Mesh optimization for CFD analysis of a spark-ignition engine featuring a deep Miller cycle and high power density

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1 Introduction

The work illustrated in this Master Thesis has been the result of the study conducted during the internship at Leonardo Engineers for Integration. In detail, it is a CFD simulation performed using Ricardo Vectis software and carried out on a high compression ratio gasoline engine designed to be used in a Range Extender hybrid vehicle. My CFD analysis is the prosecution of a study conducted, first, by Vincenzo Bottari on a different chamber and piston geometry, designed to work with a lower compression ratio than the current one, later improved by Marzia Trane, who has worked on the actual CAD geometry.

In both previous works, some of the necessary input data to set up the three-dimensional CFD simulation were obtained from the one-dimensional model created by Carlos Mariani and subsequently optimized by Salvatore Chierchia, using Ricardo Wave software.

More specifically, my study starts from the Geometry used in Vectis (Phase5) by Trane, appropriately improved in some points, and from the results of the one-dimensional CFD analysis performed by Chierchia. Moreover, even though I have used Vectis software, it was decided to use an improved solver version of Vectis (Phase5), which is called Vectis Vsolve, involving a series of operations to modify the geometry in order to solve several interface problems between one version and another.

Nevertheless, an optimization work of the results obtained by Trane, using Vectis Vsolve, at the end was configured as a work of correction and improvement of the STL geometry available in the model and the generation of an improved calculation grid, Polyhedral instead of Cartesian. This difficulty and other problems due to the limitations caused by the Covid-19 emergency, led us to consider it
appropriate to use the CFD simulations conducted by me to correct the available geometry and so stopping the work on the geometry mesh generation and setting of the simulation parameters in VSOLVE model.

Therefore, as future works, a complete simulation on the current geometry is expected and then a Wave-Vectis co-simulation will be performed in order to obtain more accurate results than those achievable with a 3D simulation conducted only on Vectis.

Finally, in addition to my study on the three-dimensional model, a process of optimization of the results obtained by Chierchia was performed by my colleague Luigi Siodambro, also with the aim to improve the previous results in order to allow a future Wave-Vectis Co-simulation.

### 1.1 Internal combustion engine

The system being treated here is a Turbocharged Spark-Ignition Four-Stroke Engine featuring a Miller Cycle.

This type of thermal driving machines makes it possible to produce work by converting the heat generated by the oxidation process of a fuel (gasoline in this case) into an oxidizer (oxygen contained in the intake air), which takes place inside the engine combustion chamber, without requiring the use of an external component, such as a boiler. In fact, the working fluid consists of a mixture of fuel and air, before combustion, and the products of the oxidation of the fuel into air, after this process, which thanks to consecutive cycles of expansion and compression exchanges mechanical energy with the moving parts of the machine (piston).

For these reasons this type of engines are called “Internal Combustion Engine”.

Moreover, in classifying engines according to how the combustion process is started, the engine studied is a Spark Ignition Engine.

In fact, the fuel used is gasoline and the combustion process of the air-gasoline mixture is activated by the spark generated between the electrodes of a spark plug.

Being characterized by very fast combustion, which ideally occurs at a constant volume, these are also called Otto Engines.

On the other hand, regarding the way how the exhaust gas is changed, our engine is configured as a four-stroke engine, since the working cycle lasts four strokes of the piston, i.e. two revolutions of the crankshaft, and the intake and exhaust phase lasts more than half of the entire working cycle, achieving an excellent fluid change.
Finally, the following figures illustrate the main geometrical parameters of an internal combustion engine and an example of an actual Otto Cycle for a 4-stroke engine, demonstrating how it deviates from the ideal Otto cycle.

Figure 1-1: Actual Otto Cycle and Ideal Otto Cycle comparison for a four-stroke cycle engine.
1.1.1 Turbocharging

The maximum power an engine can make available at the shaft depends principally on the quality of fuel it is able to burn (with the highest possible degree of efficiency) inside the cylinder. This process itself depends on the amount of air that can be introduced into the cylinder at each cycle. For this reason, if intake air is compressed to a density higher than that of the external ambient, it would be possible to increase the power delivered by the engine with all other parameters and dimensions being the same. In fact, the purpose of turbocharging is precisely to increase fresh charge in the intake manifold compared to that realized in a naturally aspirated engine, and in the engine, I studied, this is achieved by the use of a compressor (three 6-stage axial turbochargers).

Nevertheless, it is good to define how differences Turbocharging from Supercharging:

The fundamental difference between these two systems is the power supply.

In a volumetric compressor (supercharging), a belt connects it directly to the engine, thus obtaining its power in the same way as the water pump. A turbocharger, instead, obtains its power from the

\[
s(\theta) = a \cos \theta + \left( l^2 - a^2 \sin^2 \theta \right)^{1/2}
\]

Cylinder volume when piston at TC (s=l+a) defined as the clearance volume \( V_c \)

The cylinder volume at any crank angle is:

\[
V'(\theta) = V_c + \frac{\pi B^2}{4} \left( l + a - s(\theta) \right)
\]

Maximum displacement, or swept, volume:

\[
V_d = \frac{\pi B^2}{4} L
\]

Compression ratio:

\[
r_c = \frac{V_{BC}}{V_{TC}} = \frac{V_c + V_d}{V_c}
\]

Figure 1-2: Geometry of cylinder, piston, connecting rod, and crankshaft where B = Bore, S = Stroke, L = Connecting Rod Length, a = Crank Radius, \( \theta \) = Crank Angle.
exhaust gases. These pass through a turbine, which then provides mechanical energy to the compressor, which is mounted on the same Turbine shaft.

Now, remembering that in a four-stroke engine, the exhausted charge is renewed through the stroke of the piston towards the TDC and its subsequent downshift to the BDC, we define the equation of Power (P), Torque (T), and Mean Effective Pressure (mep) to show how these changes varying the air inlet density:

\[
P[W] = \frac{\eta_v \eta_f N V_d Q_{HV} \rho_a \left(\frac{F}{A}\right)}{n_R}
\]

\[
T[Nm] = \frac{P}{2\pi N} = \frac{\eta_v \eta_f V_d Q_{HV} \rho_a \left(\frac{F}{A}\right)}{2\pi n_R}
\]

\[
me p[Pa] = \eta_v \eta_f Q_{HV} \rho_a \left(\frac{F}{A}\right)
\]

Where:
- \(\eta_v\) = Volumetric Efficiency;
- \(\eta_f\) = Fuel Conversion Efficiency;
- \(V_d\) = Displacement;
- \(Q_{HV}\) = Fuel Heating Value;
- \(\rho_a\) = Inlet Air Density;
- \(n_R = 2\) (for a four-stroke cycle engine).

So, turbocharging in a four-stroke cycle engine permit to boost the Power per unit displaced volume, simply increasing the inlet air density.

### 1.1.2 Miller Cycle

To understand better the functioning of a Spark-Ignition Engine featuring a Miller Cycle, we must spend some words about Atkinson Cycle. In fact, nowadays the term "Atkinson cycle" is erroneously used to describe a normal Otto cycle engine in which different compression and expansion strokes
are obtained by acting on the opening/closing times of the intake valves, this cycle is instead correctly
described by the Miller cycle. In both cases the compression stroke is reduced with respect to the
expansion stroke, but the Atkinson cycle achieves this by using a particular crankshaft structure. For
this reason, many hybrid vehicles such as the Honda Jazz 2013 and the Ford Escape (front-wheel
drive and 4WD), which use a Miller cycle engine, are confused with Atkinson engines. Instead, the
Toyota Prius and Lexus RC-F V8 hybrid cars use a proper Atkinson cycle engine.

1.1.2.1 Atkinson Cycle

The main problem of Otto-Cycle is to have three passive work phases out of a total of four, i.e. Intake,
Exhaust and Compression, which give a negative contribute to the production of work for the traction.
So, to solve this problem James Atkinson modified the Otto cycle by making the passive phases work
differently from the active one.

Him, by using a different geometry of the crankshaft, imposed a different duration on the compression
stroke than the expansion stroke in order to reduce losses in the passive phase to the benefit of the
overall efficiency.

So, in 1886, he developed a cycle known as Atkinson cycle which incorporated all four strokes of an
engine in just one revolution of the crank shaft using linkages. A basic model can be seen on the right
here:

![Figure 1-3: The Atkinson Cycle engine Letters Patent No.336,505, dated February 16, 1886.](image)
The connecting rod “E” drives the piston indirectly through the E-C connection, thus permitting to realize a complete four-stroke Otto cycle. The exhaust expansion stroke was 1.78 times longer than the intake stroke. This Invention was a great success to the point that the British Gas Engine company built more than a thousand of these engines between 1886 and 1893.

In modern engines, many manufacturers declare to use the Atkinson cycle in order to improve the efficiency of their motors, with the difference that the same cycle is obtained by working with the same connecting rod and crank of the Otto engine, i.e. without making a dedicated crankshaft. This adjustment is realized adopting a Miller Cycle which work featuring a Late Intake Valve Closing (LIVC), who consists of leaving the intake valves open certain degrees after the piston gets to the Bottom Dead Centre (BDC). So, the working difference between the compression and expansion phase is realized by acting on the valve timing. Hence, in the compression phase the intake valve is kept open for a greater angle of rotation of the motor shaft, so that the expansion phase enjoys a greater stroke, but at the same time it involves a reflux of part of the sucked air during the intake phase. This leads to a lower volumetric efficiency that makes the motor behave as one of smaller displacement (lower mass of sucked air contained in the same volume). So, using the Miller LIVC Cycle provides a homogeneous mixture with a smaller quantity of better nebulized gasoline, a lower temperature of the exhaust gases, less mechanical work, but also less pressure on the top of the piston. Moreover, since LIVC pushes back charge (containing fuel) in the intake port and cannot be used in combination with scavenging. Therefore, the overall effect is a higher efficiency with lower fuel consumption but less power, compensated by the increased displacement, or by the use of a small compressor, or by the addition of electric traction.

Below is a list of the advantages and disadvantages of the Atkinson cycle.

**Advantages:**
- Higher thermal efficiency compared to the conventional Otto cycle;
- Emissions reduction, thanks to the decrease in fuel consumption;
- Suited to implementation on Hybrid Electric Vehicles (HEV’s), where the lower torque produced can be compensated with an electric motor.

**Disadvantages:**
- Lower Torque output;
- Higher complexity.
It was proven that the Atkinson cycle offers higher efficiency at part-load conditions compared to the Otto cycle, for this reason, nowadays, this solution, proposed by Atkinson for a four-stroke Spark-Ignition engine, is suitable for HEV’s, where the priority is fuel consumption and emission levels reduction. Moreover, these vehicles are designed to be driven most of the time under part-load conditions, an area where the Atkinson cycle shows a compelling advantage, although it provides a lower torque at part-load conditions, so making crucial the electrical motor's role during this phase. Therefore, in a HEV both electric and ICE motors can work together, thus, at low-load conditions the electric motor will compensate the lack of ICE power, creating a perfect match.

![Figure 1-4: The RC F uses the Atkinson cycle at cruising speeds for enhanced fuel economy, and then switches to the Otto cycle at higher revolutions to realize higher performance levels.](image)

### 1.1.2.2 Miller Cycle benefits in a turbocharged SIE

The four-stroke turbocharged engines which act on intake valve timing to reduce the compression stroke duration in favor of that expansion with the same geometry of Otto Cycle, work according to a cycle called *Miller Cycle*. It was developed by an American engineer called Ralph Miller, who patented it with the number 2817322 in 1957.

This type of cycle can be carried out both adopting the EIVC (Early Intake Valve Closure) and LIVC (Late Intake Valve Closure) strategy. Although (now) the term Atkinson cycle is generally used to refer to cycles using LIVC, while the term Miller cycle for cycles using EIVC, Miller has actually patented both solutions, in combination with supercharging.

In both strategies, the aim of this represented by the possibility of trapping the same quantity of fresh charge at a lower temperature or a greater quantity of air at the same temperature. In the case of SI engine, the use of the Miller cycle is a good tool to reduce the risk of detonation in combination with turbocharging and downsizing.
As the LIVC strategy has previously been treated, let's analyze the EIVC technique, more frequently used in a Miller Cycle, which consists in making the fresh charge expand during the last portion of the intake stroke, in order to reduce its temperature and pressure. In this case, the cylinder is only partially filled with fresh charge, then expanded during the remainder of the intake stroke. For this reason, at the beginning of the compression stroke, the charge’s temperature in the cylinder is lower than that which would occur with a normal supercharging process. Moreover, since EIVC further cools the charge due to in cylinder expansion (but unfortunately reducing turbulence), giving at full load lower end-gas temperature, that can allow a more advanced spark timing, due to the lower octane demand in order to reduce Detonation risk.

To better understand this effect, let's take a practical example:
In a standard naturally aspirated SI engine that working on a conventional cycle where the valves closed at dead center, the temperature reduction realized by intake process is amplified through the compression phase in according to the following equations:

\[ T_2 = T_1 \epsilon^{m-1} \]

Where:

\[ \epsilon = CR = \frac{V_1}{V_m} \]

![Diagram](image.png)

*Figure 1-5: Graphic representation of a compression process in a naturally aspirated SIE.*

With \( \epsilon \cong 10 \), \( m=1.35 \) and a \( T_1=300K \) (external ambient temperature) it can be found that changing the \( T_1 \) by a \( \Delta T=10^\circ C \) will have a \( \Delta T' \) on the \( T_2 \) equal to \( \Delta T'=22^\circ C \) due to the compression operation:
\[ T_1' = T_1 + \Delta T \quad \text{with} \quad \Delta T = 10^\circ\text{C} \]

\[ T_2' = T_2 + \Delta T' \Rightarrow \Delta T' \cong 22^\circ\text{C} \]

This temperature difference affects considerably the speed of chemical reactions and therefore the risk of spontaneous ignition. Therefore, EICV’s idea of anticipating the intake valve’s closing considerably, allows to obtain a lower temperature of the mixture at the end of the compression, but it involves a decrease of the volumetric efficiency which can be compensated by an increase of the supercharging pressure (as mentioned above).

In fact, starting from a supercharged engine with supercharging pressure \( p_c \) and analyzing the compression process (1c→2c), we have:

\[ p_{2c} = p_{1c} \cdot \varepsilon^m \]

\[ T_{2c} = T_{1c} \cdot \varepsilon^{m-1} \]

Where \( T_{1c} \) is the temperature we have at the start of intake phase, higher the the \( T_{\text{amb}} \). So, this temperature will be the starting temperature of the compression operation, at the end of which the PMS will be reached with a \( T_{2c} \) temperature.

