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Faculty of Engineering

Master of Science
in Automotive Engineering

Master Thesis

Calibration and assessment of the GT-Power “DI Pulse” predictive model for a light duty compression ignition engine

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December 2020

Abstract

The objective of this master thesis is to create the virtual test rig for a light duty compression ignition engine by means of the zero/mono dimensional numerical modeling software GT-Suite. In this paper the predictive combustion model called “DiPulse” was assessed.

Taking into account afford mentioned points, one dimensional simulation tools have proven to be essential in the process of confiding with strict regulations that determine the engine building and calibration operation.

The engine under investigation in this paper is light duty Diesel, equipped with single stage variable geometry turbocharger, displacement of 1.6 liter, compression ratio of 16:1 and common rail fuel injection system. In order to perform the calibration of previously mentioned engine the data set of 41 operating points was provided.

The calibration procedure starts with a preliminary calibration using non-predictive combustion sub-model called Cylinder Pressure Only Analysis (CPOA). CPOA required the measured pressure traces which are then used to obtain the fuel burn rate. Imposed burn rates from CPOA are then treated as an input in the DiPulse calibration. DiPulse calibration is carried out for smaller number of operating points that represent the engine map. Calibration is composed of the optimization process during which parameters influencing the combustion process are investigated in order to minimize the factors such as Improved Burn Rate RMS error and IMEP% error. Having reach the satisfactory level of accuracy the NOx emission calibration was performed in order to match the emission levels provided with the data set. Once the calibration was completed, the validation process was performed in which operating points not considered in the DiPulse were evaluated to assess the predictive capabilities of the combustion and emission models. The final model can be implemented in subsequent studies which may include the influence of alternative fuels or fuel blends on the represented engine.

In conclusion the DIPulse multizone predictive combustion model developed by Gamma Technologies was vastly employed to perform engine calibration process. The resulting virtual test rig model can be employed to assess the influence of different engine configurations and hardware components hence shortening the experimental activity required to accomplish projects goals.

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1. Introduction

In the recent years there has been a progressive tightening of the anti-pollution regulations, which have led to strong development of internal combustion engines. The need to reduce the emissions of greenhouse gases and pollutants has forced car manufacturers to focus their attention on increasing the engine and fuel conversion efficiency and lowering its impact on the environment.

Over the last few years several new techniques has been developed to target those regulations: variable valve timing, direct injection strategies and systems, cylinder deactivation, start – stop system, improvement of air motion inside the cylinder and the most recent the ongoing electrification of the powertrain.

The numerical simulation play fundamental role in the development process of those systems. They reduce the product development times as well as costs of experimental tests, hence saving valuable resources.

One-dimensional calculation codes have proved highly advantageous as they provide great compromise between computational time and results of the analysis. GT-SUITE is the industry leading simulation tool developed by Gamma Technologies, Inc. The software allows to simulate the physics of fluid flow, thermal, mechanical, chemistry and acoustic flow, has built in libraries that can be used to build any engineering system, including but not limited to engines, drivelines, transmission and aftertreatment. It provides the possibility to model the engine and assess the thermo-dynamic mutual interactions.

Focus on this thesis was the combustion model, specifically a "DIPulse" predictive combustion model present and available in the GT-Power library was calibrated and implemented. It is a combustion model that predicts the combustion rate and associated emission for direct injection compression ignition engine with single or multi-pulse injection. This combustion model cannot predict the interactions between the jets hence if the more accurate model is required a 3D Computational Fluid Dynamic model is necessary. A 3D CFD model comes at a significant cost of computational power, which limits its use towards specific applications.

During the early stage of engine development a reliable and fast response is vital, hence 0 and 1 D simulations play fundamental role during the initial stage of the project. They can predict the evolution of the combustion process and flow inside the cylinder, they are limited however by 3D interactions: spray to spray interaction of injected fuel, turbulent motion and cycle to cycle variations are amongst those limitation. Calibration process of the parameters available within the DI Pulse model is therefore necessary to recreate reliable data when the experimental results are available. The search of right set of corrective multipliers that adapt the empirical formulas guiding the model ensuring the predictivity of the model is called calibration.

