variations and the large pressure span to cover. On the UCLouvain single-cylinder HCCI test bench, a piezoelectric sensor is used for dynamic pressure acquisition up to 150 [bar]. This sensor outputs a current signal amplified by a charge amplifier.

The measured signal is quite noisy, especially during the breathing phase, as the pressure variations are low. The uncertainty of in-cylinder pressure measurement around IVC is mainly due to the sensor being used in its lower extreme range. For the breathing phase, M. Pochet computed a lower bound, conservative in-cylinder pressure uncertainty of around 0.01 [bar] (cf. [5] Appendix A.4.2 and A.4.3). After consultation with M. Pochet and Prof. Jeanmart, we decided to set the initial pressure to 1.025 [bar] to fit the pressure curve as best as possible.

A summary of the model initial and boundary conditions discussed in Section 4.2 is presented in Table 4.1. All those values are coming from direct measurements on the experimental test bench except the piston temperature and swirl profile that are common values for ICE.

Effective compression ratio	21.65:1 [/]
Starting CAD	-146 [CAD]
Initial pressure	1.025 [bar]
Liner temperature	380 [K]
Cylinder head temperature	380 [K]
Piston crown temperature	430 [K]
Swirl Profile	3.11 [/]

TABLE 4.1: Initial and boundary conditions summary

The calibration of the simulation is made by adjusting the initial charge temperature and swirl ratio. These two values are not measured experimentally and finding the perfect combination between the two parameters turned out to be challenging.

The HCCI test bench is not equipped with an in-cylinder temperature dynamic sensor. The only information about in-cylinder temperature was the intake value from which we could approximate the BDC temperature using a correlation (cf. Section 3.3.1). However, correlations of this type are inaccurate with an estimated error close to 10%. Moreover, the initial temperature required is the one at -146 [CAD] and not at BDC. We thus started from the 0D model prediction of $T(-146 \text{ CAD}) = 370 \text{ [K]}$ knowing further adjustments of this value would be required.

As a first step, we selected couples of initial charge temperature and swirl ratio that fit the experimental motoring pressure evolution. The two parameters affecting the pressure evolution, defining acceptable pairs was done iteratively while staying within reasonable values. Afterwards, we switched to full combustion modelling including the chemical reaction model. Doing so, we observed that initial temperature close to 370 [K] led to late ignition and weak combustion. We had to focus on higher temperatures. Further combinations of SR and temperature were then investigated.

Keeping everything else constant, increasing the swirl ratio increases the heat losses and the charge thermal stratification. As a result, the auto-ignition timing is delayed and the combustion duration is extended, leading to lower values of MPRR. The initial charge temperature has also an impact on the auto-ignition timing and the pressure evolution during the compression phase. However, its impact on the MPRR is weaker. Targeting the best fit of the experimental curve, we determined by trial and error that a swirl ratio contained between 2 and 2.2 should lead to a correct prediction of the combustion behaviour. The azimuthal velocity profile ($U_y(r)$), corresponding to these ratios for a swirl profile of 3.11 and a rotational speed of 1500 RPM, is presented in Figure 4.4.

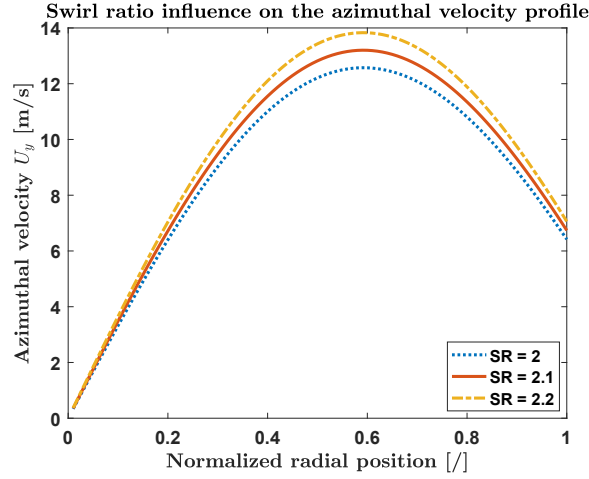


FIGURE 4.4: Swirl ratio influence on $U_y(r)$ for a swirl profile of 3.11 and 1500 RPM

The complete sensitivity study resulted in the selection of a swirl ratio of 2.1 and a starting charge temperature of 294 [K] at -146 [CAD].

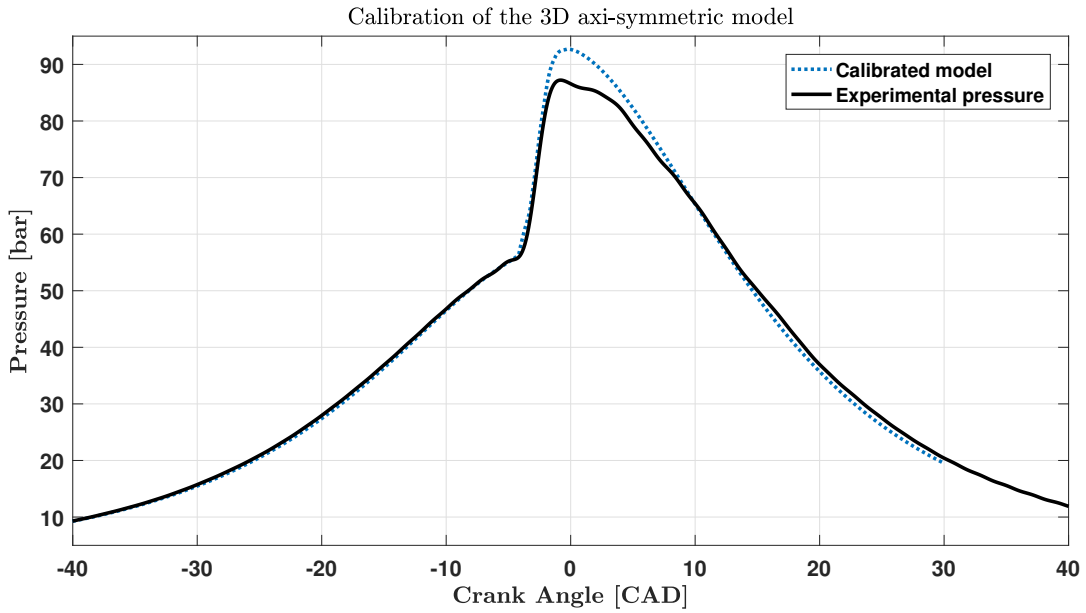


FIGURE 4.5: Experimental pressure curve and simulated pressure curve after calibration

One can observe in Figure 4.5 that the simulated pressure curve fits accurately the experimental pressure on the majority of the simulated crank window. The auto-ignition timing is well estimated and the combustion behaviour prediction in terms of MPRR seems satisfactory. Nevertheless, the simulated pressure is overestimated during the late phase of the combustion, leading to a higher maximum in-cylinder pressure. During the expansion following the combustion, the pressure is firstly overestimated due to the higher maximum pressure but evolves gradually to be slightly underestimated at the end of the simulation.

Cycle-to-cycle variations lead to a flattening of the pressure rise rate when measured on the mean pressure curve [17]. To avoid this phenomenon, the experimental MPRR is computed on each cycle and averaged. The pressure measurement has a resolution of 0.1 [CAD]. The experimental MPRR is thus determined using this resolution, leading to the computed mean value of 17.3 [bar/CAD] for the calibration.

To ensure the convergence of the numerical simulation results, the time step used in our model is fixed at 0.02 [CAD]. Computing the simulated MPRR on this reduced time step could lead to an overestimation, misleadingly denoting brutal auto-ignition. The modelled MPRR is thus computed using a time interval of 0.1 [CAD] to use the same resolution as in the experimental results. The resulting modelled MPRR value is 17.7 [bar/CAD], which is considered accurate.

It is wise to remember that the results generated and discussed in this chapter are estimations and that experimental confirmations would be desirable. The model was calibrated on the only available data with a different fuel and energetic content. Parameters such as the swirl ratio, initial and walls temperatures are selected to tune the model but were not measured experimentally on the test bench. The model convergence has its limitations and lower tolerances in terms of time step and TDAC always increase the fidelity of the results. The choices made were the results of a trade-off to reduce the running time because we had to perform the simulations with limited resources.

4.4 Simulation Results

Once the model has been precisely calibrated on experimental results, useful data are generated and observed. This section contains a compilation of the most relevant results obtained using the developed model. Firstly, the parameters used to interpret the results are presented along with the explanation of how they are computed. Then, air and pure oxygen methane HCCI combustion predictions are presented and compared for different equivalence ratios. The optimal combustion timing is discussed and the high load limit is determined. Subsequently, the influence of different parameters on the combustion MPRR is detailed. Finally, the influence of CO₂ (synthetic EGR) on the combustion duration and high load limit is investigated.

4.4.1 Description of the Interpretation Parameters

The fuel content is expressed in terms of FuelMEP in this chapter. Contrary to the 0D model, the influence of the intake charge temperature on the volumetric efficiency is taken into account. The model starts at an initial volume defined by the mesh. From the initial values of charge temperature and pressure, the model computes the mixture density using the perfect gas law. The total mass at the start of the simulation is then computed with a domain integrate of the density. Using the user-defined mass fractions of each species, the model then initialises the mass of each chemical element. The FuelMEP is finally computed from the mass of the fuel, its LHV and the engine displacement, as presented in the following equation:

$$\text{FuelMEP} = \frac{m_{fuel} \cdot \text{LHV}}{V_d} \quad (4.7)$$

Therefore, the starting charge temperature influences the FuelMEP for a set equivalence ratio.

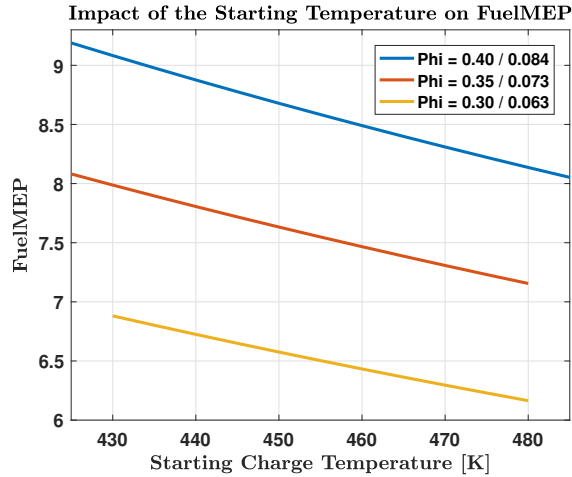


FIGURE 4.6: Impact of the simulation starting temperature on FuelMEP

Figure 4.6 shows that, for an increasing starting temperature, T(-146 CAD), the FuelMEP decreases because the total mass at the beginning of the simulation is lower. This phenomenon is explained by the decrease in charge density. The results were obtained from air and pure oxy-combustion simulations, hence the two different values of equivalence ratio for each curve. For a fixed temperature, we have the same fuel content for the two types of combustion. This confirms the factor of 4.76 between the two equivalence ratio definition (cf. Section 1.3.1).