In this case both temperature and pressure are higher than a naturally aspirated engine with same characteristics.

It’s important to underline that the IVC occurs at BDC (point 1c on figure below), as normally happens in a standard SIE.

![Figure 1-6: Comparison between a supercharged engine with the one featuring EIVC Miller cycle.](image)
The reference cycle (red curve) represents a compression process carries out in a supercharged engine. Now we will understand how turbocharging permits to overcome the loss in volumetric efficiency which affects Miller cycle, guaranteeing in any case the reduction of temperature at the end of the compression process (in order to avoid the appearance of detonation), which the Miller cycle wants to achieve. Therefore, taking the boost pressure to the value $P_M > P_{1c}$ (see graph above) and closing the IV at point M (before the BDC), the trapped charge will expand for the remaining part of the piston's downward stroke, according to a polytrophic expansion, up to the same compression start point $1c$ of the original cycle. At this point the fluid carries out the same compression process ($1c \rightarrow 2c$) as in the reference cycle.

Therefore, in terms of pressure levels, nothing will change because turbocharging has increased the pressure by the amount needed to compensate for the decrease in volumetric efficiency.

Now let's see how this "modification" is able to guarantee a final compression temperature lower than the one obtainable in a reference cycle.

As said before, $p_M$ must be higher than $p_{C1}$, so the compressor must work with a higher $\beta$ in order to bring the air to a higher supercharging pressure and consequently to a higher temperature.

$$\beta' > \beta \Rightarrow p_M > p_{1c} \text{ and so } T_{1M} > T_{1c}$$

At this point, using an intercooler, we will bring the temperature $T_{1M}$ to a value comparable with $T_{1c}$ of the original supercharged engine (sizing the exchanger appropriately).

But here, unlike the aspirated motor case, starting from point M at a temperature $T_{1M}$ (temperature at the exit of the intercooler) an expansion (for the remaining part of the intake stroke) up to $P_{1c}$ is carried out, which brings the temperature to a $p_{1M}' < p_{1c}$.

The result is that TDC will reach with a $T_{2M}$ temperature lower than the $T_{2c}$ of reference cycle, because the compression starting temperatures are different ($T_{1M} < T_{1c}$), consequently, the end of compression temperature of the Miller cycle will be lower than the original cycle:

$$T_{2M} < T_{2c}$$

To conclude, is useful make a comparison between the effect of the EIVC and LIVC strategy on the engine performance:
- At high engine speeds, the LIVC technique guarantees a reduced fuel consumption compared to the EIVC;

- At low engine speeds, EIVC achieves lower fuel consumption than LIVC;

- The advantage of LIVC comes from more advanced combustion phase and increased pumping work;

- At low engine speeds, EIVC ensures lower pumping loss than EIVC;

- EIVC is characterized by slower heat emission rate than LIVC.

Figure 1-7: Graphic representation of the two strategies performing Miller Cycle.

1.1.3 The major Abnormal Combustion: The Detonation

1.1.3.1 Combustion process on a SIE

The combustion process in a spark ignition engine allows the conversion of the fuel's chemical energy into thermal energy, thus constituting the principal phase of the engine's work cycle. The start, development and completion depend on the characteristics and speed of the chemical reactions, the mass and energy transport conditions that occur in the reaction zone and the heat exchange with the
surrounding environment. Since the oxidation reactions of the fuel take place in gaseous phase, the combustion speed is maximum when the fuel is vaporized, and its molecules are finely mixed with those of oxygen, this is why we speak of combustion in pre-mixed phase.

Generally, these are chain reactions that occur in several stages, since the role played by the intermediate active products (particles with free valences: radicals or atoms) that are formed during the reactions themselves is fundamental. The actual sequence of all the transformations that lead to the oxidation of the fuel is very complex and not yet known, however we can affirm with certainty that the speed of these reactions depends essentially on the concentration and temperature of the reagents.

Usually the reaction speed \((w_r)\) of any reagent or reaction product is expressed through the Arrhenius exponential factor:

\[
\frac{dc}{dt} = \frac{dp^n}{n^e} \exp \left( \frac{E_a}{RT} \right)
\]

Where:
- \(dc/dt\): time variation of the relative concentration of the reagent/product in question.
- \(E_a\): is a characteristic of the fuel considered and represents the energy barrier that must be overcome in order for the intermolecular bonds between the molecules of the reagent to break down to form the new one in the products.
- \(\exp (E_a/RT)\): expresses the fraction of molecules that have thermal agitation energy higher than the activation energy \((E_a)\).
- \(C\) and \(n\): are typical constants for each reaction.

However, since the combustion process is characterized by a set of reactions that take place both in sequence and in parallel, it is more convenient to refer to the concept of Effective Activation Energy, which is determined by the reaction that takes place more slowly, which therefore limits the value of the reaction speed intended as a whole.

Typical values of this activation energy for oxidation processes that characterize fuels used in engines are \(E_a = 80 \div 160 \text{ kJ/(mol*K)}\).

Therefore, a spark ignition engine is said to be feed with a homogeneous and totally gaseous air/fuel mixture when combustion begins. If the engine is running smoothly, the combustion process is started by the spark generated by the spark plug at a very precise point of the working cycle, located close to the end of the compression phase. In fact, the ignition occurs in a range between 10° to 40° of the crank angle before the TDC. Combustion is said to be normal when, starting from the point of ignition, the flame front gradually spreads to the edge of the combustion chamber without any sudden
changes in speed. As the process takes place, the fresh charge burns releasing heat that increases the
temperature of the gases, while the piston first reduces the volume in which the oxidation reactions
take place (moving towards the TDC) and then increases it by moving from the TDC to the BDC.
Therefore, the combination given by the heat generated by the chemical reaction and the volume
variation operated by the piston, determines the time course of the pressure that reigns in the cylinder.

It is possible to divide this process into three phases:

- **Incubation or flame development phase**: during this phase the part of the mixture closest to
  the spark plug begins to burn, bringing the pressure value in the chamber to a higher value
  than that reached at the end of the compression (piston to TDC).

- **Turbulent combustion phase**: unlike the first phase, during this phase there is a rapid
  propagation of the flame front, in fully developed turbulent regime, throughout the chamber.
  However, the volume remains almost unchanged, as the piston is still close to the PMS.

- **Combustion completion phase**: in this phase the combustion process is completed, as all the
  mixture contained in the combustion chamber has been burned.

1.1.3.2 Autoignition

Before talking about Detonation (or Knock), it is considered appropriate to define the concept of
autoignition. This term is used to denote a particular phenomenon that involves the starting of the
combustion process without the aid of an external source (spark plug). This condition occurs when
during pre-flame reactions, unstable partial oxidation products (peroxides, aldehydes,
hydroperoxides) are formed that release more energy than the one released by the reagent system to
the external environment. Because of this, the temperature of the mixture increases, rapidly
accelerating the various oxidation reactions. The phenomenon of autoignition, for a mixture in the
gaseous state and perfectly homogeneous, depends essentially on temperature, pressure, composition
(air/fuel) and ignition delay $\tau_a$.

This is defined as the time interval between the moment in which a mixture of a given composition
is brought under certain conditions of pressure and temperature and to the instant in which
combustion occurs. Thus, according to how it has been defined, the ignition delay is inversely proportional to the speed at which oxidation reactions happen. In fact:

$$
\tau_a(p, t) = A p^{-n} \exp\left(\frac{E_a}{RT}\right)
$$

Where A, n and E\textsubscript{a} are determined experimentally according to the characteristics of the fuel mixture in question.

So, thanks to the concept of \( \tau_a \), the influence of pre-reactions on the autoignition of the mixture can be assessed more easily.

### 1.1.3.3 Detonation Description

We can now define the concept of Detonation. It is the most important form of abnormal combustion as it limits engine performance (limiting the compression ratio and ignition advance) and imposes restrictions on fuel composition. When it occurs, there is a characteristic metallic noise, similar to hammering (called in slang "knocking on the head"), associated with power loss, vibrations and overheating that can seriously damage the engine's mechanical parts. There are two different theories to explain the onset of this phenomenon, one is based on the concept of autoignition in one or more points of the mixture which burns last, before it is reached by the flame front; the other, instead, believes that detonation occurs when the advancing flame front, after reaching sound speed, turns into a shock wave which, due to a forward speed significantly higher than normal, burns the remaining part of the mixture.
Figure 1-1: Normal combustion process in a SIE in comparison with one characterized by the onset of detonation.

However, the first theory is the one with the most experimental confirmation. As previously explained, auto-ignition occurs when, in one or more points of the end gas, due to particular conditions of temperature and pressure (the mixture is never perfectly homogeneous in all its points), the pre-fire reactions occur faster, determining the auto-ignition of the mixture before the fresh charge is reached by the flame front. Locally, a strong release of heat occurs, generating a strong peak of pressure which is transmitted at sonic speed to the rest of the fresh charge, causing the subsequent autoignition.

Therefore, this chain reaction means that starting from the point where the autoignition has occurred, the phenomenon extends to the rest of the fresh charge, as if another flame front was produced. As a result, the pressure waves repeatedly reflected on the chamber walls produce vibrations in the mechanical parts of the engine which are transmitted to the outside in the form of the characteristic metallic noise. By plotting the pressure trend as a function of the crank angle in a diagram, in the case of detonation will appear oscillations with amplitude gradually decreasing over time. The frequency varies between 5 and 15 kHz and depends on the propagation speed of the pressure waves and on the path travelled between two consecutive reflections.
Figure 1-2: Typical trends of pressure inside the combustion chamber in function of crank angle, in case of normal combustion, strong and weak detonation.

Depending on the percentage of mixture that self-igniting, the detonation can be more or less intense and may occur in several consecutive cycles. Obviously, longer is the duration of the phenomenon and higher is the pressure peak reached (up to $20\div30\%$ of $P_{\text{max}}$), greater will be the damage caused. In fact, the shock waves, by removing the gas film adhering to the walls, increase the thermal loads (greater heat flow to the outside) which, together with the alternating mechanical stresses, lead to breakage due to hot fatigue of various engine components.

For example, as a result of detonation, the lubricant layer between the cylinder and liner is removed, causing a creep between two components which, together with the corrosive action of the exhaust gases, leads to severe wear of the component.

Nowadays, detonation can be better controlled thanks to the adoption of an accelerometer or acoustic sensor that is calibrated on the frequency band typical of this phenomenon, in order to detect the appearance of the knock.

In fact, as soon as the metallic noise is heard, the detonating cylinder is identified (during his combustion phase) and the control system acts by decreasing the advance on ignition and increasing
the richness of the mixture. In addition to this detection tool, however, a mathematical model exists to detect the occurrence of the detonation in the fresh charge (before the arrival of the flame front). In order to define this model, we must remember the concept of ignition delay \( \tau_a \), an index of the time required by chemical reactions to reach autoignition, and the conditions of pressure and temperature of the fresh charge not yet reached by the flame front must be known. Indeed, even in the case of normal combustion, if detonation does not occur, it simply means that the conditions of \( p \) and \( T \) (\( p < 4 \text{ Mpa} \) and \( T < 900 \text{ K} \)) are such that the ignition delay of the final portion of the mixture is greater than the time taken by the flame front to reach it.

Thus, setting the engine operating conditions and fuel characteristics, we calculate the value of the progress rate \( \varphi \) of each reaction at each instant and his critical value \( \varphi_c \) to predict when detonation appears. In fact, knowing that \( d\varphi/dt \) can be estimated from the measurements of \( \tau_a \) (on a fast compression machine) and approximating the function \( \varphi(t) \) (increasing from 0 to \( \varphi_c \)) to its chord, we have that:

\[
\frac{d\varphi}{dt} = f(\varphi, p, T) \sim \frac{\varphi_c}{\tau_a(p, T)}
\]

Subsequently, assuming \( \varphi_c \) independent from \( p \) and \( T \), it is possible to define the integral function of the autoignition delay:

\[
I(t_c) = \int_0^{t_c} \frac{dt}{\tau_a(p, T)}
\]

Where the final instant coincides with \( t_c \), where \( \varphi = \varphi_c \) and \( I(t_c) = 1 \) such that the cycle is detonating; instead if \( I(t_c) < 1 \) the denotation does not occur in the cycle considered.