The calibration phase of the project utilizes the vast data set of experimental results. Experimental results include engine main performance parameters, pressure traces averaged over 100 consecutive cycles, engine geometry and fuel composition. It allowed for the preliminary calibration in a Closed Volume Analysis, Only (CPOA) mode and subsequent calibration of the multiplier coefficients typical for DI Pulse, through a built-in Design Optimizer.

Once a reliable and robust predictive combustion model was obtained, the model calculating NOx emissions has been implemented and coupled with combustion model. After calibration of the emission parameters the model was able to replicate the NOx concentration with satisfactory accuracy.

2. Theory

Internal combustion engines can be classified into two large families, by virtue of the type of combustion process that takes place within them: spark ignition (SI) engines and compression ignition (CI) engines.

Compression ignition (CI) engines draw the air into the cylinder during the intake stroke, compresses it to allow the fuel injected when piston is nearing TDC to self-ignite. It is possible only when the temperature inside the cylinder at the moment of injection is higher than the ignition temperature.

The air-fuel mixture is prepared in the cylinder. Given high reactivity of the fuel they do not require the additional ignition source (External heat source might be used during the cold start, to heat up the air coming into cylinder). Once injected into the combustion chamber, jet disintegrates into drops though interaction with gas in the cylinder (this action is called atomization), the drops mix with air creating a mixture suitable for combustion. As the droplets quickly vaporize being surrounded by hot air they create the fuel vapor which ignites spontaneously while the injection event still takes place, as fuel combust as it is fed in to the cylinder. The self-ignition of the 1st portion of the fuel accumulated in the combustion chamber causes sudden pressure increase which excites the engine structure.

2.1 Combustion in Diesel engines

The basis for the combustion examination are the changes of pressure in terms of crank angle degree. Combustion process in the CI engine can be divided into 4 main groups.

- Ignition delay
- Premixed phase
- Mixing controlled phase
- Late combustion phase

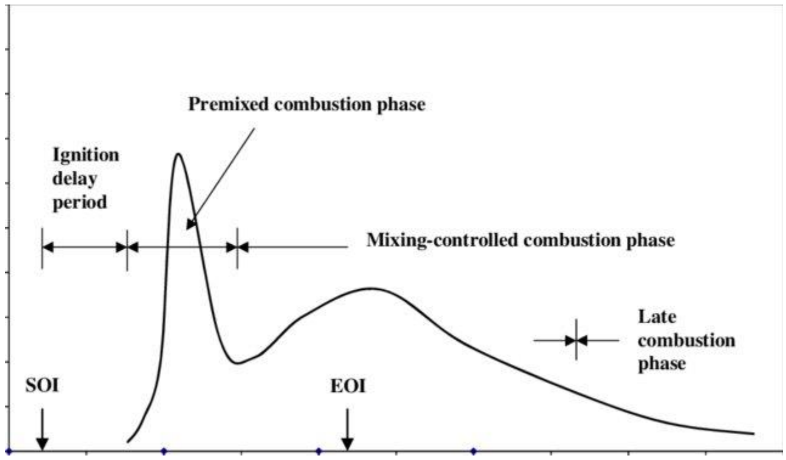

Figure 1: Combustion process in Diesel engine [1]

Ignition delay corresponds to the period between Start Of Injection (SOI) and the first sight of autoignition, Start Of Combustion (SOC). It is characterized by relatively slow oxidation reactions, pressure and temperature change corresponding to polytropic compression (indicated cycle compression curve does not deviate from compression curve) and increasing velocity of injected fuel. Period of ignition delay needed for self-ignition is caused by a necessity to prepare the fuel for ignition. It includes heating up the fuel droplets to the moment of total or partial vaporization, heating up said fuel vapor to the self-ignition temperature, preliminary oxidation reactions leading up to self-ignition. Ignition delay is sometimes called delay period while the crank angle revolution corresponding to it is called delay angle. The more fuel gets into the cylinder during the ignition delay period, or due to the lower cetane number (which influences the ignitability of the fuel), or due to the higher engine speed the more rapid pressure rise is and harsher the engine work is. To improve the combustion process and allow for greater engine speed multi-injection strategies are employed.