Using OpenFOAM run-time data processing with the implemented Qdot functionObject, the simulation computes and outputs the heat release rate for each time increments in each cell. Performing a volume integral of these returned values at each time step allows us to have the complete HRR value over the whole mesh at each time step. Further integrating with regards to the time step provides the cumulative heat release curve that allows to define the combustion timing parameters such as CA10, CA50 and CA90 (cf. Section 2.3). These parameters enable the observation of the impact of several factors on the ignition timing and the combustion duration. For reference, an example of heat release rate and cumulative heat release obtained with the model is represented in Figure 4.7. For the sake of brevity, the results are interpreted in terms of CA10, CA90 and DOC but the cumulative heat release curve is not plotted for each simulation.

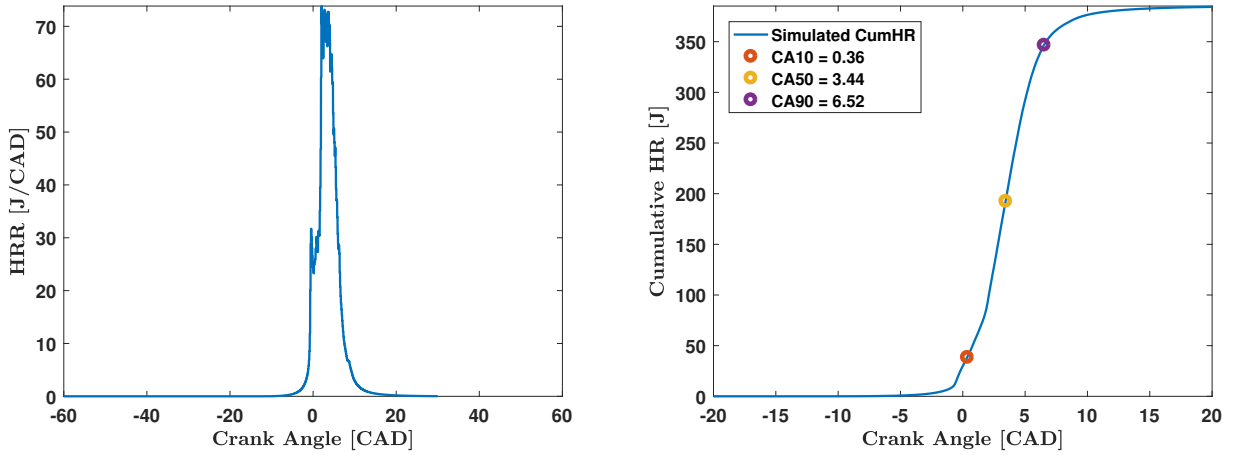


FIGURE 4.7: HRR and cumulative HR for oxy-combustion with $\phi=0.084$ and $T_{\text{start}}=435$ [K]

The heat release rate (HRR) curve graphed in Figure 4.7 is globally correct but the first bump is non-physical. In reality, the HRR curve is expected to be composed of a monotonic increase leading to a maximal value and followed by a monotonic decrease in the late stage of combustion. This observed inaccuracy is linked with the AramcoMech1.3 chemical kinetics mechanism. The strange behaviour of the heat release rate during the early phase of combustion leads to imprecision in the cumulative heat release. The combustion pressure thus increases in two steps, which is particularly observable for low-load results. The impact on the combustion timing parameter determination is small. As the MPRR values are more critical for high load operations, this imprecision is judged minor even if non-physically correct.

From the cumulative heat release curve, an image of the combustion efficiency can also be derived. Indeed, its maximal value ($Q_{\text{gross max}}$) depicts the total heat energy released by the charge during the combustion. The heat release mean effective pressure (QhrMEP) can be computed by dividing the determined maximum heat release, $Q_{\text{gross max}}$, by the cylinder displacement (V_d). The combustion efficiency (η_c) is then obtained by the ratio of QhrMEP on FuelMEP. As HCCI combustion is triggered by auto-ignition, high values of the combustion efficiency ($\eta_c \geq 0.9$) are expected. Combustion with $\eta_c \leq 0.9$ is regarded as unsatisfactory in the following results as low values of the combustion efficiency indicate an incomplete combustion.

The considered research engine being originally a naturally aspirated single cylinder engine, the in-cylinder peak pressure limit is set at $P_{\text{max}} = 100$ [bar] to ensure it withstands the combustion.

HCCI engines narrow operating range and their high load limit have been detailed in Section 1.2.4. In short, the rapid HCCI combustion process causes brutal pressure rise rates that can result in critical engine noise and mechanical damage. This phenomenon is named ringing. In practice, to decrease the pressure rise rate, low fuel content are used in HCCI engines, causing low power density. The technicians from the UCLouvain IMMC laboratory have extensive experience with HCCI combustion experimentation. For them, 15 [bar/CAD] is the outermost limit in terms of MPRR. They hardly ever surpass 12 [bar/CAD] as intense noise is produced by such brutal combustion. We have proven that our model faithfully represents the combustion behaviour but still comports some approximations. Therefore, a conservative ringing threshold is set at $MPRR = 10$ [bar/CAD].

To determine the optimal auto-ignition timing, the net IMEP is not computable as we don't have the pressure data over the full 720 [CAD] cycle. The gross IMEP is thus computed between -180 and 180 [CAD] with the following equation:

$$IMEP_g = \frac{-1}{V_d} \cdot \int_{-180}^{180} p \cdot dV \quad (4.8)$$

However, it has been observed in Figure 4.5 that the 3D axisymmetric model overestimates the peak in-cylinder pressure and later undervalues the expansion pressure. Moreover, as stated previously, the simulation starts at -146 [CAD] and ends at 30 [CAD] in an effort to reduce the long required computational time. Prior to the effective IVC, the in-cylinder pressure is assumed constant at 1.025 [bar]. The later part of the expansion, from 30 to 180 [CAD], is approximated by an isentropic expansion with a constant ratio of specific heat ($\gamma = 1.3$) selected to fit the experimental pressure at the exhaust valve opening (EVO). An example of extended pressure curve using these assumptions is represented in Figure 4.8. In reality, the expansion is far from isentropic, due to cylinder wall heat losses reducing the charge temperature. The ratio of specific heat is hence increased leading to a negative impact on the pressure. Nevertheless, because the simulation stops at 30 [CAD], the charge mean temperature is not defined for CAD further than this end point so gamma correlations could not be used either. Trying to fit the EVO experimental pressure by selecting γ accordingly is a way to take into account this pressure loss. However, the expansion pressure is still underestimated in the first part then overestimated in the later part of the expansion. The $IMEP_g$ value being sensible to the late expansion phase, its estimated value is not considered accurate. Still, the computed $IMEP_g$ value allows a comparison between numerical results despite the above-described approximations.

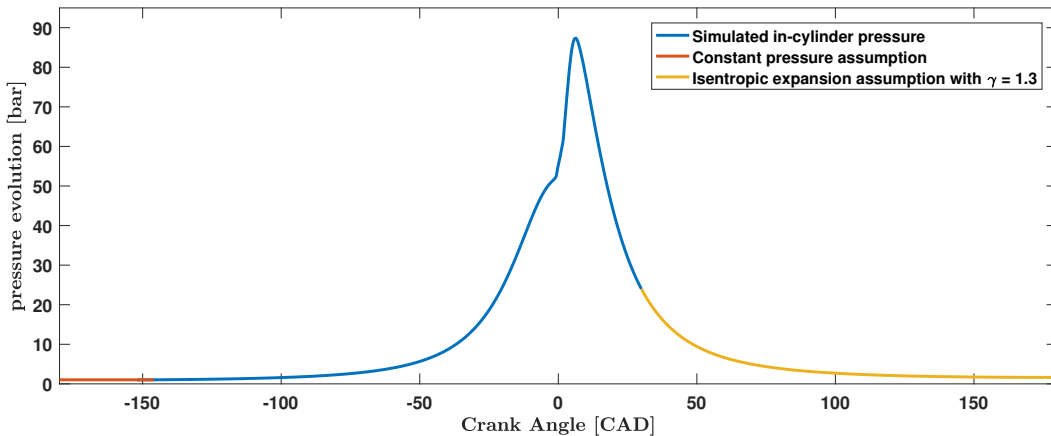


FIGURE 4.8: Extended pressure curve for oxy-combustion with $\phi=0.084$ and $T_{start}=435$ [K]

4.4.2 Methane Air and Oxy-combustion Results

The decisive goal of the 3D model is the comparison between air and oxy-combustion behaviour. Simulation results for these two types of combustion are presented in this subsection for different equivalence ratios. The aim was to observe similar combustion with the same fuel content and ignition timing to isolate the effect of using pure oxygen as oxidiser on the MPRR. However, fixing the equivalence ratio similarly to what has been done in the 0D model does not exactly fix the FuelMEP as it has been demonstrated in Figure 4.6. For a set equivalence ratio, the start of combustion is controlled by the starting charge temperature, $T(-146\text{CAD})$, that is modified by steps of 5 [K]. This choice was made to reduce the number of runs required as the computing time exceeded 48 hours in the worst cases.

Results for $\phi = 0.3 / 0.063$

The simulated combustion obtained with the equivalence ratio of 0.3 (and corresponding 0.063 in oxy-combustion) are relatively weak and lead to low values of peak cylinder pressure. For reasons of clarity, only the pressure curves with the optimal combustion timing are represented in Figure 4.9, for both combustion types.

For our high compression ratio engine, FuelMEP varying around 6-7 [bar] (depending on the starting temperature) lead to low engine loads illustrated by the estimated IMEP_g in Figure 4.11. The equivalence ratios of 0.3 and 0.063 are thus on the low load side of our HCCI engine, contrary to what was expected by the 0D model results. Methane having a high octane number, the ringing limit is expected to be located at higher loads. As we are interested in finding the high load limit, higher fuel contents are then simulated. Nevertheless, the results obtained for these corresponding fuel contents deserve to be observed thoroughly.

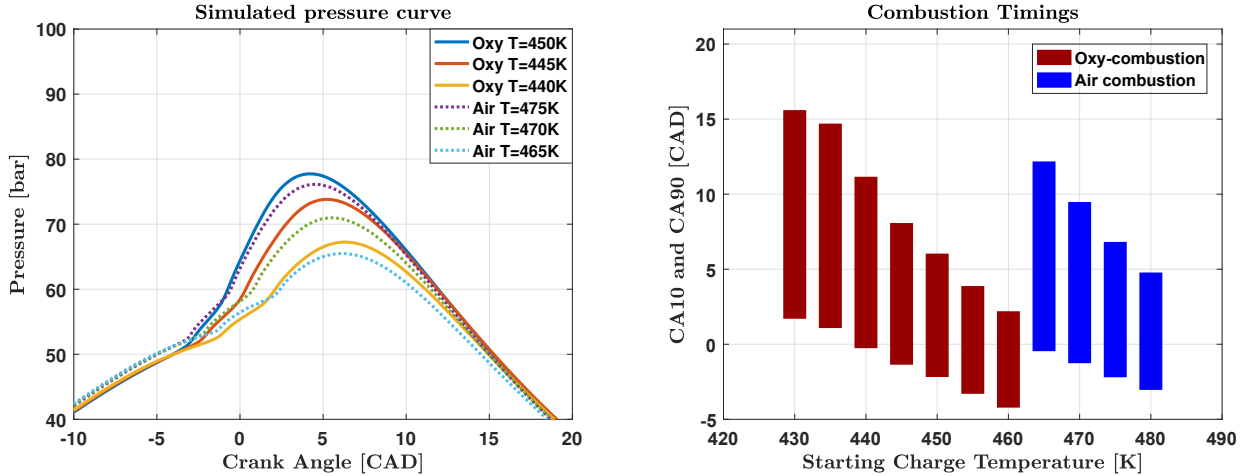


FIGURE 4.9: Air and Oxy-Combustion Simulation Results for $\phi = 0.3/0.063$: Pressure evolution and combustion timing

The graph on the right in Figure 4.9 illustrates the combustion timing for both air and pure oxy-combustion with respect to the simulation starting charge temperature, $T(-146\text{ CAD})$. Each vertical bar represents the interval between the start and the end of combustion (CA10 & CA90). The length of each bar thus depicts the total duration of combustion (DOC = CA90 - CA10). This graph confirms that, for the same SOC timing, oxy-combustion auto-ignition occurs with an

internal charge temperature reduction of approximately 20-25 K in comparison to air-combustion. This observation was also depicted using the required T_{BDC} with the 0D model. For similar CA10, the duration of combustion of an oxy-combustion is shorter. The combustion timing graph also exhibits the impact of the start of combustion on the total combustion duration. An advanced combustion is quicker and, the later the auto-ignition is, the longer the combustion gets. This technique can be used up to a point to reduce the combustion brutality.