Finally, a list of the most important factors that favor the onset of the detonation:

- A mixture with high chemical reactivity, i.e. characterized by high octane number;
- High compression ratio;
- The introduction of a greater quantity of mixture for each work cycle;
- An increase in the temperature of the inlet mixture
- A high spark advance on ignition, which increases the pressure in the chamber more quickly;
- Poor cooling of the final portion of the fresh charge by the walls of the combustion chamber.
1.2 Overview on Vectis VSOLVE

VECTIS is a software developed by Ricardo Software, that allows to perform a complete Computational Fluid Dynamics (CFD) analysis for the solution of advanced 3D industrial fluid flow and heat transfer problems, specifically for automotive industry applications. The innovative feature is that this software contains a fully automatic Cut-Cartesian mesh generator, a multi-domain solver capable of running on arbitrary unstructured meshes and an advanced graphical user interface (GUI) to prepare the geometry and visualize simulation results. The study of fluid flow behaviour is done by solving the fundamental equations of conservation and chemical species. These are first discretized for the VECTIS mesh using the finite volume method, and then solved completely implicitly by coupling variables and non-linear effects incorporated using iterative or predictor-corrector methods. It is possible to calculate transient or stationary flows. Time-dependent geometry, such as moving valves and pistons, are correctly accounted for within the VECTIS mesh structure. However, in the VSOLVE version (the current version) the mesh is realized on the background geometry, which consists of the static parts of the model in the maximum extension configuration (e.g. PMI in the case of an ICE). A further difference is found in the VSOLVE mesher, called vmesh. This is a fully automatic mesh generator that allows you to generate structured and unstructured Cartesian, Tetrahedral and Polyhedral meshes. The study of fluid flow behaviour is done by solving the fundamental equations of conservation and chemical species. These are first discretized for the VECTIS mesh using the finite volume method, and then solved completely implicitly by coupling variables and non-linear effects incorporated using iterative or predictor-corrector methods. It is possible to calculate transient or stationary flows. Time-dependent geometry, such as moving valves and pistons, are correctly accounted for within the VECTIS mesh structure. However, in the Vsolve version (the current version) the mesh is realized on the background geometry, which consists of the static parts of the model, taken in the configuration corresponding to the maximum displacement of the moving parts (e.g. BDC in the case of the engine Liner and maximum lift condition for the valves). A further difference is found in the VSOLVE mesher, called vmesh. This is a fully automatic mesh generator that allows you to generate structured and unstructured Cartesian, Tetrahedral and polyhedral meshes. In any case, a more detailed description of the software functionality will be made in the following chapters, dedicated to the various phases of the work carried out. The following flowchart provides a brief overview of the setup process (from start to finish) for a typical CFD simulation within VECTIS.
1.2.1 Brief description of the PHASE5 version

In figure 34 it is represented a diagram that summarizes the working procedure required to execute the CFD simulation on Phase5. A calculation using VECTIS consists of five individual programs or phases. These are:

- **Phase1** – Geometry import and preparation → The same for VSOLVE version
- **Phase2** – Mesh generation → Corresponding to vmesh
- **Phase4** – Mesh linker → Corresponding to vpre
- **R-Desk PHASE 5 plugin (GUI)** → Corresponding to R-Desk solver setup
- **Phase5** – CFD solver → Corresponding to VSOLVE

Each phase will be presented and discussed in more details in the following chapters.
With regards to the part related on the setting of simulation parameters in the solver, the user interface (GUI) is quite similar in both versions, while there are additional functions, which allow to improve the quality of the results, and an innovative solver technology in VSOLVE compared to PHASE5. Some of these improvements are shown below:

- **Dynamic shear cell method for moving geometry simulations** - This feature provides support for cylinder simulations and other moving geometry applications. The functionality is available for any type of background mesh (e.g. Cartesian, multifaceted, etc.). belong to a family of fixed background grid methods. In these methods, the solid boundary (body) moves along a fixed background grid so that the flow domain includes within it the part of background grid delimited by its moving and fixed boundaries. The geometry of the boundary surface must be provided by Lagrangian reference points or by a level-based representation and the update of the cut cells can be done in the narrow band of cells around the moving boundary;

- **vsurf** - a new surface re-meshing tool which offers an autonomous surface re-triangulation capability for using different mesh types, such as Tetrahedral and Polyhedral;
• **Improved solver and numerical solution process** - The improved Generalised SIMPLE algorithm offers better convergence, while substantial remodelling of gradient limiting methods and the linear solver available in vsolve speed up the simulation process;

• **Zonal Simulations** - VECTIS vsolve now offers multi-zone simulations where zones can be connected or disconnected at the prescribed simulation times;

• **Simulation control options** - new time base options have been added to provide support for multi-cycle simulations and flexible ways to define simulation duration, and new options for adaptive time stepping;

• **New mathematical models** for the calculation of turbulence, spray, wall fill, combustion and so on.

To conclude this section, the substantial differences between the two software have been found in the part related to the mesh generation.

As we will see later, VSOLVE requires only a model geometry in STL (at a specific motion configuration), on which the computational grid is represented, then generated through the vmesh command. This command (combined with vsurf) also allows the conversion of the grid from one structure to another (Cartesian - Tetrahedral - Polyhedral), the default format is Cartesian, as for Phase5.

On the other hand, Phase5 requires 5 starting STL geometries and generates the mesh using different interfaces. The geometries are generated through the tool "In-Cylinder Geometry Generator" and the mesh is managed through "Crosslink".

- **In-Cylinder Geometry Generator**: allows the user to automatically generate geometries for all topologies in a moving boundary configuration. In the case of an internal combustion engine, it allows the user to generate the system configuration in correspondence with the valves opening and closing moments. Before using this tool, the starting geometry file must be characterized by: all open valves, the geometry must be painted, and the motion files must be available for all valves and pistons.

- **Crosslink**: In the presence of moving components for which a motion boundary condition is assigned, the mesh will be moved too and therefore it is appropriate to set limits on distances.
that the boundaries can be moved before the mesh becomes too distorted, or the cell aspect ratio become too large. At this point, the solution can be remapped to a new undistorted mesh, corresponding to the next motion instant. This is known as crosslinking. It can also be used to map a solution to a new mesh when a drastic change in geometry occurs. An example of this is in the calculation of an engine intake and compression stroke. At the closing point of the intake valve, the intake ports disappear completely from the calculation, which requires a new mesh. To use crosslinking, a calculation is divided into a number of time-regions. Each time-region is defined by its start and end times and by the mesh which is used for that period.

2 Computational Fluid Dynamics

Fluid dynamics is the science which studies the behavior of fluids under various conditions, these are governed by partial differential equations which represent conservation laws for mass, momentum, and energy, i.e. Navier-Stokes equations. So, *Computational Fluid Dynamics* (CFD) is intended as a tool that allows to study systems characterized by fluid flow, heat flow, and chemical reactions associated with them, by using a computer-based simulation that replace the PDE equation systems (which governs them) with a set of algebraic equations which can be solved more easily.

Therefore, by using CFD is possible:

- To simulate the behavior of fluids with considerable savings in lead time and resources compared to conventional methods;
- To conduct experiments without disturbing the flow, unlike other measuring instruments;
- To study systems under hazardous conditions at and beyond their normal performance limits;
- It can be used to compare various solutions and direct the project towards the most appropriate one;
- Practically unlimited level of detail and results.

However, it has some limitations:
- It needs an adequate knowledge of the simulated phenomena and numerical models available;
- Although technological progress ensures a constant increase for calculation resources and numerical methods efficiently, not all phenomena can be simulated adequately (large systems, complex phenomena, time-dependent problems);
- It needs to be combined with other resources (experimental analysis) for validation and verification.

All commercially available CFD software has a simplified interface that allows the user to type in problem parameters to be studied and to analyze the results obtained.
In addition, all of them are divided into the parts:

- **Pre-processor**
  Thanks to this tool it is possible to define all preliminary operations for setting the parameters related to the simulation.
  It starts by defining geometry of interest, called computational domain that is subdivided in a set of subdomains in turn subdivided in cells (control volumes or elements) of finished dimension, that go to constitute the computational grid (or mesh) where numerical calculation is performed. The solution to a flow problem is defined at nodes inside each cell and its accuracy depends on the number of cells in the grid.
  In general, a larger number of cells give a better and more accurate solution, but the cost in terms of computing hardware resources and calculation time is quite higher.
  A good mesh definition often is not uniform, in fact it will result tighter in the regions of the domain characterized by remarkable gradients and/or where flow variables considerably vary in the space, while the grid will be gradually coarser where flow variables vary less from one point to the other of the domain.
  After mesh definition and generation, it proceeds to the definition of fluid properties, the physical and chemical phenomena that must be studied are specified and finally the boundary conditions for the cells coinciding with the domain surfaces are defined.

- **Solver**
  After discretizing the fluid domain in elementary cells in order to obtain the calculation grid, we pass to the definition of the physical model (for example, the equations of motion + the equation of energy + the equations of species) and the discretization method of the equations.
  It consists of an iterative method that allows to solve numerically the equations of Navier-Stokes and those of the turbulence model, constituting the physical model.
The iterative calculation is interrupted once the prescribed degree of accuracy has been reached. The Navier-Stokes equations, although providing a continuous description of the analyzed phenomenon, cannot be solved directly (solution in closed form) except for very simple cases. Therefore, discretizing in space (and eventually in time), a finite number of points (finite differences) or volumes (finite volumes) is defined where solving algebraic equations derived from the constitutive equations.

There are essentially three discretization methods:

- **Finite Difference Method (FDM):** was the first adopted in fluid dynamics field and still used in some specialized CFD codes. This strategy is used to solve numerically differential equations by approximating the derivatives of unknown functions to finite difference equations. Indeed, knowing the unknown function values at reference points, which coincide with the mesh nodes located on the coordinate axes (at the edge), we use Taylor's series developments to calculate the "variation" of the unknown function between one grid node and the next. It is mainly used for ordinary differential equations, even if the method is used as a pattern of advancement in time for partial derivative problems.

- **Finite Element Method (FEM):** is a numerical method to look for approximate solutions of problems described by Partial Differential Equations (PDE) of an unknown function of multiple independent variables, reducing them to a system of algebraic equations. It consists in discretizing the domain by creating a grid (mesh) composed by finite elements of coded shape (for example: triangles for 2D domains and tetrahedra for 3D domains). On each of these elements, the solution of the problem is assumed to be expressed by the linear combination of functions called basic functions or shape functions valid to describe local the variation of unknow flow variables. Usually polynomial functions are used, so that the overall solution of the problem is approximated with a piecewise polynomial function. The coefficients number that identifies the solution on each element is therefore related to the grade of the polynomial chosen. This, in turn, governs the accuracy of the numerical solution found. But, when the piecewise approximating function for the unknown flow variable “x” will replace the governing equation, these will not coincide, and this generates a residual, which is a measurement of approximation errors. These residuals are minimized by multiplying for weighting functions and integration on the finite element. At the end of this
process it’s possible to obtain a set of algebraic equations for unknown coefficients of approximating functions.

In general, the finite element method can be used to solve partial derivative equations when the domain has a complex shape (like the chassis of a car), when the domain is variable (a solid state reaction with variable boundary conditions), when the accuracy required to the solution is not homogeneous on the domain (a crash test on a car requires greater accuracy at the point of impact) and when the solution sought lacks regularity.

- **Finite Volume Method (FVM):** is a method which consists in the integration of differential partial equations on a finite control volume on whose contour boundary conditions are imposed. In this way the equations governing the unknown flow variable are expressed in integral form for each volume element. The first step consists in splitting the domain in so many elementary volumes, subsequently the relationships (in integral form) that connect between them the various bordering volumes are defined and finally the system of algebraic equations so defined is resolved for numerical way with the aid of the computer. So, from a numerical point of view the FVM is a generalization of the FDM in the sense that the set of finite elementary volumes can be reduced to finite difference pattern, with the difference that the latter is based on nodal relationships for differential equations, while the FVM is a discretization of governing equations in integral form. Moreover, the volume integrals in partial differential equations are converted into surface integrals using the divergence theorem, for the reason that they contain a term of divergence, which represents the flux (of the unknown variable) across the surfaces of each finite volume, and since the flow entering a given volume is identical to the flow leaving the adjacent volume, these methods are conservative. This characteristic enforces conservation of quantities at discretized level (i.e. mass, momentum and energy), which remain conserved also at a local scale. Instead, non-conservative schemes are generally less accurate than conservative ones, particularly in the presence of strong gradients. To conclude, we have to affirm that finite volume method is currently the most widely used approach in CFD calculation through computer, principally because finite volumes domain partitioning takes full advantage of using an arbitrary mesh to approximate complex geometries.

- **Post-processor**

When the iterative process for solving the governing equations has come to an end, the simulation is complete and the CFD software allows to visualize the results obtained.
This is the part of CFD codes that has grown considerably over the years. In fact, in recent decades, thanks to the increasing use of CFD software in engineering and the availability of workstations with considerable performances and graphics capabilities, it has become necessary to equip CFD software with versatile data visualization tools.

In particular, now is possible to visualize on computer monitor domain and mesh geometry, vector plots, 2D and 3D plots, particle tracking, color postscript output, is possible to manipulate geometry in terms of selecting visualization options (translation, rotation, scaling) and fixing errors on the geometry in STL format.

Recently, the possibility to add animation for dynamic result display has been included.

After having described the components of any CFD software, let's see which numerical methods can be used to solve the flow equations. As already said the main use of CFD is to solve Navier-Stokes equations and the equations connected to them (turbulence). These equations can be solved analytically only in very simple cases, characterized by laminar flow and simple geometries (spheres, flat plates), while the resolutions of real cases, in which turbulent flows frequently appear, necessarily require a numerical approach.

Therefore, there are several methods to solve Navier-Stokes equations, and since they are generally operations with a high computational cost, more and more refined model-based approaches have been developed:

- **Direct Numerical Simulation (Direct Numerical Simulation: DNS):** consists of discretizing the domain in space and time using grids of arbitrary size and performing calculations on them. It allows to obtain more accurate results but has a very high computational cost.

- **Reynolds Averaged Navier-Stokes (RANS):** this method allows to study the motion in turbulent regime as formed by an average motion and its fluctuation in time so the quantities of the flow equations are averaged in a certain time interval. In this way the calculation times are significantly reduced because the scales of the average motion are significantly greater than those of the turbulent motion. They require the use of further equations (e.g. the k-ε model) to complete the problem.

- **Large Eddy Simulation (LES):** it consists in numerically calculation of the behavior of the largest turbulent scales and modelling the smallest ones (Sub-grid Scales or Kolmogorov's
scales). It provides more accurate results than RANS and has at the same time a computational cost significantly lower than DNS, for this reason it is a method in strong development.

2.1 Governing Equations of Fluid Flow

The equations that describe the behavior of a fluid in motion inside a machine coincide with conservation laws of mass, momentum and energy, expressed in differential form at each mesh node, finite volume, or element in which the domain is split according to the chosen discretization method. Since the dimensions considered in engineering are (usually) equal to or greater than the micron, the molecular structure of the matter can be neglected, and the fluid can be considered a continuous body. So, the properties used to describe the behavior of the fluid are assumed macroscopic and dependent on time and space. Therefore, to define the governing equations of the fluid flow behavior, let's consider infinitesimal cube of dx, dy and dz dimensions, where the positive verses of the coordinates are shown in figure 2-1

![Figure 2-1: Fluid portion used to describe the governing equations](image)

Fluid proprieties we consider are pressure \( p(x,y,z,t) \), desity \( \rho(x,y,z,t) \), temperature \( T(x,y,z,t) \) and velocity vector \( \mathbf{u}(x,y,z,t) \). The values of these quantities at the center of each face of the cube are taken as reference values, while their value in the other points of the face (at the same time \( t \)) are defined by partial derivatives \( \frac{d}{dx} , \frac{d}{dy}, \frac{d}{dz} \) of the function considered, depending on the direction between the reference point and the other. So, an accurate analysis of the changes in mass, momentum and energy in the fluid element due to flow through the boundaries and (eventually) due to influence of sources inside it, allows to define fluid flow equations.

First, Let's start by defining the **mass conservation equation**.
\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} + \frac{\partial (\rho w)}{\partial z} = 0
\]

This is obtained by equalizing the rate of increase of mass inside the infinitesimal cube (first term of equation), with the mass flow rate of the fluid through the cube faces (the other terms of equations), and after a series of steps we obtain the expression shown above.