Premixed phase corresponds to the period between SOC and moment when all the fuel accumulated in the cylinder during the ignition delay burns. The fuel air mixture ignites in multiple points across the cylinder and burns rapidly in few crank angle degrees, which makes it almost constant volume combustion. Rapid rise of pressure and fast temperature rise influence the NOx emission. NOx formation during premixed combustion may not be significant but that portion of the gas is compressed to the higher pressure and temperature which enhance the oxidation process resulting in NOx formation. Injection time can be shorter or longer than ignition delay. Ignition delay shorter than injection time results in the smaller pressure rise while higher pressure rise is achieved for ignition delay longer than injection time. Influence of ignition delay on maximum pressure and pressure rate can be seen in the figure.

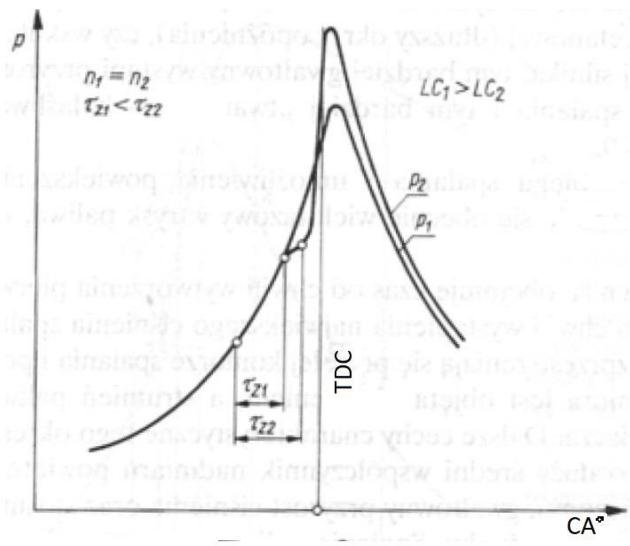

Figure 2: Ignition delay influence on combustion process [2]

Mixing controlled phase – starts after fuel accumulated in the cylinder during the ignition delay has burned during premixed phase. Fuel burns as it is injected into the cylinder, meaning the burning rate is controlled by the rate at which fuel is injected. Heat Rekease Rate (HRR) reaches its second peak at lower intensity as NOx continues to form in high temperature burned gas, while due to local lack of oxygen soot may start to form.

Late combustion – Takes place during the expansion stroke after the end of injection. Late combustion is a source of efficiency losses and as such should be avoided, on the other hand it has an application during the Diesel Particulate Filter (DPF) regeneration. During this phase the mixing rate of fuel and air decreases, as well as temperature in the cylinder and chemical kinetics slow down. [3]

2.2 Diesel jet development

A conceptual model describing the evolution of the combustion and jet characteristics was developed at Sandia National Laboratories by John E. Dec. The model describes the origin and formation mechanism of the main pollutants emitted by a compression ignition engine. The most important pollutants in the Diesel engine are nitrogen oxides (NOx) and particulate matter, referred to as PM or soot. To evaluate the formation of these pollutants the interaction of fuel spray with high pressure and temperature air needs to be investigated.