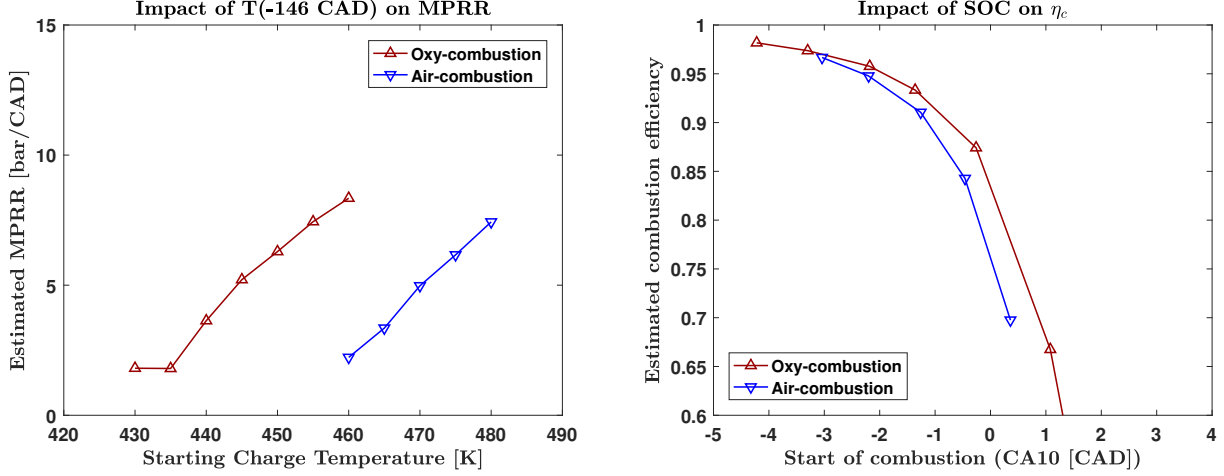


FIGURE 4.10: Impact of T(-146 CAD) on MPRR and of SOC on η_c for $\phi = 0.3/0.063$

The MPRR values computed for these weak combustion are far from the ringing threshold set at 10 [bar/CAD], even for large timing advances. The first graph in Figure 4.10 shows the influence of the starting charge temperature, and indirectly of the combustion timing, on the combustion MPRR. Increasing the initial charge temperature advances the start of combustion. The more advanced the combustion is, the more brutal the pressure increase becomes, as the piston compression influences the combustion.

Reducing the starting charge temperature is beneficial for increasing the overall efficiency of the system, but it retards the auto-ignition timing. If this timing is too retarded, the combustion won't be complete due to bulk quenching, as the in-cylinder temperature drops during the expansion. This phenomenon is more severe for low fuel content and is represented on the second graph of Figure 4.10 by the rapid decrease of the combustion efficiency. If we exclude combustion with $\eta_c \leq 0.9$, oxy-combustion with Tstart lower than 440 [K] and air-combustion with Tstart lower than 470 [K] should be disregarded.

The $IMEP_g$ is estimated to determine the optimal auto-ignition timing for a set equivalence ratio. The value also allows to have an idea of the HCCI engine power density under different conditions. A too advanced auto-ignition timing is detrimental to the gross indicated mean effective pressure because the pressure increase before the TDC reduces the mechanical work produced by the combustion. As observed previously, a too retarded auto-ignition leads to low in-cylinder pressure and incomplete combustion, which is also undesirable for the $IMEP_g$. Figure 4.11 illustrates that the optimal $IMEP_g$ is reached for a slight ignition advance of around 1 [CAD] for both combustion types. One can observe that the maximal engine load is higher for oxy-combustion. This is partly due to the higher fuel content linked to the lower required charge temperature for similar combustion timing.

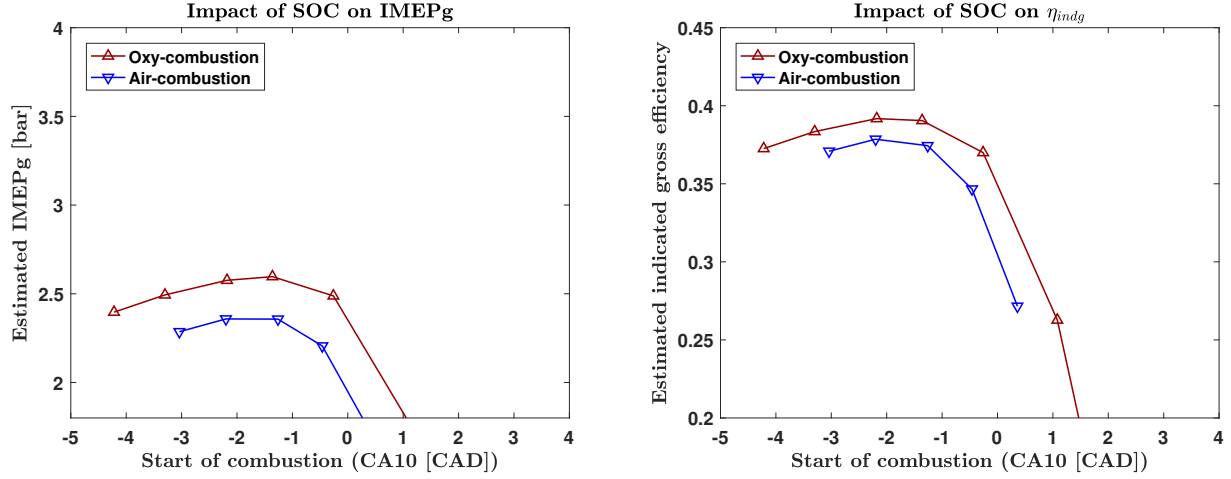


FIGURE 4.11: Impact of SOC on the estimated IMEPg and η_{indg} values for $\phi = 0.3/0.063$

To determine the optimal start of combustion independently from the varying FuelMEP, the gross indicated efficiency (η_{indg}) is used. The start of combustion has a similar impact on this parameter but the optimal value seems to be reached for slightly more advanced timings. The oxy-combustion leads to higher efficiency than their air combustion counterparts. For these corresponding equivalence ratios, the optimal combustion is obtained with $T_{start} = 445\text{-}450$ [K] for oxy-combustion and $T_{start} = 470\text{-}475$ [K] for air combustion.

Results for $\phi = 0.35 / 0.073$

Given the low loads reached with the simulation results for $\phi = 0.3/0.063$, higher fuel contents were progressively investigated to find the oxy-combustion high load limit of our particular high compression ratio research engine.

Firstly, combustion with equivalence ratios of $0.35/0.073$, corresponding to a FuelMEP between 7 and 8 [bar], depending on the starting temperature (cf. Figure 4.6), were simulated. The in-cylinder pressure curves simulated for these corresponding fuel fractions are represented in Figure 4.12. Comparing these curves to the ones with lower fuel content, significant increases of the pressure rise rates and peak pressures are observed. The equivalence ratio is strongly influencing the combustion behaviour. The range of starting charge temperature does not significantly change as the equivalence ratio has a minor impact on auto-ignition timing. Therefore, the start of combustion is mainly controlled by the charge temperature, as stated in Section 1.2.3. Increasing the equivalence ratio only advances slightly the auto-ignition timing for oxy-combustion and retards it for air combustion, as observed with the 0D model in Section 3.4.1 and 3.4.3. Nevertheless, the impact is very limited and may be affected by other factors in running engines.

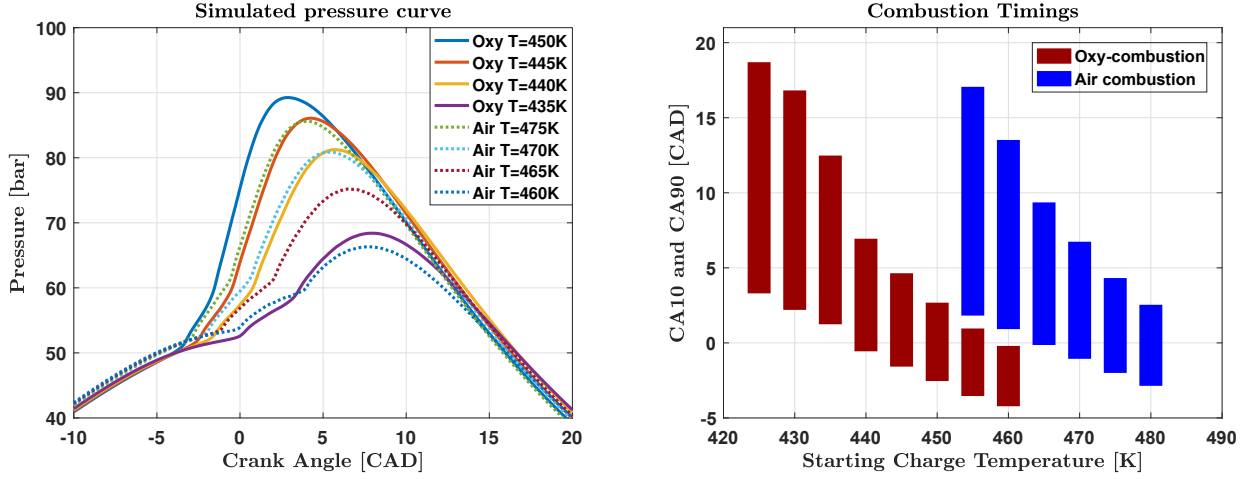


FIGURE 4.12: Air and Oxy-Combustion simulation results for $\phi = 0.35/0.073$: Pressure evolution and combustion timing