It is possible to write the previous equations in compact vector notation:

\[
\frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{u}) = 0
\]

In both cases, these express the unsteady, three-dimensional mass conservation or continuity equation in three dimensions at any point of an incompressible fluid.

For an incompressible fluid, where density is constant, the previous equation becomes:

\[
\text{div}(\rho \mathbf{u}) = 0
\]

Now, we can define the **momentum conservation equation** or Newton's second law and which states that the momentum variation of a fluid particle (Lagrangian Derivative) corresponds to the sum of the forces acting on it.

The rate of momentum increases per unit volume for a fluid particle, along the three directions \(x\)-, \(y\)-, \(z\)- is given by the following three terms:

\[
\rho (\frac{D\mathbf{u}}{Dt}) ; \frac{D\rho}{Dt} ; \frac{D\rho}{Dt}
\]

Where \(u,v,w\) are the components of the vector \(\mathbf{u}\).

Instead talking about acting forces, we can identify two types of them:

- Surface forces: like pressure and viscous forces;
- Body forces: which are gravity force, centrifugal force, Coriolis force and electromagnetic force.

Talking about surface forces, we can affirm that the stress state of the fluid element is defined through the nine components of the strain tensor. Here viscous stresses are indicated with \(\tau_{ij}\) while normal tensions are denoted by \(p\) for the reason they are pressures. The usual suffix notation \(i-j\), for viscous stresses, is adopted to indicate that the stress component acts in the \(j\)-direction on a surface normal to the \(i\)-direction. Regarding the body forces, instead, these will not be treated in detail and therefore
they will be grouped all in the term $S_{Mi}$ ($i = x, y, z$ depending on the forces components taken into account), defined as the source of the momentum per unit volume of the body forces along $x, y$ or $z$.

Now it is possible to define the expression of the conservation law of momentum, subdividing it into its components defined along the three Cartesian axes.

- **The $x$-component of momentum equation:**

  \[
  \rho \frac{Du}{Dt} = \frac{\partial (-p + \tau_{xx})}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + S_{Mx}
  \]

- **The $y$-component of momentum equation:**

  \[
  \rho \frac{Dv}{Dt} = \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial (-p + \tau_{yy})}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} + S_{My}
  \]

- **The $z$-component of momentum equation:**

  \[
  \rho \frac{Dw}{Dt} = \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial (-p + \tau_{zz})}{\partial z} + S_{Mz}
  \]

All that remains now, is to define the **energy equation**.

It is achieved starting from the first law of thermodynamics that states that the time variation of a fluid particle energy is equal to the sum of the heat flow associated with the fluid particle and the work done by it.

The expression of this equation is as follows:
\[ \frac{D\mathbf{E}}{Dt} = -\text{div}(\rho \mathbf{u}) \]

\[ + \left[ \frac{\partial (u \tau_{xx})}{\partial x} + \frac{\partial (u \tau_{yx})}{\partial y} + \frac{\partial (u \tau_{zx})}{\partial z} + \frac{\partial (v \tau_{xy})}{\partial x} + \frac{\partial (v \tau_{yx})}{\partial y} + \frac{\partial (v \tau_{zy})}{\partial z} + \frac{\partial (w \tau_{xz})}{\partial x} + \frac{\partial (w \tau_{yx})}{\partial y} + \frac{\partial (w \tau_{zy})}{\partial z} \right] + \text{div}(k \text{grad}T) + S_E \]

The rate of increase of energy is represented by the term on the left side, which is a Lagrangian derivative of energy. Often the term E is done by the sum of internal (thermal) energy of fluid, kinetic energy \( \frac{1}{2}(u^2 + v^2 + w^2) \) and gravitational potential energy.

The total rate of work done on the fluid particle by surface stresses is expressed by the following terms:

\[ -\text{div}(\rho \mathbf{u}) + \left[ \frac{\partial (u \tau_{xx})}{\partial x} + \frac{\partial (u \tau_{yx})}{\partial y} + \frac{\partial (u \tau_{zx})}{\partial z} + \frac{\partial (v \tau_{xy})}{\partial x} + \frac{\partial (v \tau_{yx})}{\partial y} + \frac{\partial (v \tau_{zy})}{\partial z} + \frac{\partial (w \tau_{xz})}{\partial x} + \frac{\partial (w \tau_{yx})}{\partial y} + \frac{\partial (w \tau_{zy})}{\partial z} \right] \]

The total heat flow associated with the fluid particle due to heat conduction across element boundaries is given by the term \( \text{div}(k \text{grad}T) \) and finally \( S_E \) represents the effects of potential energy changes due to the gravitational force, in fact is the source of energy per unit volume per unit time.
3 Hybrid Vehicles

Since the end of the 20th century, the automotive industry has changed rapidly due to the growing attention to economic and environmental aspects related to the consumption of fossil fuels (gasoline and diesel), thus promoting the development of vehicles that can significantly reduce fuel consumption and even using alternative power sources.

Fossil fuel use has decreased mainly for two reasons:

- The constant increase in the price of oil, due both to the scarcity of supply sources and to the great demand at a global level. In fact, oil is the main non-renewable energy source used and, at the current state of knowledge of the subsoil, it is expected that oil reserves could last for another 50 years compared to current consumption.

- Pollutant emissions from the combustion process in internal combustion engines have harmful effects on the environment (global warming and acid rain) and on our health too.

The main pollutant gases emitted by internal combustion engines are:

- Carbon dioxide (CO2): it is a gas slightly heavier than air, it is not poisonous because it is stable, but an atmosphere with a high percentage of carbon dioxide causes asphyxia due to lack of oxygen. However, the main problem associated with this gas is that it is one of the so-called "greenhouse gases", i.e. in the upper atmosphere it forms a cover that retains the
reflected solar rays of the Earth, thus contributing to global warming with the negative consequences that we all know by now.

- Carbon monoxide (CO): it is an odourless, colourless and unstable gas because it tends to associate with oxygen (O); it is therefore very poisonous if inhaled and in smaller doses it causes heart disease and tumours of the respiratory system. It is highly flammable and constitutes an explosive mixture in certain percentages with air.

- Sulphur oxides (SO2) and nitrogen oxides (NO3, NO2): they are mainly present in the exhaust gases of diesel vehicles. In the presence of rain and high air humidity they combine with water creating highly corrosive acids (sulphuric, nitric and nitrous) that have a negative impact on the soil (deforestation) and human health.

- Unburned Hydrocarbons (HC): they originate from incomplete or low temperature combustion of fuels. One of the most important is benzopyrene, which is found in the exhausts of vehicles with diesel engines. The consequences are worse than those of particulate matter in terms of human health.

- Particulate Matter (PM): they consist of solid micro particles in suspension, classified PM10, PM2.5 and PM0.5. They originate from the combustion of wood, coal and petroleum products (excluding LPG and methane). These are highly carcinogenic, especially those of smaller size (PM 2.5 and PM0.5) because they enter directly into the lungs and blood causing cancer and serious cardiovascular diseases. However, their concentration in the exhaust gases can be reduced by the application of suitable filters, which is obviously an added cost.
Since 1970, the European Community has issued directives for the containment of polluting emissions from vehicles, establishing stringent limits of air pollution for manufacturers who must comply with the so-called "euro standards". These currently provide for six classes, from the most polluting for older exhaust systems (Euro1, Euro2, Euro3 no longer in production) to the least polluting for the latest generation of exhaust systems (Euro4, Euro5 for newly produced cars, Euro6 for models produced from 2014). Currently, the reduction of emissions is achieved through the use of exhaust systems equipped with the Retrofit system (reduces the level of pollutant emissions by 50%) or with Catalytic Converter (which chemically transforms pollutants at the input, into other less polluting substances at the output) in engines with cycle eight and with particulate filter (FAP) in diesel engines.

Nevertheless, despite modern internal combustion engines are characterized by considerable performance compared to the past, they are not yet able to reverse the upward trend in pollutant emissions because the number of vehicles is also constantly increasing. Therefore, thanks to an intense research activity carried out with the aim of reducing polluting emissions, without renouncing the high performance provided by an ICE, electric (BEV) and hybrid (HEV) vehicles have been introduced on the market.
An electric car's propulsion system consists exclusively of an electric motor, powered by the chemical energy stored in one or more rechargeable batteries, which make it available to the engine in the form of electric energy. Their use ensures a series of advantages, which include higher overall energy efficiency, the possibility of using renewable energy sources, reduction of polluting gas emissions, reliability and noiselessness. On the other hand, electric vehicles are characterized by a low autonomy, long charging time, poor battery life and significantly lower performance than an internal combustion engine.

Hybrid vehicles, instead, have been developed in order to combine electric motor advantages with those of the internal combustion engine. In fact, the propulsion system consists of the combination of a thermal engine and one or more electric motors, which work in synergy or separately (depending on the hybridization type).

IC engine is powered by a fuel that can be gasoline or diesel, while electric motors, instead, exploit the energy made available by a battery pack that can be located either on the vehicle ground, thus lowering the car's center of gravity for better weight distribution, or in the rear, usually under the load surface of the trunk.

The hybrid electric propulsion systems allow the combustion engine to operate at maximum efficiency even in non-optimal driving conditions, such as departures, overtaking, low speeds moments and situations characterized high power demand, where the greatest fuel consumption and the highest amount of pollutant emissions are recorded.

The fuel efficiency at each running condition is higher than a conventional combustion engine for the following reasons:

- The electric motor and its piloting system are characterized by an efficiency significantly higher than that of an internal combustion engine, we speak of efficiencies close to 90% against 35-40% that would be obtained at full regime in a diesel engine;
- The vehicle can be used only in the electric mode (zero emission vehicle ZEV).
- When the vehicle has to stop temporarily, the combustion engine can be switched off, therefore ensuring considerable energy saving.
- The presence of electric engine as auxiliary power source permits to choose a smaller ICE (downsizing) or a longer final transmission ratio (down-speeding), without neglecting high performance;
- It grants an optimal control over the operating points and transients of engine operation, providing the thermal motor with the necessary torque to work under better working conditions;
- The electronic control selects the engine speed to optimize fuel consumption according to the battery charge status and vehicle power demand;
- The power transmission from the electric motor to the gearbox provides greater energy savings than the hydraulic power transmission.
- The electric motor acts as a power unit for charging the batteries, while the vehicle brakes (regenerative braking).

Nevertheless, we have to consider the limits of this technology too:

- Hybrid vehicles are much more expensive than conventional vehicles, in particular due to the high purchase cost of specific components, such as batteries, transmissions and electric motor;
- These vehicles have a greater construction complexity than one with a thermal engine, especially due to the presence of additional control systems for the electrical part;
- For the presence of batteries and auxiliary electric motor hybrid vehicles have the disadvantage of having a considerable additional weight.
- In conditions of constant driving at high speed (extra-urban driving), the advantages of the electric motor are nullified, since it is deactivated (over 50 Km/h), to avoid wasting the batteries in situations that do not require electrical assistance, with the aggravation of carrying around the "dead weight" of an electric engine almost unused.
- Due to the reasons listed above, a hybrid vehicle involves a reduced drivability and the need to correct your driving style in order to optimize fuel consumption and battery life.

### 3.1 Hybrid Vehicles Typologies

Before proceeding with the HEVs classification, a brief description of its constituent elements is considered appropriate:

- **Internal combustion engine**: characterized by a lower power compared to a conventional vehicle and equipped with modern systems to reduce pollutant emissions and increase efficiency;
- **Fuel tank**: primary energy source of the vehicle;
Electrical Machines: one or more electrical machines equipped with advanced electronics to work as engines for torque suppling, and, as generators for energy recovery;

- **Batteries**: they constitute the secondary energy storage system on board the vehicle and are also able to store the kinetic energy recovered;

- **Transmission**: gearbox (stepped or continuous CVT) and clutch.

There are essentially two classification criteria for hybrid propulsion systems: according to the "Hybridization Degree" and according to HEV power train configuration.

The degree of hybridization is defined as the ratio between the maximum power of the electric motor and the overall maximum power installed on the vehicle (\( P_{EM} \) - Maximum power of the electric motor + \( P_{ICE} \) - Power of the thermal motor):

\[
HF = \frac{P_{EM}}{P_{EM} + P_{ICE}}
\]

For conventional vehicles, the hybridization factor is zero, whilst in the case of electric vehicles, it has a value equal to one, so all possible hybrid vehicle configurations are included between these two values.

### 3.1.1 Classification according to Hybridization Degree

Depending on the degree of hybridization and the capacity of the hybrid system to store energy, three different levels of hybridization have been defined:

- Full HEV;
- Mild HEV;
- Micro HEV.

- **Full hybrid (Full HEV)**

When the electric system alone is able to move the vehicle on a complete standard driving cycle (0.5 < HF < 0.7). A driving cycle represents a set of vehicle speed points versus time. It is used to assess fuel consumption and pollutants emissions of a vehicle in a normalized way, so that different vehicles can be compared.
Specifically, this type of hybrid car has the classic thermal engine, gasoline or diesel, one or more high power electric motors and batteries of sufficient capacity to allow the car to travel a distance of about 50 km in purely electric mode, i.e. zero emissions. The two engines are normally coupled through a continuously variable CVT transmission or through an automatic converter or double clutch transmission. The electronic piloting system which controls the engines operation, permits them to work in conditions of maximum efficiency. For this reason, both thermal and electric motors or together can be used for traction, as in those non-optimal driving conditions in which the thermal motor is "helped" by the electric one.

Another important function is that of the "Inactive Distribution", which when no torque is required to the thermal engine, keeps the valves in a rest position, so that the ICE stops without really shutting down. Finally, we have another function, common to all types of hybrid vehicles, regenerative braking, which in the deceleration and braking phases allows to use the electric motor as a current generator, so as to recharge the battery pack by exploiting the kinetic energy that would otherwise be lost as heat.

In this category, we can also include HEV Plug-in, as they are hybrid vehicles that perfectly reflect the characteristics of the full hybrid, with the only difference that they add a charging socket for recharging a battery pack characterized by greater capacity, thus allowing the car to travel a longer distance in purely electric mode.

- Mild hybrid (Mild HEV)

In this case the electric system alone is not able to perform a complete standard driving cycle (0.25 < HF < 0.5). These vehicles mount, in addition to the thermal engine, also an electric motor/generator as in the case of full hybrid, with the difference that it has less power because in this case the traction in purely electric mode (ZEV) is used only for starting from standstill and to cover a few hundred meters.