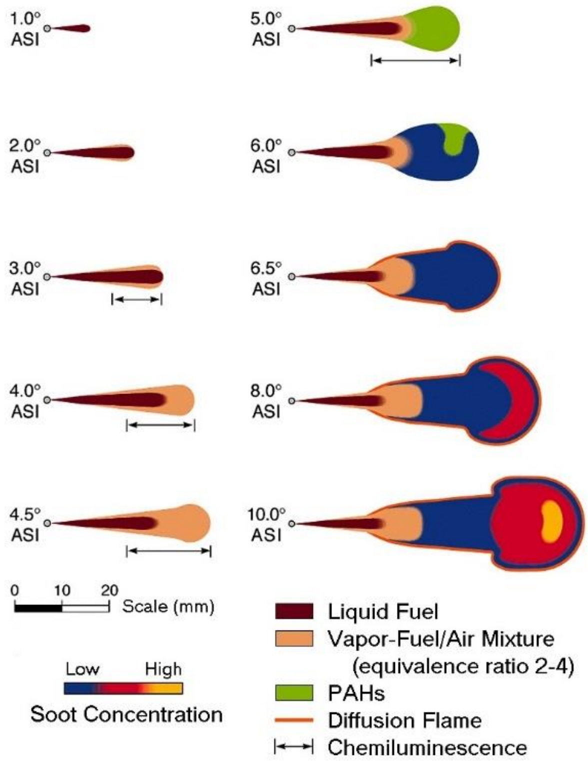

Figure 3: Conceptual model for DI diesel combustion [3]

Looking at the figure, once the liquid jet reaches certain penetration, it is no longer able to advance further as it begins to evaporate. Liquid fuel penetration length is a useful parameter to know it order to avoid the interactions between in-cylinder walls and fuel jet. Its length depends on the air temperature inside the cylinder (liquid fuel penetration decreases with increasing air temperature as vaporization occurs faster), injector's orifice diameter (penetration increases with the diameter size), inlet cylinder pressure (penetration decreases with higher inlet pressure). As the injection advances air is entrained and fuel vaporizes which creates a vapor fuel - air mixture first at the sides of the liquid fuel and then downstream of it. The equivalence ratio of the fuel vapor – air mixture is between 2 and 4, which means that initial premixed combustion occurs in rich conditions, while the overall mixture inside the cylinder is extremally lean. It is possible due to the high reactivity of the fuel molecules and high temperatures surrounding the spray. At 5.0o fuel breaks down and large Polycyclic Aromatic Hydrocarbons (PAHs) form in the leading portion of the jet, it corresponds to the rapid rise in heat release rate indicating the premixed burn phase. Between 5.5o and 6.5o diffusion flame forms at the jet periphery separating the fuel-rich combustion products and surrounding air. For the reminder of the premixed phase jet continues to penetrate across the chamber. Soot concentration increases, with its highest concentration towards the head vortex of the jet. As combustion transitions into Mixing controlled phase (10.0o), soot concentration increases in the head vortex but overall shape of the jet does not change significantly.

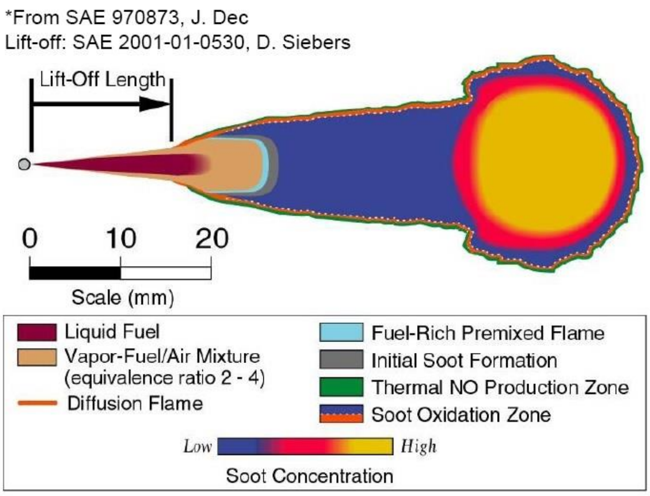

Figure 4: Mixing controlled burn schematics [3]

During the combustion soot is thought to form in two ways:

- During the rich premixed phase local shortage of oxygen leads to the initial soot formation,
- When the products of rich premixed combustion burn out in the area close to the diffusion flame.

NOx formation

During the premixed phase local lack of oxygen does not promote reactions leading to NOx formation, it is however very important to future NO formation. As the portion of the gas that burned during the premixed combustion is then compressed to higher pressure and temperature. NO first appears in the thin layer surrounding the diffusion flame and it continues to be present outside the soot region of the jet until the early burn-out phase of mixing controlled burn. NO forms in the lean side of the diffusion flame and hot spots of combusted gases.

2.3 Fuel injection systems

Engine efficiency and fuel conversion efficiency is mainly limited by the development of technologies related to fuel supply system. The best way to control the combustion process is through the injection system.