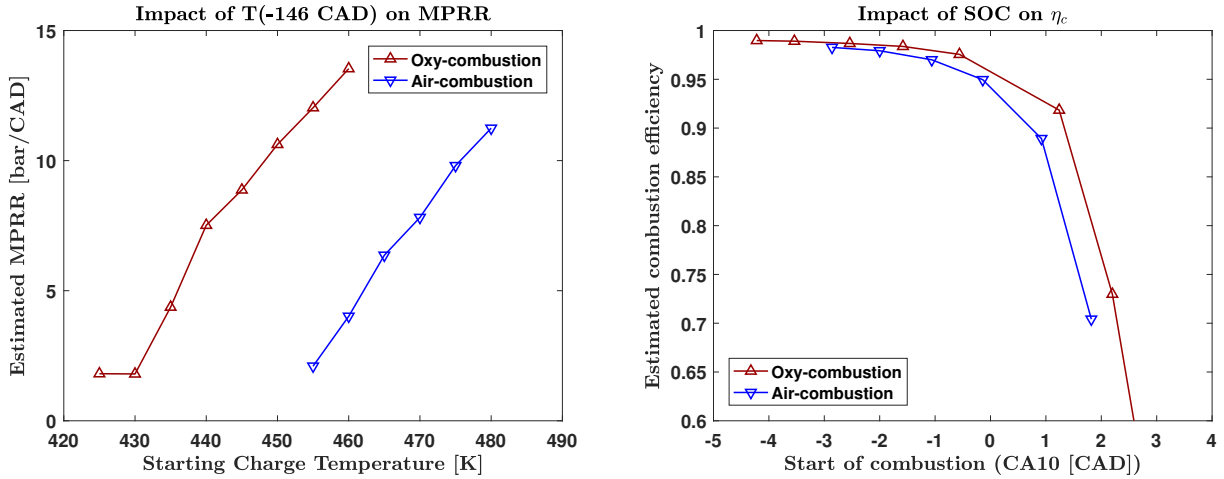


FIGURE 4.13: Impact of T(-146 CAD) on MPRR and of SOC on η_c for $\phi = 0.35/0.073$

The combustion timings represented on the second graph in Figure 4.12 follow the same tendencies observed at a lower equivalence ratio in Figure 4.9. The required temperature difference between air and oxy-combustion for the same auto-ignition timing is unchanged at approximately 20-25 [K]. Moreover, the impact of the start of combustion on the total combustion duration is still significant. Finally, for a similar CA10, oxy-combustion DOC is again smaller than air combustion DOC. The increase in equivalence ratio significantly reduces the DOC of both types of combustion for comparable start of combustion. This reduction in DOC is linked with the higher pressure rise rate.

As expected, the MPRR values in Figure 4.13 are higher due to more brutal combustion. This puts in evidence the strong impact of fuel content on the combustion pressure rise rates. However, the ringing threshold is only reached for high temperatures that leads to premature auto-ignition. Figure 4.13 also illustrates the strong impact of the starting charge temperature, hence of the ignition timing, on the MPRR. The more advanced the combustion is, the larger the MPRR gets. For comparable SOC, the MPRR seems to be higher for pure oxy-combustion but the

difference is much less striking than what was predicted by the 0D model. The sensitivity of the MPRR on various parameters is investigated more precisely in a following subsection.

For higher fuel contents, the maximum values of the combustion efficiency are higher. Indeed, they lead to higher combustion temperature that allows a more complete oxidation of the charge. The steep drop in combustion efficiency for retarded timing is still experienced. Although, the drop is observed at slightly later timings than previously. The cause of this drop is still the in-cylinder expansion accompanied by a sudden drop of charge temperature, leading to bulk quenching. The right graph in Figure 4.13 indicates that oxy-combustion has a higher combustion efficiency. If we exclude combustion with $\eta_c \leq 0.9$, oxy-combustion with Tstart lower than 435 [K] and air-combustion with Tstart lower than 465 [K] should be disregarded.

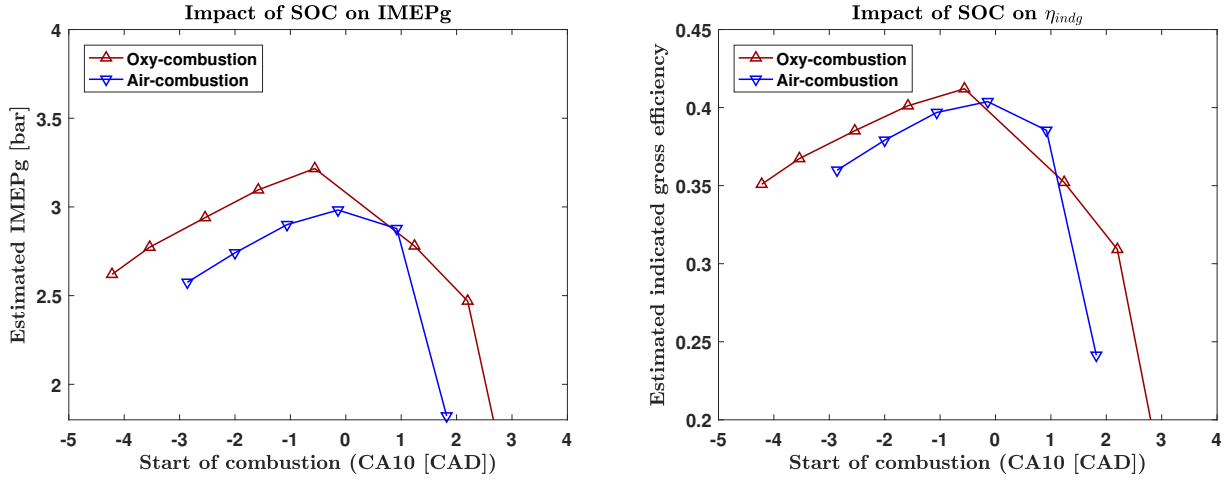


FIGURE 4.14: Impact of SOC on the estimated IMEP_g and η_{indg} values for $\phi = 0.35/0.073$

The values of IMEP_g computed from these simulations at higher equivalence ratio indicate higher engine loads. This increase of estimated engine load with the fuel content is expected as the combustion releases more heat, leading to higher values of pressure. Even though an advanced ignition timing increases the maximum combustion pressure, for more brutal combustion, the advance is more detrimental to the IMEP_g as the pressure rise before the TDC is enhanced. The optimal start of combustion is thus located at a lower advance for these higher fuel contents. The IMEP_g drops once more for retarded starts of combustion as a result of lower combustion efficiencies and lower pressure peaks.

To remove the impact of FuelMEP variations, the optimal timing is determined using the gross indicated efficiency. Looking at the right graph in Figure 4.14, the optimal SOC timing seems to be located around the TDC for both air and oxy-combustion. A higher efficiency is although noticed in oxy-combustion. The optimal oxy-combustion is reached when Tstart = 440 [K]. The corresponding MPRR has a value of 7.54 [bar/CAD] and the estimated IMEP_g is 3.21 [bar].

Results for $\phi = 0.4 / 0.084$

The ringing threshold is not reached for FuelMEP varying around 7-8 [bar] so further simulations with a higher ϕ of 0.4/0.084 were conducted. These equivalence ratio values lead to a FuelMEP varying from 8 to 9 [bar] (cf. Figure 4.6). The simulated pressure curves graphed in Figure 4.15 depict more powerful and brutal combustion, due to the FuelMEP increase.

All the tendencies described in the two previous results subsections are confirmed by the figures given below.

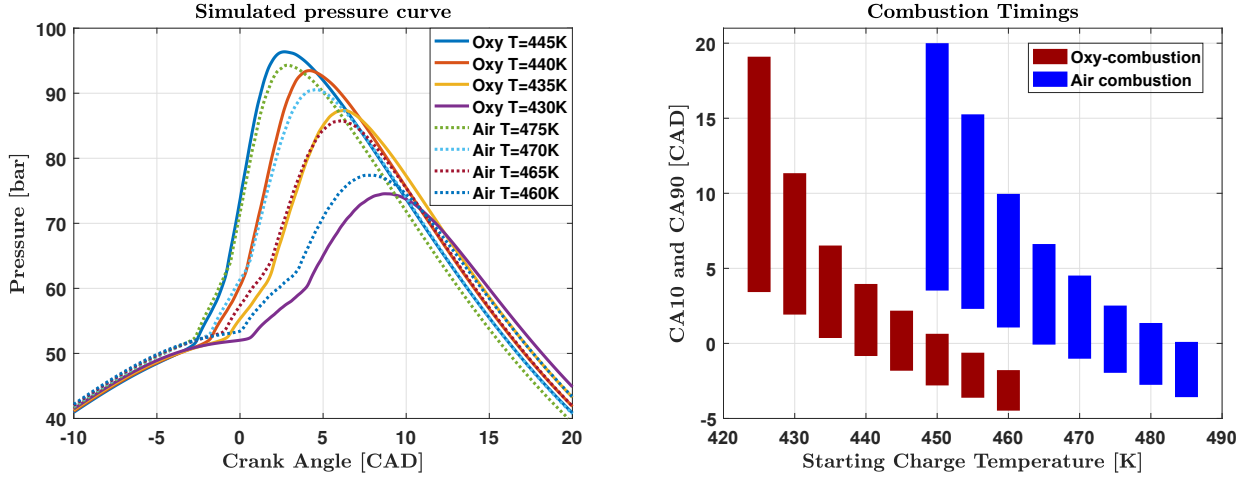


FIGURE 4.15: Air and Oxy-Combustion simulation results for $\phi = 0.4 / 0.084$: Pressure evolution and combustion timing

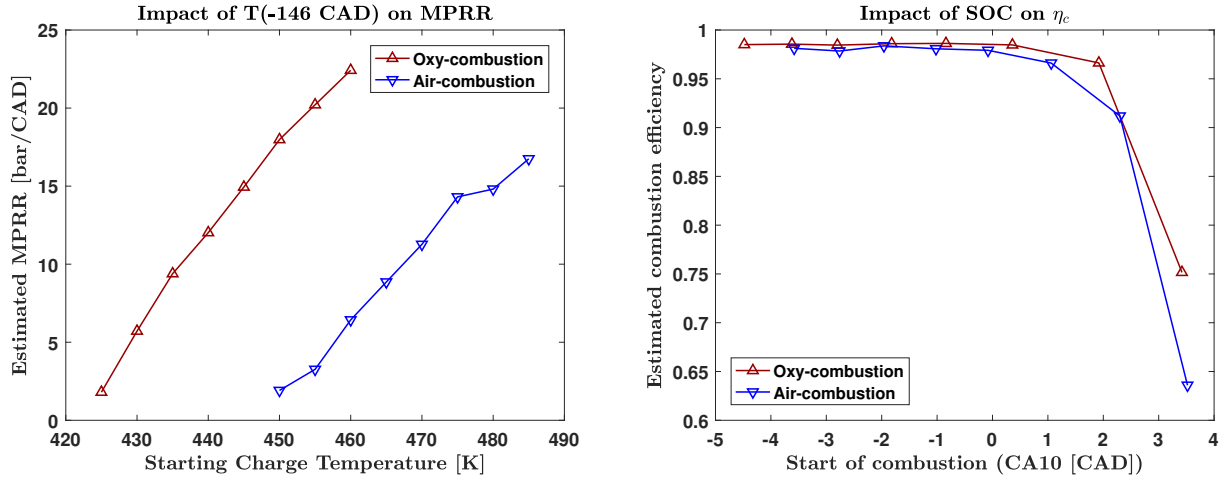


FIGURE 4.16: Impact of T(-146 CAD) on MPRR and of SOC on η_c values for $\phi = 0.4/0.084$

The higher charge energetic content further reduces the duration of combustion as it can be observed on the second graph in Figure 4.15. The impact of the CA10 on the DOC is really magnified here and the difference in $T_{BDC}(CA_{10}=TDC)$ is still around 20 [K], as predicted by the 0D model.