However, the novelty of the mild hybrid system is to have a 48 Volt electric system which, replacing the high voltage system (400 Volt) of the full hybrid systems, goes alongside the classic 12 Volt electric system (of conventional vehicles). This design choice has allowed to adopt 48 Volt engines and battery packs up to 4 times more powerful than those of 12 Volt and to contain the voltages so as to reduce costs, overall dimensions and weight of the wiring.

As for the full hybrid, the electric motor allows the power supply for traction, in addition to the thermal motor, to cover the torque peaks (for example at startup). During deceleration or braking, on the other hand, it acts as a brake to charge the battery with energy that would otherwise be lost, obviously they are also equipped with Start&Stop systems,
they guarantee regenerative braking and the possibility to keep the valves in the rest position, deactivating the ICE (without turning it off) when no torque is required. Therefore, we can conclude that the Mild Hybrid are vehicles suitable for use in urban areas, where they can reduce fuel consumption by up to 30% compared to a conventional vehicle.

- **Micro hybrid (Micro HEV)**

When a conventional vehicle is equipped with auxiliary systems that allow the recovery of a part of energy in situations where it would be completely dissipated ($0 < HF < 0.1$). This type of vehicle, indeed, is not a hybrid car in the strict sense of the word, as it does not have an electric motor for traction, which is provided exclusively by the internal combustion engine. Therefore, what makes it different from a conventional vehicle, is the presence of a modified electric system that allows to reduce fuel consumption. In fact, this allows to implement the Start&Stop function, allows energy recovery during braking (regenerative braking), energy absorption during slowdowns and energy saving through the automatic shutdown system in case of long stops.

They have larger alternators with electronic management and oversized batteries, in order to store the electrical energy obtained from the regenerative systems with which the vehicle is equipped. Moreover, thanks to the greater amount of electric energy available, all services and accessories can be powered without burdening the thermal engine in terms of power and consumption.

### 3.1.2 Classification regarding power train configuration

We can distinguish many types of hybrid vehicles considering the configuration of the powertrain construction scheme, on which depends the layout of the various main elements, such as electric engines, thermal engine, batteries, gearboxes and clutches.

The two main solutions are called series hybrid and parallel hybrid, while a third can be obtained, starting from the previous two, to get more complex and optimized engine architectures. No standard solution exists for the optimal size ratio of the internal combustion engine and electrical system, the best choice includes complex compromises between power, cost and performance. Therefore, these three configurations will be analyzed, as follows.
• **Series Hybrid Electric Vehicles (SHEV)**

These are HEV equipped with a propulsion system, which consist of an internal combustion engine (ICE), a generator, one or more batteries and electric motors. The peculiar characteristic of this HEV configuration is the absence of mechanical connections between the ICE and the wheels, in fact the traction to the wheels is provided exclusively by the electric motor, connected to them by an appropriate transmission system. The internal combustion engine, therefore, is used exclusively to power the generator and recharge the batteries; the generator in turn supplies electric power to the electric motor.

The presence of high capacity batteries allows the vehicle to travel for many kilometers in purely electric mode (ZEV), simply turning off the ICE when the level of battery charge is optimal, moreover even in this case it is possible to exploit the additional amount of energy is provided by regenerative braking. This combination (ICE-batteries-electric engine), allows to overcome the principal problem of electric vehicles, whose autonomy is linked to the presence of charging stations, not yet widespread.

![Schematic of series hybrid electric vehicles (SHEV).](image)

*Figure 3-3: Schematic of series hybrid electric vehicles (SHEV).*

Let's analyze the advantages and disadvantages of this technology:

**Advantages:**

- The thermal motor, being mechanically decoupled from the wheels, can be designed to work at a fixed point (constant speed of rotation) in its optimal operating conditions (maximum possible efficiency), avoiding the losses that would occur during transients in case it supplies driving power. By contrast, the electric motors, that delivering a high torque (maximum) already from zero engine speed and not suffering a strong reduction in efficiency at varying...
engine speed, are made to operate over the entire rotation speed range, allowing at the same
time to reduce the need for a complex transmission;
- Electric motor torque characteristic allows to have a high torque already from zero rotation
speed, without suffering a significant efficiency reduction by varying engine speed. In this
way the electric motor is able to work in conditions of maximum efficiency for every
operating condition, allowing at the same time the elimination of the multi-speed gearbox;
- By adopting a pair of electric motors for the two driving wheels, rather than just one for both,
it is possible to eliminate the differential.
- Up to 30% saving on fuel consumption
- Up to 60% reduction of pollutant emissions
- Less maintenance is required

Disadvantages:
- In the thermal-electric-kinetic conversion, however, a large part of the energy is lost, causing
the efficiency of this type of construction scheme to collapse. For this reason, the hybrid series
is ideal for vehicles that require continuous braking and restarts, while it is not very suitable
for vehicles that operate at constant high speed;
- The electric generator adds cost and weight to the traction system;
- The traction motor must be dimensioned according to the maximum power of the vehicle,
resulting in a higher cost and weight and additional overall dimensions.

• Parallel Hybrid Electric Vehicles (PHEV)

In this HEV configuration both electric and thermal engine are connected to the driveline in order to
produce driving torque. The traction can be only electric, only thermal or given by the union of both
motors (when ICE needs), while the batteries can be recharged both through the regenerative braking,
guaranteed by the electric motor, and through the current generation guaranteed by the thermal motor.
Therefore, due that both motors (electric and thermal) are connected to the wheels, when the power
required by the transmission is higher than the output power of the ICE, the electric motor is turned
on in order to fill the lack of the ICE, instead if the power required by the transmission is lower than
the output power of the ICE, the remaining power is used to charge the battery. The distinctive feature
of this type of HEV is the combination of electric motor and electric generator (able to convert the
mechanical power of the MCI into electric power) in a single unit, usually located between the internal
combustion engine and the transmission, exactly where the flywheel and the clutch are located. The
construction scheme of this HEV is featured by the majority of hybrid vehicles in circulation; it is shown in the figure below.

![Figure 3-4: Schematic of parallel hybrid electric vehicles (PHEV).](image)

Let's analyze the advantages and disadvantages of this technology:

**Advantages:**
- Compared to SHEV, the total efficiency is higher when driving at cruising speed and on long-distance highway routes;
- Better performance during acceleration is granted because of the combined power from both engines;
- System with high operating flexibility in the transition from electric to thermal motor functioning;
- Only one electric machine (EM and generator combination) is required;
- The nominal power of the electric machine is usually in the range between 5 and 20 kW, considerably lower than the one required by the SHEV.

**Disadvantages:**
- Typically, a PHEV runs in purely electrical mode at low speed, until the battery's state of charge reaches a predetermined low level, usually 30%;
- Quite complicated system;
- Although the electric engine-generator permits removing both the starter motor and the alternator, it needs a continuously variable transmission (CVT) or an automatic gearbox with converter or double clutch in order to operate;
- The ICE no longer works at fixed point as it did for the hybrid series, so its efficiency is reduced at low speeds;
- Since the engine is not disconnected from the wheels, the battery cannot be recharged when the vehicle is stationary.

**Combination of parallel and series HEVs**

In this case the combination of the two patterns previously seen, the serial and the parallel one, is verified. The system, in fact, consists of two electric machines, a generator and an electric motor and a thermal engine, working with gasoline or diesel. The constructive modality with which the hybrid parallel to the series configuration is changed (and vice versa) can vary from vehicle to vehicle. For this reason, we will analyze the architecture of the Toyota Prius HSD (Hybrid Synergy Drive) as a very clarifying example. In this hybrid car the mechanical coupling between the thermal engine, the two electric cars and the final drive shaft has been realized through a planetary gearbox and a reduction gear. This transmission allows three different degrees of freedom which are selectively blocked by an electronic control unit depending on the battery charge status and driving phases. The first degree of freedom is occupied by the thermal motor and the electric motor-generator, the second degree by the second electric motor (responsible for traction) and the third by the final transmission to the wheels. So, by varying the locking of the three degrees of freedom, the planetary gearbox allows to pass from one configuration to the other.

This type of transmission, called e-CVT (electronic continuously variable transmission), works in a similar way to the CVT system.
This configuration also guarantees:

- Kinetic energy recovery both braking and descending;
- The ICE has a smaller operating range, allowing it to work in conditions of maximum efficiency;
- ICE on/off management for ZEV operation;
- Possibility to implement the plug-in function;
- Reduced size of the thermal motor;
- Reduction of fuel consumption.
3.2 Our Hybrid Propulsion System: Range Extender

The Range Extender is a type of series hybrid, indeed even in this case the traction is supplied exclusively by the electric motor, powered by high capacity batteries or by absorbing energy from a generator in turn fed by the thermal engine, or by exploiting both energy sources.

If the battery charge level is optimal it is possible to move in ZEV mode, without requiring the intervention of the thermal motor, which (as already said) has only the function of recharging the battery pack, since it is not connected to the wheels.

This solution allows to reduce fuel consumption up to 30% and pollutant emissions up to 60% compared to a traditional vehicle. Moreover, the Range Extender system solves all the main obstacles to the diffusion of electric vehicles, proposing an ecological and at the same time an economic solution: a great autonomy in electric mode (up to 300 km), without depending on the presence of charging columns and at an affordable price compared to that of a traditional vehicle.

To conclude, this hybrid version is considered an evolution of a pure electric one. As the name suggests, these vehicles are designed to have an "extended range" in electric, guaranteed by the presence of the thermal engine and fuel tank, which act as a "charging station for batteries". In fact, on-board battery recharging opportunities allow the use of an electric car even for long highway stretches, not possible today with a purely electric vehicle, especially due to the lack of power line availability for recharging batteries along the road.

The thermal engine that will be studied in this thesis work, is intended to work in a range extender hybrid vehicle and the representation of its construction scheme is shown in the figure below.

![Diagram of the Range Extender system](image)

*Figure 3-6: The layout of the model we will study*
In this scheme, we have a 125cc aeronautical boxer turbocharged engine with four cylinders, designed to work at fixed point at constant revolution speed of 8500 rpm, reaching a peak combustion pressure of 350 bar.

This spark ignition engine is able reach 12 bar of boost pressure by using three axial compressors, each one made up of six stages, chosen for granting higher isentropic efficiency than a centrifugal compression group. Each compressor is followed by an intercooler, placed downstream of each one, with the task of lowering the intake air temperature at the end of each compression stage, so that it is not too high inside the combustion chamber.

The thermal motor is followed by a five-stage axial turbine, mounted on the same compressor shaft, with the aim of exploiting the thermal energy (still high) of the exhaust gases to produce mechanical power, of which a part is used to feed the compressors and the remaining is converted into electrical power to power one of the electric motors, precisely the EM2.

All the power produced by the thermal motor, instead, is used to recharge the on-board battery pack and to supply power to the EM1.

<table>
<thead>
<tr>
<th>Bore</th>
<th>37</th>
<th>mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stroke</td>
<td>29</td>
<td>mm</td>
</tr>
<tr>
<td>Displacement</td>
<td>0.125</td>
<td>l</td>
</tr>
<tr>
<td>N. of cylinder</td>
<td>4 - V 180°</td>
<td>-</td>
</tr>
<tr>
<td>Firing order</td>
<td>1 - 2 - 4 -3</td>
<td></td>
</tr>
<tr>
<td>Engine speed</td>
<td>8500</td>
<td>rpm</td>
</tr>
<tr>
<td>Turbo shaft speed</td>
<td>200000</td>
<td>rpm</td>
</tr>
<tr>
<td>Boost pressure</td>
<td>12</td>
<td>bar</td>
</tr>
</tbody>
</table>

*Figure 3-7: Table resuming the principal engine characteristics*
4 Geometry Preparation

As specified in the beginning chapter "Introduction", my work has focused on the implementation of the model in the new Solver version of Vectis, called VSOVE, and to perform a CFD simulation through this.

In particular I worked on the same geometry used in the simulation carried out by Trane, with the difference that before analyzing and modifying properly the parameters, in order to improve the results, it was necessary a long editing process on the STL geometry. In fact, the STL file that I used, has been conceived for being implemented in Phase5, not in VSOLVE, having an operating logic for the simulation process on the input geometry, different from the first one. In fact, using the same STL file (and mesh) on which Phase5 was able to realize the simulation without giving calculation errors, in VSOLVE various stops of the computational process have been verified, due to the geometric interferences between various components of the mesh, that did not allow the iterative calculation to reach convergence.

In the following chapters the work I conducted will be explained in detail.

4.1 Engine CAD Model

A multidimensional CFD simulation consists in solving Navier-Stokes equations on a particular geometry, which must be provided in STL (acronym of Standard Triangulation Language) format, which consists in approximating the surfaces of the CAD model using a triangular network, more or less dense, depending on the desired level of detail. So, starting point is the CAD model realization of the system studied. The complete assembly of the thermal engine, including the intake and exhaust ducts, has been executed through the Cad software "PTC Creo Parametric 3.0", by the various thesis students during their thesis work at Leonardo Engineers for Integration.

The bill of components consists of:

- Cylinder head;
- Piston surface;
- Intake/Exhaust Poppet valves;
- Spark Plug;
- Injector;
- Intake and Exhaust ducts.
Among the components that are assembled with the cylinder head, a key role for the successful CFD simulation is played by the piston surface and the spark plug. Therefore, greater construction precision is required in the design of these components. The rest of the assembly does not affect the quality of the results very much, so less precision does not affect them. We can conclude this introduction speech claiming that poppet valves, injector and intake and exhaust ducts were designed by Vincenzo Bottari, spark plug and piston, instead, were realized by Lorenzo Sguaitamatti, after Chierchia optimization study.

Let's proceed with the description of each one of these components.

### 4.1.1 Cylinder Head

The Cylinder head of the engine was designed by De Virgilio, applying the results obtained from the structural and thermal analysis he carried out during his thesis. This component has already been used in the previous simulation of Bottari and Trane and will be used in this thesis too. This geometry is equipped with four poppet valves, all with the same diameter of 14 mm and a valve angle of 40°, and a pent-roof combustion chamber, which ensures relatively high power for displacement and faster combustion time of the fuel-air mixture. The following images show a detailed representation of the cylinder head:
4.1.2 Poppet Valve

A sketch of one of the mushroom valves is provided in the figure below, with attached dimensioning, in order to have a more precise idea of its section and overall dimensions.