Considering single injection event main calibration parameters are injection pressure and injection advance.

- Retarding the injection reduces the ignition delay and the importance of premixed burn, it is commonly used method for effective NOx emission reduction, as it reduces the maximum temperature and pressure in the process. The trade-off is brake specific fuel consumption (BSFC) and soot increase.

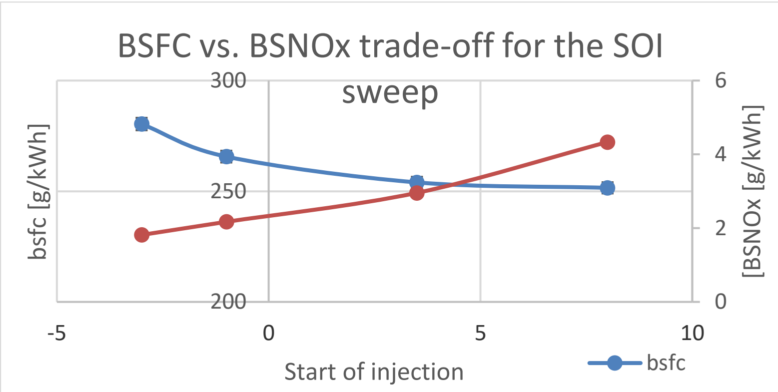

Figure 5 Start on injection trade-off

- Increasing the injection pressure allows for a better jet atomization and air entrainment, which leads to better fuel consumption and reduction in soot formation. On the other hand NOx, combustion noise and peak cylinder pressure are increased.

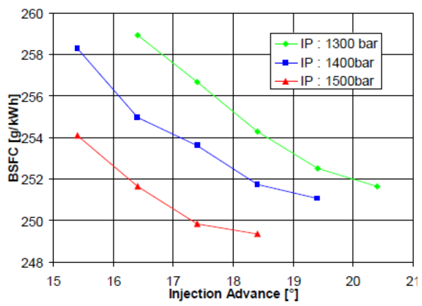

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Figure 6: Injection pressure trade-off [4]

Ignition delay should be minimized, to limit the rapid heat release rate during the premixed phase and consequently prevent too steep pressure increase. From the point of view of thermodynamic efficiency combustion should occur as close as possible to TDC. The compromise between these two requirements can be reached through injection rate shaping.

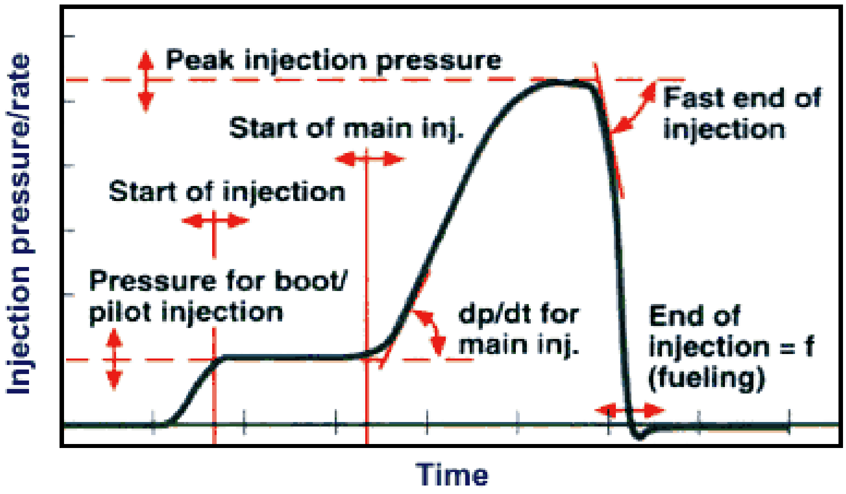


Figure 7: Injection rate shaping [5]

One continuous injection with two different injection rates realized through pressure modulation without throttling fuel flow near spray holes. During the ignition delay small amount of fuel should be injected into the combustion chamber which is represented by boot injection in the figure. This should lead normalized heat release and pressure rise during the premixed burn phase. Injection rate ramps up during the mixing controlled burn.