The Maximum pressure rise rate values presented in the first graph of Figure 4.16 grow with an increasing starting charge temperature as the timing is advanced. For a set temperature, so an almost set timing, the MPRR goes up with the equivalence ratio. At this last fuel content, the high load limit is exceeded for slightly advanced combustion. Starting temperature higher than 470 and 435 [K] should be disregarded for air and oxy-combustion respectively. Fortunately, looking at both graphs of Figure 4.17, the optimal combustion occurs for a timing close to the TDC or even slightly retarded, thus for lower temperature than the above-mentioned limits.

The positive impact of an increasing equivalence ratio on the combustion efficiency is proven in the second graph of Figure 4.16 as values up to 98% are reached. The high values of η_c are maintained for later auto-ignition timings as high energetic contents lead to higher in-cylinder temperatures reducing the bulk quenching risk. Even so, the combustion efficiency eventually drops due to the in-cylinder expansion.

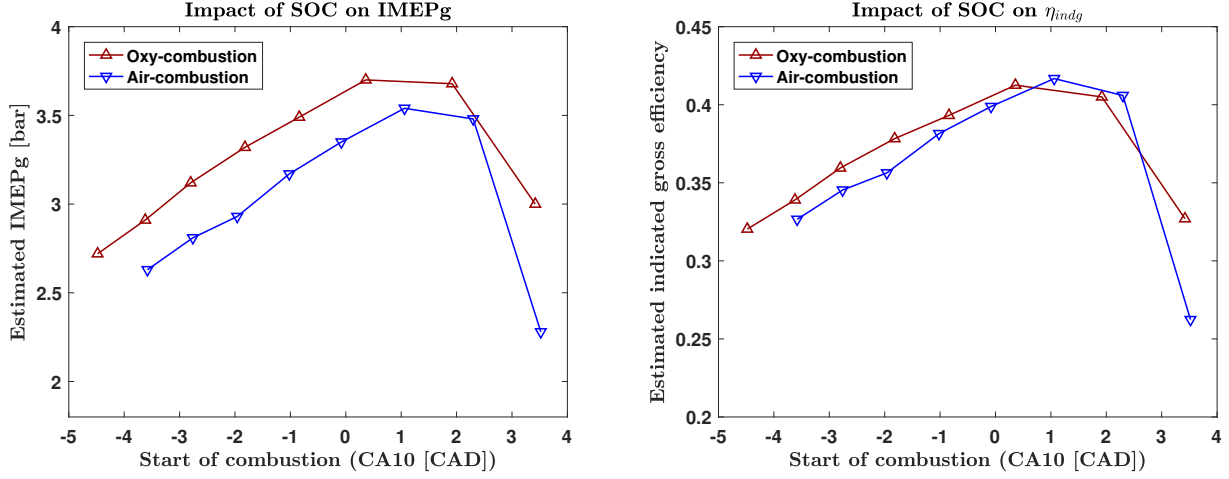


FIGURE 4.17: Impact of SOC on the estimated IMEP_g and η_{indg} values for $\phi = 0.4 / 0.084$

The estimated IMEP_g values for the optimal timing are still increased compared to the values obtained with $\phi = 0.35/0.073$. The engine load seems to be proportional to the amount of fuel in the mixture as an increase in the optimal gross IMEP of approximately 0.5 [bar] is observed for each step increase of equivalence ratio. However, one should remember that the IMEP_g arise from an approximation of the expansion and should not be considered perfectly accurate. The estimations are used to compare numerical results on a correct basis.

Looking at the indicated gross efficiency plot in Figure 4.17, we observe that, for higher loads, the optimal timing is moved to later SOC. The efficiency obtained for the two types of combustion are comparable even though the optimal is reached for barely later SOC for air-combustion.

The optimal oxy-combustion is obtained for a CA10 around the TDC. An MPRR of 9.392 [bar/CAD] is estimated for this combustion with CA10 = 0.36 [CAD] and a FuelMEP of approximately 9 [bar]. As a consequence, the equivalence ratio of 0.084 is considered as the reasonable high load limit for pure oxy-combustion in our specific HCCI engine.

For air combustion, on the other hand, the optimal timing $CA10 \approx 1$ [CAD] leads to an estimated MPRR of 6.43 [bar/CAD]. Hence, the high load limit of conventional combustion is located at higher equivalence ratio than oxy-combustion in this particular engine. This is partly due to the higher temperature required leading to lower values of FuelMEP.

As explained in Section 4.4.1, because our simulation stops at 30 [CAD], the IMEP_g estimation is based on an approximation of isentropic expansion with $\gamma=1.3$ kept constant between 30 and 180 [CAD]. When a combustion starts later in the expansion, the mean in-cylinder pressure is higher at 30 [CAD]. Late burning of the charge leads to lower pressure peaks but higher mean expansion pressure. This second effect is amplified with higher fuel content. An observation of the (p,V) diagram in Figure 4.18 highlights the beneficial impact of the expansion pressure on the IMEP_g value. The diagram is limited on the x axis to clearly indicate the difference between the curves. Up to the BDC volume of 455.46 [cm³], a later combustion timing (lower

Tstart) will have a slightly higher expansion pressure. Nevertheless, this positive impact is quickly surpassed by the negative influence of the low pressure peak. In the particular case of a pure oxy-combustion at $\phi=0.084$, the optimum is reached with a CA10 = 0.36 (Tstart = 435 [K]). The constant γ value may slightly impact the optimum location as later combustion leads to higher temperature at 30 [CAD] but also increased wall heat losses.

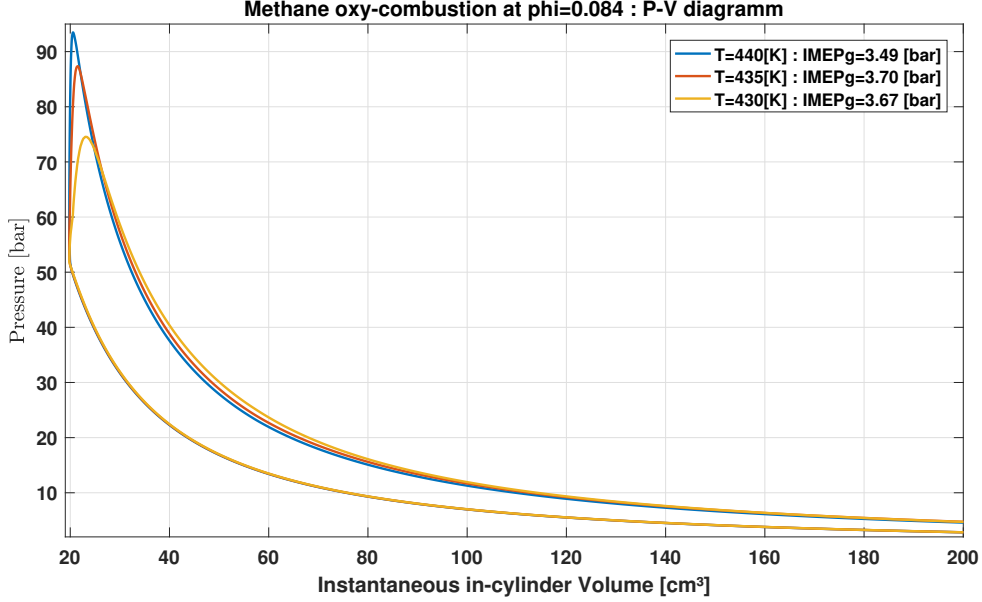


FIGURE 4.18: (p,V) diagram for the optimal oxy-combustion at $\phi = 0.084$

4.4.3 Sensitivity Analysis of Different Parameters on MPRR

In the previous results subsections, computed combustion MPRR values were represented with respect to the starting charge temperature linking the values to the pressure curves with ease. However, this representation does not allow a direct comparison between air and oxy-combustion simulations as a same starting charge temperature is linked to the same fuel content but different combustion timings.

The influence of the start of combustion on the estimated MPRR value for different equivalence ratios is represented in Figure 4.19. This representation allows to study the impact of the combustion timing and fuel content on the MPRR. However, a fixed equivalence ratio does not perfectly fix the FuelMEP as discussed earlier. By only plotting points higher than MPRR = 3 [bar/CAD], we disregard weak and incomplete combustion.

The strong impact of the ignition timing is striking and increases with the equivalence ratio. Indeed, if the charge auto-ignition occurs during the compression stroke, the pressure increase due to the combustion is enhanced by the piston compression leading to a higher value of MPRR. In the case of HCCI combustion, this timing is mainly controlled through the charge intake temperature and, in the case of our simulations, T(-146 CAD). Depending on the equivalence ratio acting on the combustion intensity, the optimal combustion timing varies slightly, as observed in the previous section.

For a fixed combustion timing, an increase of the equivalence ratio results in an increase of the combustion pressure rise rates for the two combustion type. For equivalence ratios in

the low-load range, the MPRR values obtained for air and oxy-combustion are comparable at corresponding ignition timing. However, as it is observable in Figure 4.19, increasing the charge fuel content has a stronger impact on oxy-combustion MPRR values. Hence, the Ringing limit is reached sooner for HCCI pure oxy-combustion.

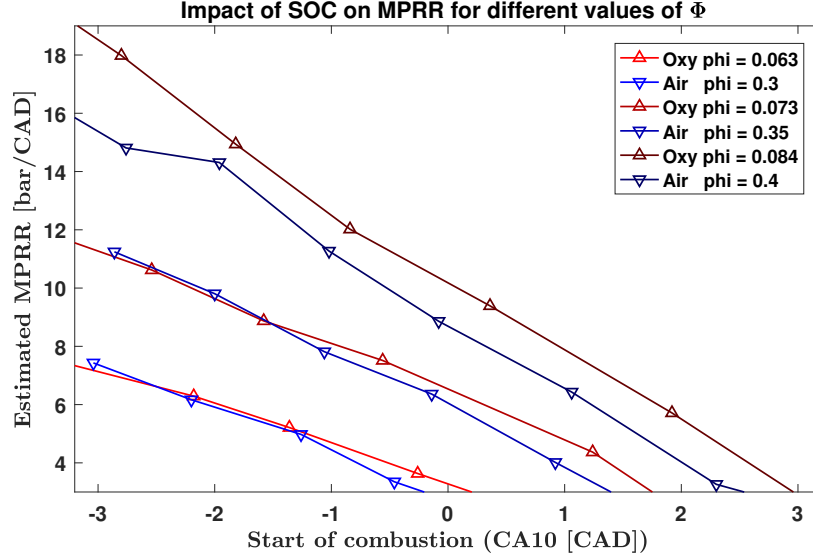


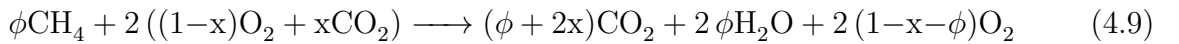
FIGURE 4.19: Influence of SOC and Φ on the MPRR for air and oxy-combustion

The mixture composition has an impact on the MPRR values via the oxidiser choice and the fuel content. The addition of carbon dioxide in the intake flow also influences the combustion behaviour. This effect is investigated in the following subsection.