CAD models, designed by Creo Parametric, are showed in the following figures:
In the Bottari model the valve motion curve is the same used for the 1D Wave model, where for both valves (intake and exhaust) a maximum lift of 4.5 mm is reached. On the other hand, in the Trane model, the maximum lift for intake and exhaust valves is not symmetrical. In fact, for the exhaust valves there is a maximum lift (measured along the axis of the valve) of 4.5 mm, as in the previous model, instead for the intake valves this value has been lowered to 2 mm. This choice was the result of a compromise between the results obtained by Chierchia and those obtained by Mariani, both working on model 1D with Wave. In particular, Chierchia analysis, mainly aimed at fuel consumption improvement, led to unacceptable results in terms of net power, as well as sub-optimal intake valve lift values.
<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>EVO</td>
<td>120°</td>
<td>IVO</td>
<td>340°</td>
</tr>
<tr>
<td>EVC</td>
<td>375°</td>
<td>IVC</td>
<td>520°</td>
</tr>
</tbody>
</table>

*Figure 4-6: Table reporting Crank Angle values at which valve opening and closing occurs*

### 4.1.3 The Piston Surface

Piston surface used by Bottari, had a hemispherical shape and provided a compression ratio of about 9 (actually 8.88), as it was consistent with the results of the 1D analysis conducted by Mariani on Wave. Its shape was modified several times according to certain design specifications, including minimization of the unburned portion of the fresh charge and reducing detonation risk.

*Figure 4-7: Bottari's Piston Surface*

In the Trane model and therefore also in mine, the piston surface that has been adopted, is the one designed by Sguaitamatti, based on the study he conducted. In fact, in this case, this one has a pent roof shape, in order to achieve a much higher compression ratio of 21. Choosing the optimal shape for the piston surface is the result of a long study process that takes various factors into account. Here we proceed with the description of some of the most important aspects involved in the design phase. A fundamental requirement that an internal combustion vehicle must ensure is the reduction of pollutant emissions, caused mainly by the incompleteness of the combustion process. This problem can be partly solved by maximizing the volume occupied by the piston surface. In this way the air-fuel mixture is concentrated within smaller area, making lower the probability that part of it will fit into the interstices between the chamber and the piston, thus remaining unburned.
Another parameter that should not be overlooked is the risk of detonation. To overcome this problem is necessary that on piston surface there are no sharp edges and small curve radius, where very high temperatures would be reached causing self-ignition. Obviously, in order to ensure proper functioning of the system, there must be no interference between piston and valves during their movement, which would cause irreparable damage. Finally, it is necessary that the part of the piston top closest to the spark plug, at the TDC, has a hemispherical depression, so that it pushes the mixture towards the spark plug seat during piston rising.

Below, the piston surface shape is showed.
4.1.4 Spark Plug

In this model the spark plug has the same position as in Bottari's, it is positioned at the center of the cylinder head. But in our case, it was chosen another type of spark plug, which differs to have two side electrodes (also known as the "ground strap") instead of only one. The spark plug is a key component for the efficiency of the combustion process and therefore it is necessary to ensure that it does not get excessively dirty and replace it when necessary. In fact, malfunctioning can occur if the external temperature is so low that the spark plug cannot be properly warmed up or if an excessive layer of unburned gas is deposited on the spark plug surface. To avoid these problems, it is recommended to choose a spark plug with a suitable degree of thermal insulation for your application and to clean it periodically.

The used spark plug is NGK 1633 LMAR9D-J and in the following figures its characteristics are exposed.

Figure 4-10: Spark plug geometry

![Spark plug geometry](image)

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thread size</td>
<td>10 mm</td>
</tr>
<tr>
<td>Thread pitch (A)</td>
<td>1.0 mm</td>
</tr>
<tr>
<td>Gasket seat diameter</td>
<td>16 mm</td>
</tr>
<tr>
<td>Reach</td>
<td>26.5 mm</td>
</tr>
<tr>
<td>Hex size</td>
<td>9/16&quot; (14 mm)</td>
</tr>
</tbody>
</table>

Figure 4-11: Spark plug CAD model

![Spark plug CAD model](image)
4.1.5 Injector

The injector used is a Bosch HDEV5 high resistance model that can handle pressures of up to 200 bar. Based on the results obtained by de Virgilio, due to the limited dimensions of the cylinder head and the high pressures in the chamber, it was decided to choose an indirect injection configuration.

Figure 4-12: Injector specifics

- Max. 500 bar
- Multi hole
- Flow rate at 100 bar: up to 1,640 g/min (n-heptane)
- Spray angle 8 to 20°

Figure 4-13: Injector CAD model and its position in the chamber
4.1.6 Intake and Exhaust Ducts

The CAD model of the chamber including the intake (on the left) and exhaust ducts (on the right) is shown in Figure 4-14.

The dimensions of the ducts are the same as those of the 1D model created by Mariani, however, the Intake and Exhaust ambient have been made in a different shape.

As stated in Trane's thesis, this design choice is due to the fact that the spherical shape they originally had (and that was adopted by Bottari) did not allow the calculation to reach convergence in areas where the curvature varied. For this reason, it was decided to modify the geometry by slicing the sphere through a plane and giving the edge of the duct an almost conical shape. In this way, the inlet pressure and temperature values are assigned to the extreme surfaces of the ducts.

Figure 4-14: Intake and Exhaust ambient and their connections with the Chamber
This operation was performed by Bottari before starting to work on Vectis. In particular, the initial STL file was obtained from CAD model, after having arranged the moving parts in the following configuration: exhaust and intake valves left open and the piston in TDC position. This design choice will be justified in the next chapter, where the comparison between PHASE5 and VSOLVE operating procedure will be briefly discussed. Going back to the STL file generation, we can say that the starting point is the conversion of the model assembly from .prt format, which is the standard format used by PTC Creo Parametric, to STL format. The conversion is done automatically by the software. However, the user can modify two process parameters in order to obtain a more appropriate triangulation depending to the use of the geometry that will be performed.

Process parameters on which the user is going to act are:

- **Chord Height**: is defined as the maximum admissible distance between the model's CAD version and that of the STL format. All surfaces of the parts are covered by this criterion and this distance is measured in the native units of the CAD model. The choice of this restriction arises from the fact that an STL file approximates the geometry surfaces using triangles. Therefore, the conversion will be better when higher is the number of triangles used and smaller their dimensions are. The quality of the triangulation depends precisely on this parameter, which in our model is 0.006 mm.

- **Angle Control**: used to set the desired tessellation density to approximate those points on the model that have a small curve radius. Deeper is the tessellation and higher will be the file resolution, which in turn increases the size of the file. This value can be set between 1 (most accurate) and 0 (minimum). In our model was port equal to 1. In fact, an excellent detail level of the duct and combustion chamber surfaces is required, to ensure more accurate results in the CFD simulation.
4.2 Starting STL Geometries

As mentioned above, the analysis conducted by Trane has been configured as a continuation of Bottari's one. The substantial difference between these two models consisted in the lift law of the intake valves, in the design of the piston surface (flat - convex) and in the shape of the intake and exhaust ambient. Both of my colleagues have used the PHASE5 version of Vectis, so in their models the starting STL geometries were five. Below will be listed only geometries related to Trane model, being my thesis work, the continuation of her study. We know that the necessary geometries were created using the "In-Cylinder Geometry Generator" tool.

As specified in Trane's thesis, the starting geometry for the generation process was imported by setting the model time to 0°, corresponding to an open valve configuration. The first four geometries, generated by Trane, represent the configuration in which the piston is positioned with a specific crank angle, corresponding to the four opening and closing points of the intake exhaust and valves. Finally, the last geometry is that represents the configuration of the moving parts at 110°, an instant chosen as initial for the previous CFD simulation, which I also have chosen. Below the geometries created by Trane are shown:

The study should begin with the exhaust process, so that the combustion process in the chamber can be simulated correctly. The exhaust phase begins when the exhaust valves are opened, at 120° with the current valve lift law. However, rather than starting from the precise moment in which this process occurs, it was considered appropriate (already in the Trane model) to start the CFD analysis when the chamber does not communicate neither with the Intake nor with the Exhaust ambient, precisely 110°.
Let's continue by showing the others engine configuration:

*Figure 4-16: Geometry at 120° corresponding exhaust valves closed and intake valves opened*

*Figure 4-17: Geometry at 340°, when both intake and exhaust valves are opened*
Figure 4-18: Geometry at 375 with IV closed and EV opened

Figure 4-19: Geometry at 520° with both Intake and Exhaust valves are closed
4.2.1 Choice of the starting STL file

This choice was guided by the characteristics required to the STL file, by the VSOLVE importation tools, in order to correctly run the simulation. Initially we decided to start from the 110° geometry, as it happened for the previous work. On this, the computational grid in Cartesian format had been drawn, subsequently generated through the vmesh command and then converted in polyhedral format. The problems arose when, once the geometrical preparation was finished, the VSOLVE interface for setting the parameters of the CFD simulation was used. In particular, the process of generating the Background Geometry was not successful, step necessary to correctly perform a zonal simulation of the combustion process inside an ICE.

In fact, using 110° geometry, the BG geometry thus generated had unacceptable geometric characteristics. Consequently, this choice was discarded and thanks to a careful study of the functioning of the BG geometry, carried out by making attempts on the available geometries (not being possible to start directly from CAD), the 340° geometry was chosen. This in fact had the necessary characteristics for the correct realization of the BG geometry, allowing to pass to the next steps of the simulation.

Below is proposed a diagram that briefly summarizes the main operations performed on the 110° geometry.

These operations are:

1. Geometry importation;
2. Fixing STL error;
3. Mesh definition;
4. vsurf – Surface remeshing;
5. vmesh – Mesh generation;
6. Checking for errors caused by "In-Cylinder Geometry Generator";
7. Fixing geometry errors;
8. Final result after correction process.

These steps were fundamental for the understanding of the operating procedure that distinguishes VSOLVE from PHASE5.
4.3 PHASE1

Phase 1 is the first of the VECTIS pre-processing tools that cover all the necessary steps required for importing the model geometry into the solver vsolve. More specifically, Phase 1 allows the import, manipulation and modification of geometry, including the definition of the boundary region and mesh setup tools in order to realize computational grid for specific types of simulation, such as internal combustion engine simulation.

For Phase 1 description Vectis Vsolve 2019.2 manual was used.

Let's list some basic functions:

- It allows geometry importing from an external source and convert it into a format acceptable for the Vectis meshing generator;
- Allows to identify the various regions of the geometry as different boundaries for CFD simulation;
- To define additional geometric positions to be used in calculation requiring for moving meshes (In-cylinder geometry generator);
- To define the global mesh and control parameters for the mesh generation;
- To run the mesh generator and visualize the resulting mesh
Phase1 GUI consists of the main toolbar, the main menus, the OpenGL canvas, the information area and the tool panels.

Currently, the following file formats can be opened:

- ASCII VECTIS Triangle file,
- binary VECTIS Triangle file
- VDA File
- STL File (both binary and ASCII)
- phase5 mesh file (viewing only)
- VECTIS mesh set-up file (associated with the current model)

All of these may be imported by selecting the Open option from the File menu.
When a new file is imported, the user will be select whether to replace the existing model with the new one or to merge the new model with the old one, as showed below:

![Query](image)

*Figure 4-22: Command that manages how to import a new file, if one is already open.*

After selecting the previous option and before importing the model, the nodes are merged to eliminate duplicate or very close nodes. Then the program asks the user to choose the tolerance for this merging process. The default tolerance is such that the merge does not delete triangles. In addition, it is also necessary to specify the model time expressed in crank angle, in order to define the position of the piston within the imported geometry. In this case, the time has been set to 340° CA, for the reasons mentioned in the previous chapter.

![Import Geometry](image)

*Figure 4-23: Setting "Model Time" and "Merge tolerance".*

Then the model, in one of the listed formats, is imported into the software, whose graphical interface allows us to visualize its reticular structure, made up of triangles.
As it can be noticed showing at Figure 34 (Chapter 4.1.6), the STL file has been slightly modified (by Bottari) compared to its CAD version, because some of the cylinder and head surfaces were useless for the CFD analysis of the combustion process (surfaces no in contact with fluid), besides the fact that they would have significantly weighed down the simulation run process.

To manipulate and edit the imported geometry, the tool panel can be used. It consists of three main modules:

- **General View Options Panel**: allows user to easily handle how the model can be displayed. The viewing options appear on the left side of the canvas when the application first starts up;
- **Triangle Creation Operations**: Allows the user to perform any editing operation on the triangular grid structure of the model. These tools were used in the preparation phase to fix typical generation errors characterizing an STL file;
- **Mesh Set-up**: a separate toolbar equipped with several functionalities for setting the global mesh lines that the mesher uses as a basis for mesh generation. In this section you can also
specify any refinement blocks in those areas where greater accuracy of the iterative calculation is required.

Figure 4-25: Three Main part of Tool Panel

4.3.1 Repairing STL generation errors

This section of the program is concerned with producing a triangular surface model that meets the requirements of the VECTIS mesh generator. In fact, the procedure for exporting the STL model from the CAD model is often characterized by errors due to the fact that the curves of the CAD model must be transformed into a surface formed by triangles only. The main errors that occur are:

- Triangles intersecting each other;
- Presence of unconnected boundaries (open surfaces);
- Sides of adjacent triangles not properly connected to each other, causing holes, or overlapping or cut surfaces (called "Bad Edges");
- Imperfect surfaces, the original CAD shape was not reproduced;
- Flat features.

Figure 4-26: Some of the errors found in the STL model.

In presence of these errors, the mesher is not able to generate the calculation grid on the model, therefore they must be eliminated. Some of these processes can be completed automatically by the phase1 Auto Stitch command, in other cases it is necessary to act manually for removing these defects. To check these errors on the model, the following commands of the "Operation" bar can be used:

- **Check for self-intersection**: Intersection between the triangles of the reticular structure are present. IF PRESENT, it is not possible to start the mesher;

- **Check for unstitched**: Presence of edges or surfaces NOT CONNECTED (isolated) to the rest of the model. IF PRESENT, it is not possible to start the mesher;
- **Check for flat features**: Error that does not allow conversion (and re-triangulation) of the mesh from one structure to another (Cartesian - Polyhedral). IF PRESENT, it does not prevent the mesher from generating the Cartesian grid.