Splitting the injection event into multiple injections was made possible thanks to the Common Rail system. Common rail is a direct fuel injection system controlled electrically by set of signals including:

- Engine speed,
- Fuel pressure
- Gas pedal position
- Air pressure and temperature as well as boost pressure
- Fuel and coolant temperature
- Vehicle speed
- EGR rate

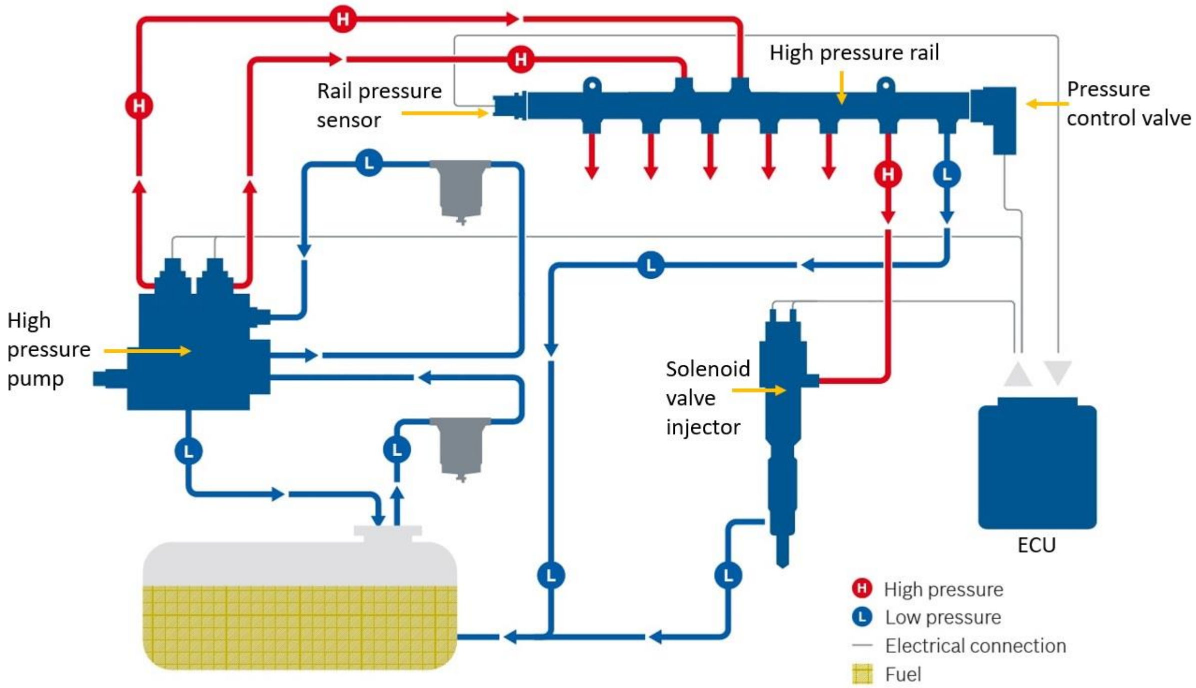


Figure 8: Common rail system schematics [6]

There are several circuits in this system that have different pressure levels. Starting from the tank there is an electric low pressure pump, which transfers the fuel through the fuel filter to the high pressure pump. High pressure pump is decoupled from the injectors, it feeds however the high pressure rail (accumulator, common rail) through which the injectors will be fed at constant and adjustable pressure. The fact that high pressure pump is decoupled from the injectors allows for a pressure setting inside the rail that is independent of engine speed and fits the operating characteristics in the most suiting way. The rail is positioned on the engine head and the fuel is injected into the cylinders by means of electro-hydraulic injectors (solenoid injectors are being replaced by piezo injectors, which are faster and better suited to work with high injection pressure). Rail size needs to be carefully chosen to limit the influence of pressure fluctuations, which may lead to inaccuracies in desired and actual fuel injection volume.

Electronic Control Unit (ECU) controls the pressure inside the rail thanks to the rail pressure sensor, pressure control valve and high pressure pump using the suitable injection and engine maps. It also controls the injection events (time and duration its duration) by sending the electrical signal into the injector which after some hydraulic delay starts the injection. Injections pressures are very high and range from 100 to 2000 bars (and even more for most recent advanced systems).