4.4.4 Methane Oxy-combustion with EGR

The last simulations conducted with the 3D axisymmetric model aimed to prove the benefits of using EGR in oxy-combustion. To that end, methane oxy-combustion with a pure flow of carbon dioxide were simulated.

As a reminder, the complete oxy-combustion of methane with our simulated EGR is represented in Equation (4.9)



The EGR used is x , the molar proportion of carbon dioxide with respect to oxygen, ranging from 0 to $1 - \phi$ while staying under $1 - \frac{2}{9.52}$, as previously discussed. According to this definition, the EGR rate does not affect the FuelMEP. A modification of intake temperature, on the other hand, would slightly change the FuelMEP because the charge density of the engine is affected, as previously mentioned.

Firstly, using the same starting charge temperature of $T(-146\text{CAD}) = 460[\text{K}]$, the impact of EGR on the combustion behaviour is investigated. As confirmed in the previous section, oxy-combustion leads to more violent combustion compared to air combustion. The introduction of CO_2 at the intake helps to reduce the maximum pressure rise rate by two combined effects. First of all, the carbon dioxide acts as a heat buffer and postpones the charge auto-ignition.

CO_2 then continues to absorb heat during the combustion and thus slows down the oxidation reaction kinetics, spreading out the combustion. These two effects on the ignition timing and the combustion duration are observable in the two graphs of Figure 4.21.

Figure 4.20 exhibits the behaviour of EGR on the pressure evolution while the starting temperature is kept at 460 [K] and the equivalence ratio at 0.084. Along with reducing the MPRR by delaying and extending the combustion, the EGR rate reduces the maximum in-cylinder pressure. The EGR rate of 10% leads to an incomplete burn ($\eta_c=0.675$) because the ignition is too retarded for this given equivalence ratio.

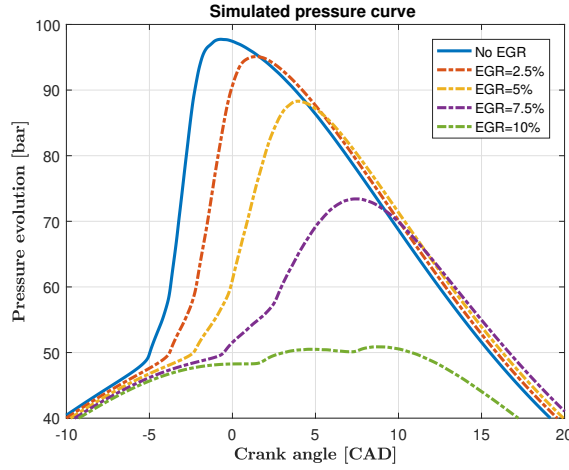


FIGURE 4.20: Influence of the EGR rate on pressure evolution for $T(-146\text{CAD})=460[\text{K}]$ and $\phi=0.084$

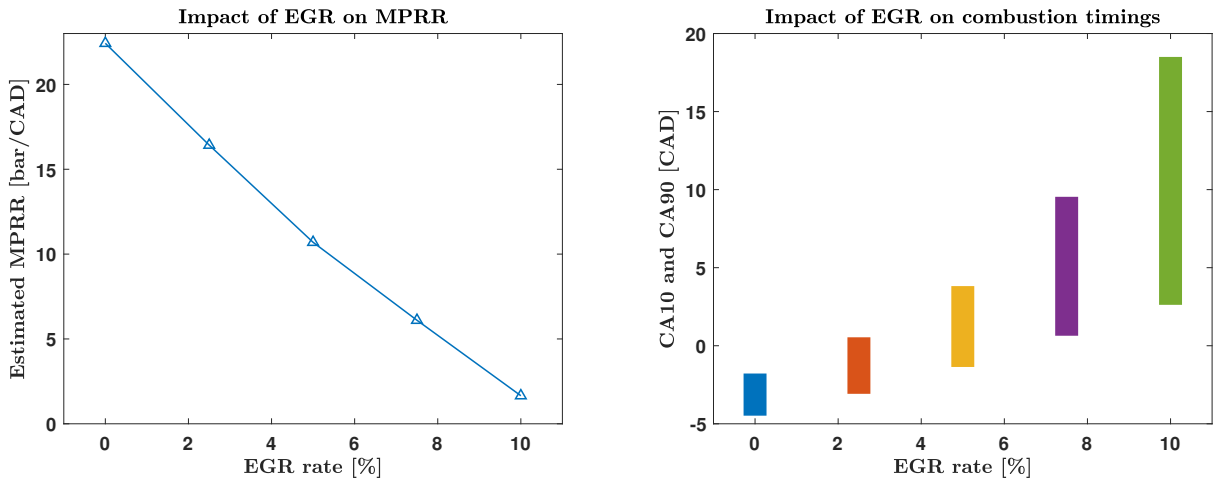


FIGURE 4.21: Impact of EGR on MPRR and combustion timings for $T(-146 \text{ CAD}) = 460 [\text{K}]$ and $\phi = 0.084$

These tests compare the behaviour of different EGR rates at a constant fuel content. The optimal IMEP_g was reached for EGR = 7.5% at 3.39 [bar] which is slightly under what was computed for the optimal pure oxy-combustion at 3.7 [bar] for the same equivalence ratio and comparable ignition timing. That difference is partly due to the slight difference in FuelMEP

linked to the difference in starting charge temperature. Moreover, as stated previously, CO_2 absorbs a certain quantity of the combustion heat. However, the EGR seems to have a very limited impact on the gross indicated efficiency with $\eta_{\text{indg}} = 0.399$ for the optimal combustion with EGR and $\eta_{\text{indg}} = 0.412$ without EGR.

The main effect of the EGR perceived in our simulations is the postponement of the ignition timing that, in itself, inevitably increases the duration of combustion.

As the MPRR experienced at the optimal combustion timing were acceptable in the previous simulations, it was eventually decided to increase the equivalence ratio gradually to improve the power density of the engine. By increasing gradually and simultaneously the fuel content and the EGR rate, higher values of estimated IMEPg are reached while maintaining reasonable pressure rise rates.

For the sake of continuity, the model parameters were left unchanged. We discovered that, for early auto-ignition timing, the simulation results do not converge at high fuel content. This can be linked to the mesh refinement, the time step or even the TDAC tolerances selected. However, further refinement of these parameters would lead to an important increase in the computation time. The convergence issue is accentuated as the equivalence ratio increases because the combustion gets even more brutal. The following represented results are therefore the best results we could achieve without experiencing a convergence issue, even though the ignition is significantly retarded and the pressure rise rates are relatively soft. Luckily, the optimal start of combustion in terms of IMEPg is retarded as the fuel content increases. Despite the above-mentioned limitation, considerable engine load improvements were obtained using EGR.

Φ	FuelMEP [bar]	EGR rate [%]	CA10	CA90	MPRR [bar/CAD]	IMEPg [bar]	η_{indg}
0.084	8.98	0	0.36	6.52	9.40	3.70	0.412
0.095	9.94	2.5	1.40	7.40	9.59	4.04	0.406
0.105	10.98	5	3.66	12.66	5.24	4.56	0.415
0.116	12.02	6.25	4.84	13.66	5.25	4.92	0.409
0.126	13.05	7.5	6.74	17.35	4.52	5.31	0.407

TABLE 4.2: Conditions optimising the IMEPg compared to the optimal pure oxy-combustion

Table 4.2 presents the conditions that optimise the engine load (IMEPg) for higher values of fuel content with EGR. Besides the pure oxy-combustion, which started at 435[K], all the presented results have a starting charge temperature of 440 [K]. The estimated gross indicated efficiency is approximately constant, allowing a proportional increase of the IMEPg with the FuelMEP. As the fuel content increases, the optimal start of combustion is quite importantly delayed, also helping the reduction of pressure rise rates. A late ignition of the charge is beneficial in terms of mean pressure during the expansion phase even if the peak pressure is reduced. However, the optimum is quickly surpassed as a too late ignition of the charge reduces the combustion efficiency. The advantage of higher experienced mean expansion pressure is indeed hindered by the lower peak pressure. All the results presented in the above table are almost complete combustion with $\eta_c \geq 0.95$. The maximal simulated FuelMEP of 13.05 [bar], corresponding to $\phi = 0.6$ for air combustion, lead to an IMEPg value of 5.31 [bar]. This represents a leap of 43% in gross engine load over the high load limit observed in pure oxy-combustion.

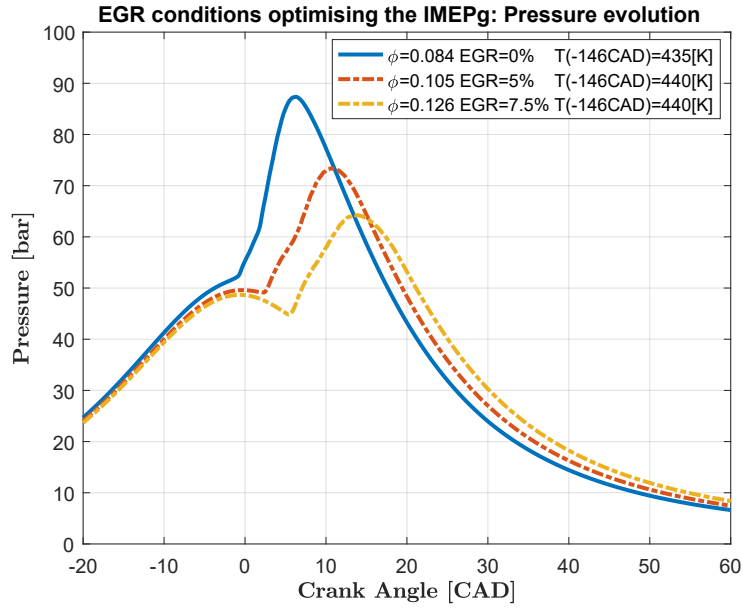


FIGURE 4.22: Influence of the EGR rate and equivalence ratio on pressure evolution

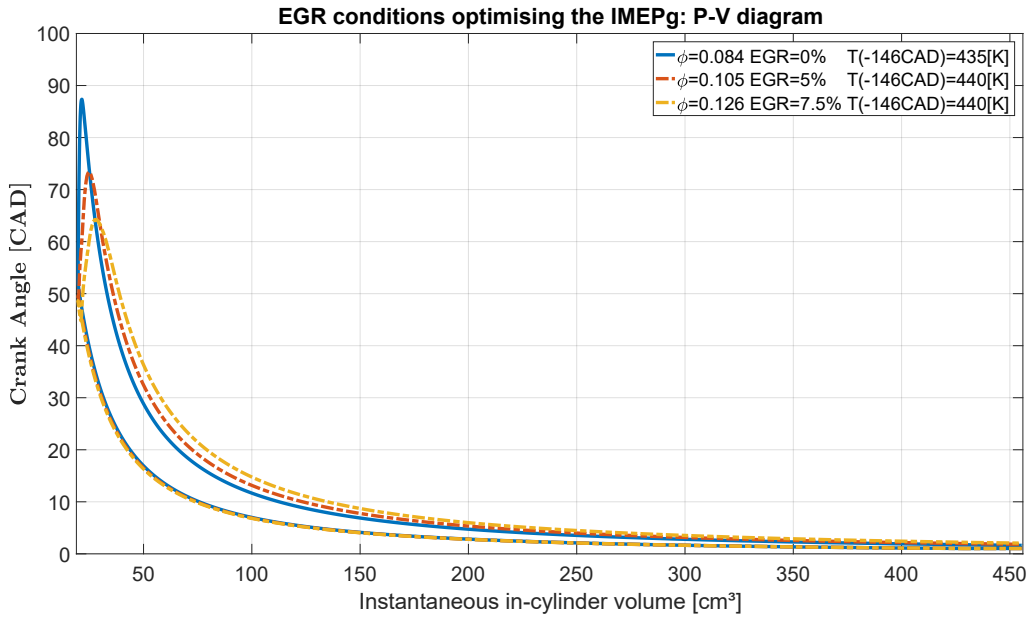


FIGURE 4.23: Influence of the EGR rate and equivalence ratio on a P-V diagram

Figure 4.22 exhibits the pressure evolution for different conditions optimising the IMEPg with different EGR rates while Figure 4.23 illustrates the corresponding P-V diagram. The P-V diagram from the start of the compression to the end of the expansion phase gives an adequate representation of the IMEPg. Even though the peak cylinder pressure is achieved without EGR at lower equivalence ratio, the slower combustion experienced with EGR helps to maintain a higher pressure during the expansion. The mean pressure during expansion thus increases, which helps reach higher values of IMEPg.