They can be corrected manually, using the tools in the "Triangle Creation Operations" panel:

- Cap Hole
- Delete Triangle
- Create Triangle
- Join Triangles

Below are some images that allow you to understand how to use the tools available to correct errors:

*Figure 4-27: Phase1 reparation tools*
4.3.2 Boundary conditions

At the end of all editing operations of the STL geometry of the model, which have allowed to obtain a fully stitched and triangulated surface, the user can now pass to the boundary identification step of Phase 1, by selecting: “Operations > Boundary Painting > Part and Boundary Panel”. This operation must be done before going to the Background Geometry Generation and before setting the mesh definition parameters. The setting of boundary conditions consists in identifying all the various regions of the surface as different boundaries of the model, depending on the role it has for the system functioning (engine in this case). To modify, add, delete a boundary condition and associate it to a specific surface of the model, the user can select the commands in the boundary panel shown in Figure 4-29. The software automatically associates a different color to each condition to the boundary that is added. You can display the boundary colors in one of two ways. First, using the Outline Colors section of the Viewing Options pop-up menu and set it to Multi will allow you to see the boundary color shown as lines. You can also turn on Show Surfaces, available in the Viewing Options tab, as well as on the toolbar.

![Colorful model (normal pointing outwards) with its different Boundary Conditions.](image)

*Figure 4-28: Colorful model (normal pointing outwards) with its different Boundary Conditions.*
Figure 4-29: Boundary conditions defined in the model
The association of the various BC to the model surfaces has been performed using the "Paint Face" function, consisting in selecting those triangles that are part of a surface that lies within the "Auto paint angle" value that has been specified, 45° is the default value.

Setting boundary condition is one of the most important step to set up a successful CFD simulation. In fact, these permit to identify the various zones of the model where the behavior of the fluid is studied.

A total of 27 boundary conditions have been defined, with some differences from the previous model, due to some geometric changes that will be treated later on.

The various components of the engine studied are:

- Combustion Chamber;
- Piston;
- Liner;
- Exhaust Ducts;
- Intake Ducts;
- Exhaust Ambient;
- Intake Ambient;
- Intake Valves;
- Exhaust Valves.

Each of them has been associated with a boundary condition, except for the valves, which have 4 boundary conditions:
4.3.2.1 Setting of Boundary types

Once defined which triangles are associated with each boundary, it is also necessary to specify the boundary type. These may be:

- Wall
- Zero gradient (symmetry plane)
- Inlet/Outlet
- Cyclic symmetry

In our model we have 25 Wall type conditions, of which 18 have a motion condition, and the last two are Inlet/Outlet boundary type, such as exhaust and intake ambient.

In/out conditions are also called "Open conditions" and are defined in correspondence of those surfaces of the domain through which the fluid enters or exits through. Usually here, it is necessary to define the fluid flow rate value and the direction of motion, or temperature and pressure, as in our case, where the thermodynamic conditions of inlet and outlet engine ports are prescribed. Wall type conditions, instead, are associated with all those solid surfaces that delimit the domain of the system, giving a shape to the fluid flow. They usually require heat flow or temperature specification. For these BC, in case a surface corresponds to a moving element of the model, such as valves and piston, is also necessary to define the motion condition.

Four different types of movement can be specified:

- Unspecified;
- Time-dependent displacement from file;
- Piston motion;
- Interpolated.

For all those conditions corresponding to a static component, no motion conditions need to be specified. The piston motion is defined selecting the "Piston Motion" option for specifying some geometrical parameters and motion direction by defining the verse of normal. The Liner, differently from Piston, requires only the insertion of the normal verse (motion direction), because its motion condition is "Interpolated".

Instead, for all valve wall, seat and head conditions, the option "Time dependent displacement from file" must be selected and the .mot file that defines the motion has to be added.

Finally, for valve steam the motion will be "Interpolated" as Liner and for valve port seat no motion conditions must be specified, because they are static. When a moving element is in contact both with a fixed component and with a moving one, the variation of its position over time must ensure contact with them at all times. For this reason, its motion condition is called "Interpolated".
The settings entered for each moving element are shown below:

- **Valve (wall, seat, head)**

![Figure 4-30: Valve wall, seat and head motion condition.](image)

- **Valve Stem**

![Figure 4-31: Valve stem motion condition.](image)
• Liner

![Liner motion condition](image1)

**Figure 4-32: Liner motion condition.**

• Piston

![Piston motion condition](image2)

**Figure 4-33: Piston motion condition.**
In this chapter the process that led to the generation of the polyhedral mesh on the geometry we considered will be illustrated. A final subchapter will be assigned to briefly explain the operations carried out on the Solver VSOLVE. This choice is due to the fact that the simulations conducted were used exclusively to correct the defects on the geometry, which prevented VSOLVE from working.

The substantial difference from previous models is that the mesh is realized on the Background Geometry obtained from the 340° geometry. So, the grid is realized exclusively on the static parts of the model, taken in the maximum extension configuration (BDC). Obviously, also the parameters related to the mesh fineness have been varied.

*Figure 5-1: Background Geometry configuration*
5.1 Background Geometry Generation

First of all, Background geometry tool can be started form the toolbar of R-Desk VECTIS GUI by clicking on the icon here displayed. As previous explained, this step is required only to perform simulation through VSOLVE.

![Image](image.png)

*Figure 5-2: The R-Desk VECTIS GUI interface is shown. It contains a GUI layout, the toolbar and the available setup panels used to define specific solver parameters.*

This operation is the starting point if the geometry has been prepared for use in PHASE5, as it separates the moving parts from the fixed parts, which will form the background geometry. If, on the other hand, we start from CAD file and so moving parts are provided separately, we proceed directly with zone splitting in order to perform a Zonal simulation. The zones are areas of the computational (fluid) domain that can become completely isolated from the rest of the computational domain due to boundary motion. For example, in an internal combustion engine simulation, the valve motion typically cuts off the intake zone, the exhaust zone, and the cylinder zone at some point during the simulation. The solver requires specific inputs that permitting to define, the zones themselves, the interfaces between the zones and the times when the interfaces become open or closed. In addition, some inputs may also be required during combustion modeling.
The following image shows the panel that is displayed by clicking on the BG geometry icon in the VSOLVE GUI. In our case both "Create BG geometry" and "Create zonal files" have been ticked since we started from a geometry ready to be used in PHASE5.

![BG Geometry generation panel](image)

**Figure 5-3: BG Geometry generation panel.**

When moving boundaries are present in the file loaded, they are detected automatically. Motion type of each moving boundary can be changed if has not been detected correctly. Four options of the boundary motion are available:

- **Stationary**, if a stationary boundary is detected;
- **Piston**, if the boundary checked is a piston;
- **Valve**, when boundary is a valve;
- **Moving**, different motion type can be taken as a general moving boundary.

By clicking on the "Generate" button the background geometry is created, the piston and valve boundaries are moved according to their prescribed movement to the maximum and minimum displacement position respectively, and then removed and stored in separate files. The valve stems
are also extended to ensure intersection with the head shell at minimum lift. Whilst the liner is extended to its maximum extension, i.e. up to the position corresponding to the BDC. The general moving boundaries are just removed from the main geometry and stored in separate files.

5.1.1 Generated Geometries

Just the names of the various files that have been generated by the "Background Geometry Generation" are shown for simplicity:

1. Cylinder.tri
2. Exhaust.tri
3. Intake.tri
4. geometry_340CA.tri_bg_main.tri → MAIN FILE containing all static parts
5. geometry_340CA.tri_bg_moving1.tri → Piston
6. geometry_340CA.tri_bg_moving2.tri → Exhaust valve 2
7. geometry_340CA.tri_bg_moving3.tri → Intake valve
8. geometry_340CA.tri_bg_moving4.tri → Intake valve 2
9. geometry_340CA.tri_bg_moving4.tri → Exhaust valve 2

Figure 5-4: Output message given by the software when BG geometry generation ends
File names are automatically chosen by the software, however, is recommended to change them in a form appropriate to the components generated, in order to avoid confusion in the following steps.

Figure 5-5: Intake zone generated by software e left separated by the rest of components.

All parts generated in this way have open surfaces (highlighted in red by Phase1) where they have been separated from the assembly and therefore must be closed. The only exception is made by the file containing all the static parts (Main geometry), which is automatically closed by the software at the point where it communicated with the piston. The edges of the head, which originally come into contact with the valve stem, must instead be closed manually.

Figure 5-6: Example of open surface in the Exhaust valve file.
Of course, at the end of this process check that one or more typical errors for STL file generation have not been involved in the process of Background geometry development. This checking process carried out using the typical phase1 features, such as: “Check for Self-intersections”, “Check for Unstitched Features”, “Check for Flat Features”. In particular, the latter, if present, does not allow to realize the redefinition of the model surfaces triangulation, object of the next work step.

5.2 Cartesian Mesh

Before proceeding to the mesh generation, we must first define the characteristics it should have, drawing the grid on the domain. We start by defining the Global Grid in Cartesian format, specifying the pitch between one line and the next along the Cartesian axes. If necessary, it is possible manually drawing some local refinement blocks in those areas of the domain where greater mesh density is required. As previously discussed, Phase1 has a separate toolbar, called “Mesh Setup”, that allows to set the global mesh lines that the mesher uses as the basis for mesh generation.

For choosing the mesh characteristics, the following parameters have been taken into consideration:

- Accuracy of the CFD solution: it depends on the number of cells which form the grid. A higher number of these will provide more accurate results;

- Calculation time: the fineness of the grid also influences the calculation time, meanwhile, the main grid should be thickened only in areas where large gradients occur or where the geometry is complex.

- The Cartesian grid cell shape must be as close as possible to a cubic shape (aspect ratio close to value 1).

- Cell connectivity does not exceed two cells connected to one cell, for reducing inaccuracy caused by numerical error.

Vectis solver can read different grid formats generated by different grid generators, but, it also offers its own mesh generator, called vmesh. It works automatically and, by default, produces a locally
refined Cartesian mesh. It allows the user to create meshes with minimal effort and in less time than other CFD software which requires an external mesh generator. Before describing the features of the calculation grid that we have defined, we briefly describe how vmesh works for generating mesh on the geometry model and, in particular, how local refining takes place at the boundaries.

5.2.1 How VMESH works

The mesh for the VECTIS solver is generated using the mesh generator vmesh. The input geometry required for the mesh generation must be a completely closed, fully connected triangulated surface which contains boundary information. As already said, Phase1 is used to supply this surface and also a file containing the meshing control parameters. It is also possible to generate meshes for phase5 solver by vmesh. When generating these meshes, the mesher needs to know that the output mesh is supposed to work with the phase5 solver (-V3 command line option must be used); the process of mesh generation is slightly different in this case. Only Cartesian meshes generated by vmesh can be used with phase5 solver.

1. The starting point is the surface definition and the set of mesh line positions defined in phase1:

![Figure 5-1: Starting point for mesh generation.](image)

2. After grid definition, vmesh calculates which global boxes have any volume inside the model geometry:
3. The program then subdivides (refines) the intersected boxes from the boundaries of the input surface, to produce a precise adjustment to the original shape.

The refinement level is controlled by the user specifying the “Global refinement depth” parameter which refers to how many times a global cell can be split into two. So, refinement depth (RD) defines the maximum possible division of global box to sub-cells, which is $2^{RD} \times 2^{RD} \times 2^{RD}$. Therefore, a refinement depth of 1 allows boxes to be split into at most 2x2x2 refined cells, and a depth of 2 allows boxes to be divided into at most 4x4x4 refined cells. A depth of 0 does not permit any refinement. Instead, to specify the refinement depth which is to be used in the global boxes which are intersected by a particular boundary, "Boundary refinement" has to be used. With this type of refinement, three variables can be set for a boundary:

- **Refinement depth at boundary refinement**: level prescribed to the boundary;

- **Refinement blending distance**: specifies an integer value that is used to control how the refinement at the boundary merges with the refinement level of the surrounding cells. Merging
is achieved by giving the boundary cells a forced refinement level less than or equal to the specified RD at boundary, and by moving away from the boundary, the forced refinement level gradually decreases. So, blending distance defines how many layers of cells must be at each forced refinement level;

- **Blend to boundary depth -1**: a Boolean information (yes/no), which specifies whether the blending should start from “refinement depth -1”. Blending distance is signed as negative value when “Blend to boundary depth -1” is switched on.

![Figure 5-7: Here a difference between "Blend to boundary depth -1" activated and not.](image)

As told, global mesh refinement level can change by external refinement block. It is called "IJK refinement block" and allows the user to set different refinement level simply by drawing (with mouse) a rectangular block over the global grid cells for those part of model which requires deeper mesh density. For each this block defined, the values DEEP and FORCE should be are defined:

- **DEEP** - is maximum allowed refinement level;

- **FORCE** - is a “forced” refinement level that commands to split the global box without testing whether the input surface intersects it or not). For example, if a box has FORCE = 1 and DEEP = 2, it will first be split global cell into a 2x2x2 set of boxes, and a further refinement level (DEEP) will then be applied only if the input surface intersects the box. Thus, it is possible to effectively have a finer mesh localized to a particular area. The forced refinement should be used with care: level 1 produces 8 cells from each global cell; level 2 produces 64; level 3 produces 512! Similarly, using too large a level of DEEP refinement should be avoided.
5.2.2 Setting up mesh: Global Grid and IJK Bocks

For our model, as it had been for previous works, it was decided to generate a main grid and three IJK blocks to perform further local refinement in correspondence with the area where the combustion process takes place, inside the engine.

The mesh guidelines have been realized by choosing a 3 mm pitch spacing in each of the three Cartesian directions:

Figure 5-8: Global mesh lines.

Figure 5-9: Global mesh detail
As mentioned earlier, three IJK refining blocks (locally) have been built to increment the number of cells in correspondence of the combustion chamber area, maintaining at the same time, a low number of global cells in the model. The first IJK block has been designed to cover an area which includes combustion chamber, the liner in its entirety, the area relating to the four valves and the part of the intake duct where the injector is mounted. The values that have been chosen are: DEEP=2, FORCE=1.

![Figure 5-10: First IJK block](image)

The second IJK block was made at the TDC zone, so it includes the valves, spark plug seat, part of the fuel injection zone and the top of the Liner. The values chosen are: DEEP=3, FORCE=1.

![Figure 5-11: Second IJK block](image)
The third and last IJK block was built in the ignition zone where spark plug is set. The values chosen are: DEEP=4, FORCE=2.