Concerning the computation of the IMEPg, the constant value of $\gamma = 1.3$ was kept to approximate the expansion after 30[CAD]. This value is already quite low even though the ratio of specific heat of CO_2 is lower, especially for decreasing temperature ($\gamma = 1.3$ at 1300[K] and 1.1 at 650[K] respectively). The maximum molar fraction of CO_2 used is 7.5% corresponding to a mass fraction of approximately 10%. The impact of the carbon dioxide addition on the charge ratio of specific heat, and thus on the estimated IMEPg, is minor.

Moreover, the accuracy of the EGR results of this subsection is limited by the reaction mechanism. Indeed, as previously mentioned, the chemical mechanism used is AramcoMech. Unfortunately, previous studies highlighted that this mechanism is not the most suited for oxy-combustion with carbon dioxide addition. CO_2 chemically influences the reaction, resulting in different reaction kinetics. Alves et al. [40] discovered that the formation of CO is greatly increased during oxy-combustion compared to air combustion due to reactions of CO_2 with H_2 and CH_x radicals. Unlike N_2 , a very large amount of CO_2 directly participates in fuel oxidation reactions, and thus the chemical kinetics of oxy-fuel combustion is strongly affected.

Hu et al. [41] compared multiple reaction mechanisms for methane oxy-combustion and proved, based on experimental results, that AramcoMech does clearly not depict correctly the evolution profile of CO compared to other mechanisms such as USC-MechII.

Even though the EGR effects observed in this section are consistent with the theory, the simulation results should not be considered flawless because of this chemical mechanism limitation. The limitations may explain the high relative effect of EGR in our results compared to the experimental oxy-combustion results obtained by Kang et al. [23] using the same EGR definition.

Conclusion

The present work has numerically investigated the potential of methane oxy-combustion in a HCCI engine. Replacing the air by pure oxygen as the oxidiser is challenging as it leads to a more reactive intake charge. However, the benefits of this technology outweighed this challenge. The absence of nitrogen results, at stoichiometry, in exhaust gases nearly only composed of a pure flow of carbon dioxide and water. This allows carbon dioxide capture useful for the methanation process. Furthermore, the increased reactivity is favourable to reduce the required intake temperature, which improves the global efficiency of the system.

The first chapter has exposed the theoretical context of the technology. The fundamental concepts of HCCI combustion have been detailed and oxy-combustion has been explored theoretically. As very few research works have been conducted on HCCI oxy-combustion, further studies had to be carried out with methane to explore the potential of this application.

The specifications and required modifications of the experimental test bench have been detailed in the second chapter. The heat release and heat losses experimental computing methods have also been exhibited. In the third chapter, a 0D single zone model has then been used to approximate the required intake conditions for air and oxy-combustion. The effect of hydrogen and carbon dioxide addition on the required T_{BDC} has also been observed. Hydrogen addition has been judged detrimental due to the increase of charge reactivity.

Towards the goals of a better comparison between methane air and oxy-combustion, a HCCI 3D axisymmetric model has been developed specifically and used in the last chapter. A better representation of the wall heat losses and non-uniformities inside the cylinder allows a more accurate combustion behaviour prediction. Calibrated with hydrogen air combustion, this model enables to estimate the ringing limit of our research engine. The use of synthetic EGR has been eventually investigated to go beyond this limit and increase the engine power density.

According to the 3D simulation results displayed in the last chapter, the increase in combustion brutality for pure oxy-combustion is lower than expected. The upper load limit is reached sooner than for conventional HCCI air combustion, but the optimal pure oxy-combustion still produces an acceptable amount of work. The methane oxy-combustion ringing limit is reached at a FuelMEP of 9 [bar] corresponding to $\phi = 0.084$. At this equivalence ratio, the optimum CA10 is slightly later than TDC leading to a MPRR of 9.4 [bar/CAD], an estimated IMEPg of 3.7 [bar] and η_{indg} of 41.2%. It has been found that the optimal auto-ignition timing is delayed for a rising fuel content. The load increase potential of EGR is proven through simulation by carbon dioxide addition in the intake despite non-negligible model limitations. CO₂ absorbs heat and extends the combustion duration, allowing the use of higher fuel content. A FuelMEP of 13 [bar] is reached numerically within the limits and leads to an estimated IMEPg of 5.31 [bar] and η_{indg} of 40.7%. Hence, an increase of more than 40% of the engine load is foreshadowed.

Outlook for Future Work

Methane oxy-combustion potential has been numerically explored for the UCLouvain research engine. The objective of this master's thesis has thus been met even though many perspectives for future development remain. Further numerical investigations on the impact of EGR on oxy-combustion could be conducted using the developed 3D model with a different chemical reaction mechanism. Nonetheless, the numerical simulation approach contains numerous approximations jeopardising the results' quality. An oxy-combustion experimental campaign would be desirable to validate, or not, the model predictions.

Being designed for multiple electrofuels, the engine is not optimised for pure methane HCCI combustion. To study the full potential of methane oxy-combustion, higher compression ratios and intake pressures, through turbo compression, should be used to reach optimal BMEP and overall efficiency but also higher power density. To do so, a different engine setup should be used as the maximum geometric compression ratio is met with the actual test bench. Moreover, turbocharging leads to higher in-cylinder pressure peaks and thus requires a more resistant engine block.

In a future experimental research, the use of water direct injection to reduce oxy-combustion high pressure rise rates could be evaluated as well as possible synergies with EGR. Alternatively, the 3D axisymmetric model could be modified to simulate water direct injection, as spray modelling is implemented in the OpenFOAM 7 toolbox.

Finally, as observed during the 3D model calibration, swirling vortices reduce the combustion brutality by increasing the thermal stratification. The effect of turbulence on combustion timing could be simulated numerically and confirmed experimentally by using different piston crowns or ports designs.

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Appendix A

HCCI Experimental Setup

A.1 Mass Flow Controller Conversion Table

Gas	Gas Factor	Orifice Factor	Density [kg/m ³]	Recommended	Allowed
Air	0.9980	1.018	1.293	Viton	Epdm/Buna/Teflon
NH ₃	0.7860	0.781	0.771	Epdm/Teflon	Buna/Teflon/Kalrez
CO ₂	0.7400	1.255	1.977	Buna	Kalrez
CO	0.9950	1.000	1.250	Viton	Buna/Epdm/Kalrez
CH ₄	0.7630	0.763	0.717	Buna/Viton	Kalrez
O ₂	0.9880	1.067	1.429	Viton	Epdm/Kalrez

TABLE A.1: conversion table for Brooks thermal mass flow controller with recommended and allowed joint material. Source J-836-D-508 Rev.D

A.2 Yanmar L100V Original Data Sheet

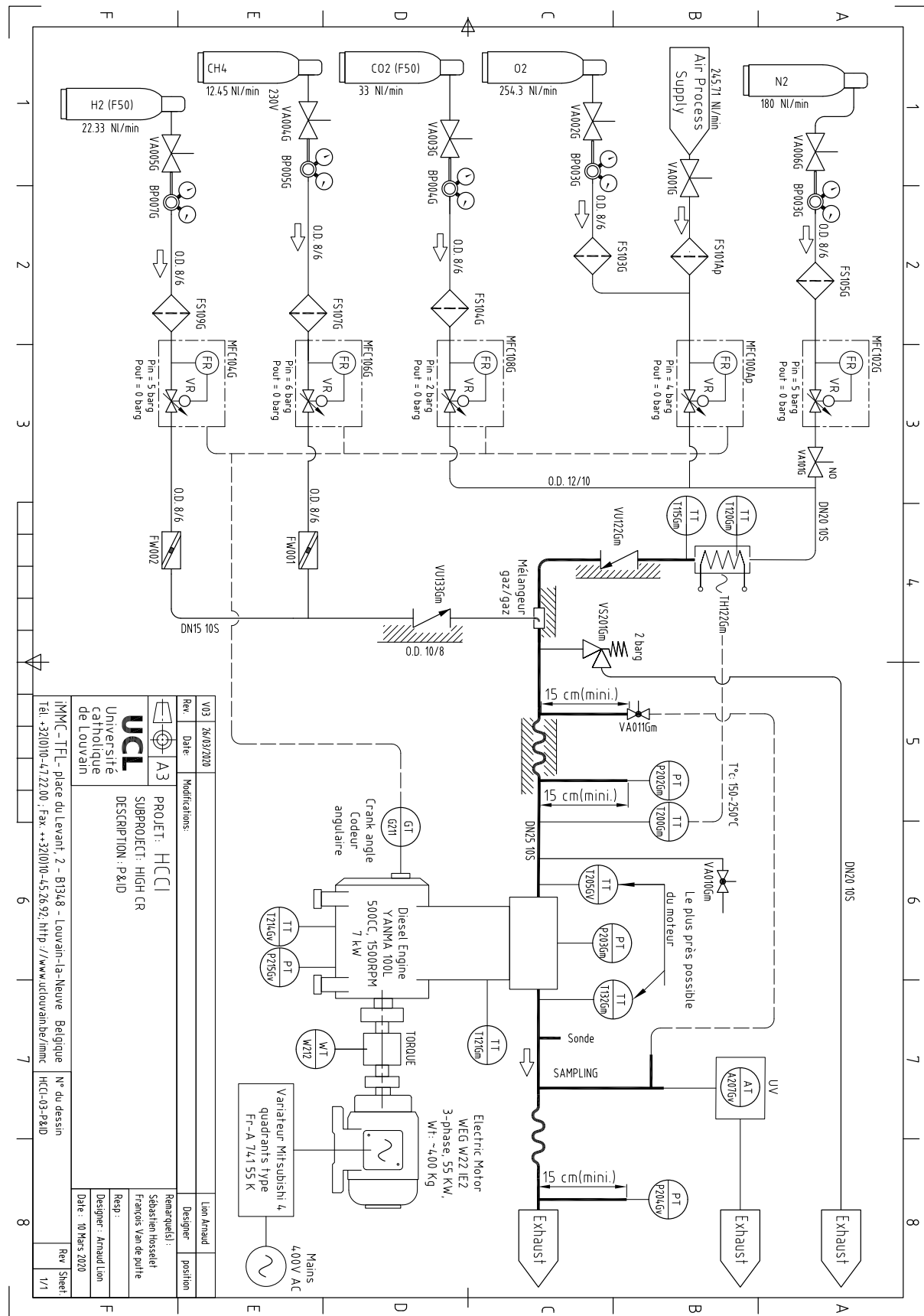


FIGURE A.1: Original Yanmar L100V monocylinder engine. ¹

Model	L100V
Engine Type	Air Cooled, 4 cycle, Vertical Cylinder
Fuel	Diesel
Number of Cylinders	1
Bore x Stroke	86mm x 75 mm
Combustion Type	Direct Injection
Total Displacement	435 cc
Aspiration	Natural Aspiration
Valves per Cylinder	2
Rated Speed	3600 rpm
Net Intermittent	9.1 Hp[6.8kW]/3600rpm
Net Continuous HP	8.3hp [6.2kW]/3600rpm
Direction of Rotation	Counter Clockwise, Viewed from PTO Side
Crankshaft Type	Straight Keyed, Tapered or Threaded
Starting System	Recoil or Recoil/12 V Electric
Decompression System	Manual Type with Auto-return Lever
Charging System	12 Volt, 15 Amps (for Electric Start Models)
Electric Stop Device	Optional, Fuel Stop Solenoid (for Electric Start Models)
Cold Start Aid	Optional, Intake Air Heater (for Electric Start Models)
Fuel Tank Capacity	4.7 liters
Brake Specific Fuel Consumption at Rated Output	279 g/kW-hr
Lubrication System	Pressure Lubrication with Trochoid Pump
Oil Capacity	1.60 Liters [0.60 Effective]
Exhaust System	Expansion Silencer with Cover
Air Cleaner	Dry-Type with Paper Element
Balancing System	Single, Counter-Rotating Balance Shaft
Length	16.2 in (412mm)
Width	18.6 in (472mm)
Height	19.4in (493mm)
Dry Weight (Recoil Start)	106.9 Lbs (48.5 kg)
Dry Weight (Electric Start)	117.9 Lbs (53.5 kg)
Noise Output @ Continuous Rating, Mean of Four Directions at 1 Meter	97 dB(A)

¹<https://www.yanmarindustrial.eu/Products/Diesel-Air-cooled-industrial-engines/L100V-75/>

A.3 Test Bench P&ID



A.4 McKinney Risk Analysis Sheet

Analyse de risque						Evolution des risques			
	Probabilité d'occurrence d'un accident	Fréquence	Gravité	Criticité	Prévention	Probabilité d'occurrence d'un accident	Fréquence	Gravité	Criticité
	0,1 à 10	0,5 à 10	1 à 100	0,05 à 10000		0,1 à 10	0,5 à 10	1 à 100	0,05 à 10000
Alimentation en gaz de bonbonnes									
Débit trop élevé au démarrage. Risque: post combustion dans l'échappement	3	6	1	18	Démarrez avec une richesse faible Casemate avec accès restreint au personnel qualifié	1	6	1	6
Fuite à la bonbonne -> création ATEX +source inflammation (élec. statique, dispositif élec., ...)	0,5	10	15	75	Isolement bonbonne : vérification étanchéité à chaque nouvelle campagne ferrules double joints et/ou raccords soudés certifié ATEX Bonbonnes en dehors de la casemate respectant le zonage ATEX	0,2	6	15	18
Fuite aux raccords ou dans la conduite d'admission -> création ATEX +source inflammation (élec. statique, dispositif élec., ...)	1	10	7	70	Vérification étanchéité à chaque nouvelle campagne ferrules double joints et/ou raccords soudés certifié ATEX	0,2	10	7	14
Oxydation de matière organique dans la canalisation d'oxygène pur (huile, graisse) menant à une inflammation locale (montée en température)	0,5	10	7	35	Canalisations, raccords, robinets certifié par AirLiquide selon la norme ISO11114 Isolement bonbonnes	0,2	6	7	8,4
Mauvaise combustion -> création ATEX dans l'échappement + source inflammation (élec. statique, dispositif élec.)	0,5	6	7	21	Flexible suivi d'un tuyaux inox résistant à la pression. Grâce à l'extraction des gazs, le tuyaux sera en dépression donc sécurisé Dilution des gaz d'échappement en ouvrant une conduite en aval de celle du banc HCCI dans le système d'extraction Casemate avec accès restreint	0,5	6	3	9
ATEX dans les analyseurs de gaz + source inflammation	0,5	10	3	15	à priori l'analyseur serait dans la casemate car il faut des gazs chaud mais besoin fréquent de les calibrer donc besoin d'entrer dans la casemate durant le fonctionnement du moteur	0,5	10	3	15
Point chaud dans la ligne - > auto-inflammation de l'ATEX	1	10	7	70	Vannes anti-retour pour isoler les résistances de l'ATEX Soupape de surpression 2 barg dégazant à l'atmosphère dans la casemate Isolation du banc moteur dans la casemate avec accès restreint	1	6	3	18
Montée en pression de la conduite d'admission Risque: explosion et conduite qui lâche. Causé par un arrêt brusque du moteur	3	10	7	210	1) Placement d'une soupape de sécurité tarée à 2 barg pour reprendre l'onde de pression dans la conduite + sécurité sur les débits MFC max + sécurité : liaison des MFC à l'arrêt du moteur. 2) Utilisation de clapets anti-retour permettant d'isoler le reste du circuit d'air et de combustible en cas d'explosion 3) Minimisation du volume entre les clapets anti-retour et l'admission du moteur 4) Casemate avec accès restreint	1	3	7	21

Montée en pression de la conduite d'admission Risque: explosion et conduite qui lâche. Causé par une défaillance des MFC	1	10	7	70	1) Placement d'une soupape de sécurité tarée à 2 barg pour reprendre l'onde de pression dans la conduite + zonage ATEX autour de la soupape + coupure automatique des gas prévue en cas de rupture + sécurité sur les débits MFC max + sécurité : liaison des MFC à l'arrêt du moteur. 2) Utilisation de clapets anti-retour permettant d'isoler le reste du circuit d'air et de combustible en cas d'explosion 3) Minimisation du volume entre les clapets anti-retour et l'admission du moteur 4) Casemate avec accès restreint	0,5	3	7	10,5
Montée en température dans résistance chauffante à l'admission, aucun risque pour le personnel	1	10	3	30	Switch mécanique et thermostat inclus dans la résistance si la température dépasse un seuil maximum Limite de la température maximum dans le "gaz heater" programmé dans LabVIEW disjoncteur sur chaque raccordement de l'armoire électrique	0,5	10	3	15
Variation non désirée du débit de combustible combustion extrêmement violente dans le cylindre menant à l'explosion de la culasse	1	10	7	70	1) coupure de l'alimentation en combustible si la valeur maximale autorisée de la pression est atteinte dans la chambre de combustion (130 bar), Limite de Pmax = 5(KW), de MPRR=120 (bar/CAD) (sécurités au niveau de LabVIEW et du PLC). + sécurité sur les débits MFC max + sécurité : liaison des MFC à l'arrêt du moteur. 2) Gestion du moteur prévue pour gérer cela. 3) Casemate avec accès restreint ATTENTION dans le cas d'oxycombustion, les limites de débits de carburants doivent être adaptées car on veut travailler avec des richesses équivalentes (4.76 fois plus petites)	0,2	10	7	14
Alimentation en air comprimé									
Surpression dans la conduite flexible reliant la source d'air comprimé au circuit d'admission. Risque: conduite qui lâche.	1	6	7	42	1) Utilisation d'un flexible en PVC résistant à des pressions jusqu'à 9 bars 2) Casemate avec accès restreint	1	3	3	9
Pièces chaudes. Risque: brûlures 1) circuit admission 2) échappement 3) Moteur lui-même	6	6	3	108	1) Le circuit d'admission se situe à la fois loin du poste de contrôle et à la fois dans la zone à ne pas pénétrer de par la présence de pièces en rotation. De plus, avant d'éteindre le moteur celui-ci tourne 5 minutes avec de l'air froid ce qui permet de refroidir le système d'admission. 2) Calorifugeage d'un maximum de parties chaudes 3) EPI obligatoire dont gants 4) Casemate avec accès restreint	3	3	1	9
Fuite de gaz d'échappement. Risque : intoxication et brûlure	3	10	3	90	Echappement fermé vers la conduite d'extraction avec ventilation forcée (plus de cône de dilution donc meilleur d'étanchéité) MODIFICATION RESTANT À FAIRE + masques avec cartouche adéquate et lunettes à disposition Fermeture des conduites d'extraction des autres bancs et du gazogène afin d'avoir un tirage maximal (sauf une pour dilution) DéTECTEUR de CO dans le hall moteur	0,5	10	1	5
Pièces tournantes									
Réglage du refroidissement par air par un clapet avec ailettes tournante à proximité Risque : Doigt broyé par les ailettes de refroidissement tournant à 1500RPM	3	6	7	126	Placement d'un grillage protégeant l'utilisateur RESTE À FAIRE Casemate avec accès restreint au personnel qualifié	3	6	1	18
Rupture du volant moteur / ailettes de refroidissement	0,2	6	15	18	1) Casemate avec accès restreint aux techniciens qualifiés lors du fonctionnement du banc 2) Le volant se situe dans un renforcement du moteur.	0,2	3	15	9

Rupture du cardan de couplage	0,5	6	15	45	Fabrication d'une protection enveloppant le cardan	0,5	6	3	9
Membres humains ou vêtements happés par pièces tournantes	1	6	15	90	Grillage de protection pour empêcher l'accès aux pièces tournantes, zone de sécurité et vêtements appropriés obligatoires Casemate avec accès restreint au personnel qualifié	0,2	6	15	18
Lubrification									
Surchauffe du circuit d'huile. Risque : moteur uniquement.	1	3	0	0	Aucune mesure nécessaire	1	3	0	0
Fuite d'huile glissante autour du banc moteur	3	3	3	27	Formation des techniciens aux risques	0,5	3	3	4,5
Suction de l'huile dans la chambre de combustion si Pin est inférieur à 1 bar	3	3	0	0	Aucune mesure nécessaire	3	3	0	0
Fuite d'huile entraînant un serrage. Risque : moteur uniquement.	1	3	0	0	Arrêt automatique du moteur si la pression d'huile est insuffisante	1	3	0	0
Electricité									
Composants qui surchauffent dans l'armoire électrique menant à un incendie ou un court circuit ou à l'explosion d'une ATEX	1	10	7	70	Utilisation d'un dissipateur à ailettes relié à l'air ambiant afin de refroidir le seul élément produisant une quantité significative de chaleur + respect du zonage Casemate avec accès restreint Disjoncteur en tête des armoires pour éviter court circuits	0,5	10	3	15
Risques d'électrocution	3	6	7	126	Formation des techniciens Armoire électrique fermée à clé avec accès restreint et dans la casemate Pictogramme de sécurité	1	2	7	14
Composants électriques qui surchauffent près des bouteilles	0,5	10	7	35	Tous les éléments électriques sont situés à plus d'un mètre des réserves de gaz	0,2	10	7	14
Acoustique									
Nuisance sonore importante	10	3	7	210	Port du casque anti-bruit obligatoire Casemate insonorisées acoustiquement	3	1	3	9

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