*Figure 5-12: The last deeper IJK block*
5.2.3 Generation of Cartesian Mesh

Then, using the values chosen for the main grid and for the refinement blocks, it has been realized a Cartesian mesh characterized by 390853 cells, of which 185431 on the boundaries and 205422 inside the model.

Figure 5-13: Cartesian mesh overview

Figure 5-14: Cartesian mesh - z slice
5.3 Polyhedral Mesh

In advanced fluid dynamics application, it is preferred to adopt a hexahedral (cartesian) mesh, i.e. made up of six faces, made up of quadrilaterals. This mesh guarantees a low numerical diffusion, especially in case the flow is perpendicular to cell faces. However, it is not always possible constructing structured hexahedral meshes for complex geometries, as well as for increasing calculation times. To overcome these limits, it is possible to adopt tetrahedral meshes, the easiest to generate, even in the case of complicated geometry, since having only four faces for each cell. However, they cannot be stretched excessively and therefore it is necessary to use a very high number of tetrahedra to obtain a reasonable accuracy. The calculation of gradients can be problematic due to the spatial position of the neighboring nodes, which can be located in same plane, since each cell is surrounded by only four others. As a result, this mesh leads to convergence errors and greatly reduce the accuracy of the solution. Polyhedral mesh, on the other hand, was introduced to combine the advantages of hexahedral (small numerical diffusion leading to more accurate solution) and tetrahedral mesh (semi-automatic quick generation) and to overcome the disadvantages of both. In fact, compared to tetrahedra, polyhedral is less susceptible to stretching, which results in a better numerical stability of the model. Compared to hexahedra, instead, it guarantees a better precision,
given a high number of close elements. Furthermore, by providing mass exchange on a larger number of faces, it reduces numerical diffusion effects caused by flows not perpendicular to the faces. So, polyhedral cells hold great promise in producing equivalent accuracy results compared to other mesh types with the added benefits of:

- Faster convergence with fewer iterations;
- More accurate solution even with a lower number of cells;
- Lower overall cell count, almost 3-5 times;
- Robust convergence for calculation of residual values;
- Lower run-times.

![Figure 5-16: Tetrahedral to polyhedral mesh conversion](image)

The polyhedral mesh is obtained starting from the tetrahedral mesh by splitting cells into several sub-volumes. For this purpose, new edges are created on each triangular face, obtained by connecting the face center (yellow points in the figure above) with the center of the edges of the same face (red points in the figure above). Then, hexahedral faces of the new polyhedral mesh are created by connecting the cell center with the sides center of two adjacent triangular faces (of the tetrahedral mesh). Altogether, for each hexahedron (one polyhedral mesh face), six triangles (faces of the tetrahedral mesh) will be needed.

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1 Taken from "Polyhedral meshing as an innovative approach to computational domain discretization of a cyclone in a fluidized bed CLC unit" written by Marcin Sosnowski, Jarosław Krzywanski, and Renata Gnatowska.
5.3.1 Surface Remeshing

Such procedure is fundamental for mesh conversion from Cartesian to Polyhedral format. The updated version of Vectis, allows to realize this conversion process through the command "vsurf", typed in the folder where is located the file on which the mesh creation must take place. In fact, vsurf is a command line tool for remeshing a triangular surface made in Ricardo trifile format (the most common geometry file extensions are .sdf and .tri). By using this tool, a new triangular surface can be created with high quality triangles suitable for generating tetrahedral mesh and remeshing of moving surfaces for wall simulations. Various commands can be associated with vsurf, permitting to control the length of triangles side realized during the remeshing process and, at the same time, to choose (if required) a different length value for the triangulation of each boundary condition forming the geometry file.

The size set for triangle side of each component, which making the background geometry, has been chosen according to the Ricardo manual. In general, higher are the gradients to which the component is exposed and higher is its importance for the simulation, so lower will be the value set to define the triangle side that defines its surface. According to this, a limit of 1mm has been set for the piston surface, 0.75mm for the valves and 1.5mm for the rest of the background geometry.

Below is an image showing the background geometry before and after the remeshing operation. The representation of the triangulation for other components is not shown for simplicity.

![Background geometry before remeshing process](image)
5.3.2 Tetrahedral Mesh Generation

After remeshing the background geometry and checking for errors in the conversion process (self-intersection, unstitched triangles and flat features), it is necessary to modify some parameters of the Cartesian grid .mesh file. Opening it as a text file, you need to modify the following parameters:

- MODEL_NAME: geometry_340CA_bg_main_remeshed.tri
- TETMSH_MAXVOLUME = 5e-10

This ensures better accuracy during the mesh conversion process. In this way a tetrahedral mesh formed by 817785 tetrahedral cells is generated on the model, while mesh faces are 1670477, whose 69814 on boundaries. Below some images allow to analyze the tetrahedral structure obtained in this way.
Figure 5-19: Tetrahedral mesh overview

Figure 5-20: Tetrahedral mesh - z slice
5.3.3 Polyhedral Mesh Generation

Starting from the tetrahedral mesh, through a simple vmesh command (-polyhedra) you can define the polyhedral mesh in the way described above.

It can be observed that in the transition from Cartesian to tetrahedral mesh the number of cells has increased significantly, while switching to polyhedral mesh the number is drastically reduced, even lower than cell numbers of Cartesian mesh.

Everything is coherent with the previous discussion, in relation to the various principal mesh structures used in fluid dynamics.

A computational grid made up of 145767 polyhedral cells is generated overall, 34905 of them are boundary cells.

The following images help you better understand the structure of this mesh.
Figure 5-22: Polyhedral mesh overview

Figure 5-23: Polyhedral mesh - z slice
6 Geometry editing for VSOLVE use

As it has already been explained, this thesis has the objective to produce a model geometry that, despite being designed for use in Phase5, can be also used in VSOLVE to perform a complete CFD simulation. After having verified the functioning of the geometry, it was not possible to use it to realize a complete CFD simulation due to various problems that arose during the Covid-19 emergency period.

6.1 Brief overview on Solver parameters setting

After generating the .GRD (grid) mesh file of the model built in polyhedral mesh, vpre command is required to be run prior to the running of the solver (vsolve).

Generally, the input grid file is initially unordered, so vpre will perform optimal cell reordering (Reverse Cuthill-McKee). The main argument is the grid file in addition to various other arguments that allow setting various options. In addition, the input mesh generated by vmesh will contain two
sets of boundary face connectivity: exact fit and IP-face (see on Vectis manual). Thus, vpre will extract a combination of these based on a face angle criterion (by default 70°). If the angle between the normal of the face considered and the face normal of neighboring cell exceeds this criterion then an IP-face is selected over the exact-fit face.

Moreover, vpre allows to define the number of processors for parallel run simulation and to transform the grid file in a zonal type file, so that a zonal simulation on the model can be carried out. In our case the number of processors used for the run has been of 24 and the simulation zones in order to permit the simulation occur separately on them, has been chosen equal to three. The zones in which the model has been broken down correspond to those specified in the BG geometry, Intake, Exhaust and Cylinder. Completed this part is switched to Vsolve, where all the parameters relative to the simulation have been entered. These will not be described given the use that has been made of the simulation results, only a diagram will be illustrates for understanding which operations have been performed.

![Diagram](image)

*Figure 6-1: Diagram showing the sequence of operation performed on vsolve, in order to run simulation*

Where the advanced operations performed on the model are:

- Definition of the Injection model (Injector)
- Spray and Wall film models;
- Ignition model definition (Spark plug);
- Setting the Combustion Model;
- Changing the "Solver Settings";
- Inserting Monitoring Points;
- Volume Sensors for the overall Control Volume and for the Zones (Cylinder, Intake, Exhaust);
- Surface Sensors (IN/OUT Edges only).
Below will be listed the operations that have been performed on the geometric model to make it suitable for use in vsolve. To each one will be dedicated a chapter, except the first one that will be treated immediately. Choice due to the fact that the first one was the simplest operation carried out. In fact, the first problem relative to the run of the simulation, is verified cause of the wrong verse that had been specified for surface normal in valves boundary conditions. In the simulation previous the inserted values had been chosen in order to work in phase5, therefore they had to be changed. The error message obtained from the software has allowed me to understand that the problem was relative to the normal direction, that had to point from the outside toward the fluid for the inner components (Valves and piston), not toward the outside like for the BG geometry!

Therefore, the values entered have been inverted:

- Normal coordinates for the Exhaust valve are (-0.766044, 0.642788, 0);

- Normal coordinates for the Intake valve are (0.766044, 0.642788, 0).

### 6.2 Piston edge issue

The second and more complicated adjustment was the one related to the Piston. This problem was found as soon as the file related to it (obtained through BG geometry generator) was loaded inside vsolve, to set the boundary motion condition. Initially the piston and the liner were connected by a flat surface, that in the case of Phase5 did not give problems, while in the case of vsolve prevented the simulation run.

In fact, once the piston was separated from the rest of the geometry by BG geometry generator, its bottom side needed to be closed (as for the other moving components) because for CFD purposes no open surfaces are allowed.
Figure 6-2: View of piston and liner edge, before correction

However, the presence of the additional annular surface between piston and liner, did not permit this operation, as the intersection between the triangles of the closing surface and those of the flat surface at piston edge would occur. Piston and Liner were in contact correctly in the CAD model. This probably occurred during the In-cylinder geometry generator process. Phase5 uses the In-cylinder geometry generator that deforms the input geometry to generate others in the required configuration. The geometries obtained in this way, are such that the contact surfaces between the various elements
always remain in contact with each other, so the displacement of the piston along the liner is realized "contracting" the liner, without the piston being separated. In this way the annular surface connecting the two edges does not create problems.

Vsolve, on the other hand, uses only a geometry obtained by extending the geometry to the PMI to the largest configuration and then generates the mesh. Therefore, if the geometry is not perfect, errors still remain not allowing the simulation to take place!

For this reason, the piston border has been corrected to coincide with that of the Liner. The following figure shows the difference from the initial situation.

![Figure 6-3: Contact area between piston and liner after modifying the piston profile for ensuring perfect matching](image)

### 6.3 Final correction: Compensation for piston misalignment and Liner redesign

This last modification, like that previous one, has been found because of an error happened during simulation process, which caused its immediate stop.

An interference has occurred between the various elements of the engine (piston, liner and chamber in such case), causing the overlapping of various cells making up the mesh of these impacting elements. When this condition occurs the cell volume became negative, causing the interruption of the iterative calculation and the simulation freezes. The interference was caused by the existing misalignment along the z axis (one of the two horizontal axes) between piston and chamber axis. In the phase5 model, this error was probably compensated by the mesher itself, since at each instant the
mesh was deformed and then adapted to the mesh corresponding to the next instant (crosslink). In our case, since the Liner was extended from the TDC to the BDC taking as reference the connecting edge with the piston, the misalignment was accentuated. This condition caused interference both between piston and liner along the stroke to the TDC and also between piston and chamber wall at the TDC itself!

This problem was solved through trial and error, since the correction was performed on the STL model, not on the CAD model, which is much less user-friendly than the second one.
1. The first step was to understand the extent of the existing misalignment. By using Phase1 tools, it was found that by imparting a translation in the opposite direction of the z-axis (0, 0.-1) with a value of 0.1mm, the gap between the edge of the chamber and the piston along z was distributed equally between the left and right of the piston. The misalignment and interference with the chamber were therefore eliminated.

![Figure 6-5: Piston and chamber coupling, after piston have been translated](image)

2. As can be seen from the figure above, the piston - liner interference still persists, so it is necessary to set the same translation given to the piston also at liner. This modification has been done taking as reference the original model where piston and liner were connected by the flat surface. It was found that by giving a translation to the edge of the piston, the liner was also moved by the same amount (being coupled). In this way the liner was also straightened. Obviously at the end of the modification the flat edge of the initial piston was deleted.
3. The last step was the liner re-design. Again, thanks to the use of the simulation, it was seen that at a certain distance from the BDC and for all the remaining distance between it and the TDC, the piston continued interfering with the Liner. Analyzing better the model, it was found that the liner, although perfectly aligned, was characterized by a triangulation such that the coincidence with the piston edges was guaranteed only at the BDC. For all other altitudes (from BDC to TDC) the triangulation was deformed. Therefore, it was necessary to redesign the liner all over again. This project was conducted taking piston base as reference, in fact only for this one the coincidence between the two edges was guaranteed. Then the base of the piston was isolated from the rest and saved in separate files, it was first shifted by a
distance equal to the difference between the current position (340°) and the TDC along the
direction (0,1,0) and then properly connected with the original base to form a liner coincident
at each point with the piston and at each altitude. Obviously also the edge of the Chamber
has been slightly modified in order to connect opportune with the new liner.

Figure 6-7: Original Liner

Figure 6-8: Redesigned Liner

Figure 6-9: Combustion Chamber adjustment
We can conclude the discussion showing the final geometry, ready to perform a complete CFD simulation using vsolve:
Figure 6-12: Final geometry, detail on piston-line
7 Conclusions

The aim of my Master Thesis work was to provide an improved version, ready to be fully featured in VSOLVE, of a geometric model of ICE for Range-Extender use. This allowed to eliminate all the imperfections that characterized the .tri file (variant of the .stl) of the model and allowing to adopt a mesh that enables reducing the running time and the accuracy of the results in full CFD simulation. The input data, such as the valve lift laws, pressure and temperature values imposed on the boundary conditions, were obtained from the one-dimensional model of the range-extender system, obtained working on the Ricardo WAVE software. The results obtained from the WAVE model have led to a substantial modification of the starting geometry compared to how it was initially conceived (Bottari model). As far as future developments are concerned, it can certainly be said that it will be necessary to carry out a complete simulation on VSOLVE. Using the improved and interference-free geometry between piston, liner and chamber and the parameters adopted in my simulations, it will be possible to make a comparison with results obtained by Trane with Phase5. In addition, it will also take advantage of the benefits that the polyhedral mesh provides. Subsequently, once the 3D model optimization part in Vectis is completed, it is expected that a co-simulation between Vectis and Wave will also be performed.

The purpose of coupled WAVE-VECTIS (1D-3D) simulation is to produce detailed 3-dimensional flow information for ICE from the VECTIS analysis results whilst also predicting the performance of the complete engine using WAVE. Specific interfaces are setup in WAVE which allow WAVE and VECTIS to communicate flow information such as the fluid pressure, temperature, and velocity at each time step, so as to allow for the prediction of transient flow fields in the VECTIS simulation.
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