In general common rail system guarantees very high flexibility of the fuel injection management:

- It allows to split the injection event thanks to electronic control of injection event
- Injection pressure is controlled independently of engine speed
- Timing and duration of injection can be constantly adjusted for maximum efficiency

Splitting the injection into multiple events is a method of reducing peak heat release rate, engine noise and emissions. Latest generations of Common Rail systems can have up to 8 injection events per work cycle. They are divided into pre-injections (pilot), main injection and post injections.

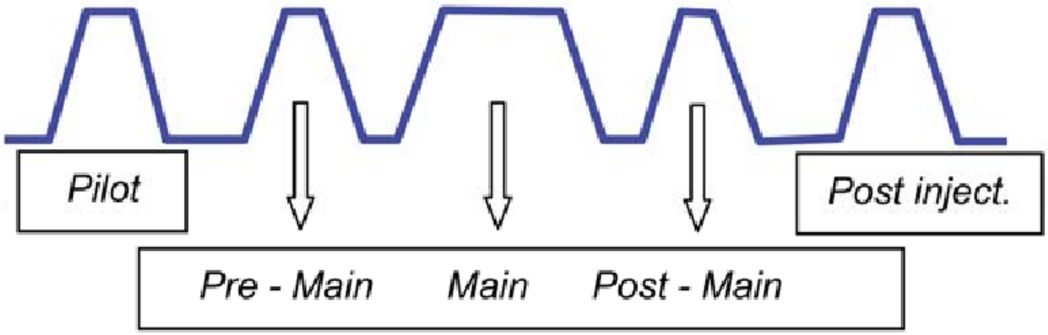


Figure 9: Multiple injection [7]

Fuel injected during the pilot injection shortens the injections delay period. It lowers the noise and therefore mechanical stresses and provide more favorable conditions for main injection. As the temperature and pressure inside the cylinder rises it enhances the air entrainment and the speed of chemical reactions during main injection. Combustion process becomes more gradual without pressure peaks which helps control the NOx emissions. The post injection which is also called late injection is crucial for aftertreatment purposes. Temperature rise due to the late combustion generated by post injection allows for soot oxidation, while the fuel is being burned. Post injection is a technique used for DPF regeneration, a device necessary to comply with emission regulations.

Pre and post injections impact negatively on the combustion efficiency. As from the energy point of view the fuel accumulated in the cylinder that burns together is closer to isochoric process and therefore highly efficient. It is required to seek compromise between the combustion efficiency and pollutant emission control.

2.4 Charge motion within the cylinder

Air-fuel mixture quality and combustion process are influenced not only by the fuel injection system but also by the construction of combustion chamber.

Direct injection compression ignition engine chamber should be designed in a way that:

- Guarantees good air-fuel mixing and a combustion process with small excess of air
- Shortens the ignition delay to lower the maximum pressure inside the cylinder.

Desired intensity of turbulent motion is achieved by particular design of the combustion chamber, piston bowl and intake ducts. Turbulent motion can be created during intake, compression and power stroke.

Swirl motion

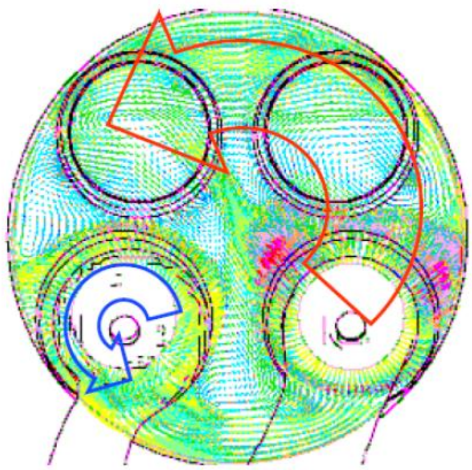


Figure 10: Swirl motion, cylinder top view [11]

Swirl is rotary motion of air about the cylinder axis (or axis parallel to it) in combustion chamber. This motion is obtained through the shape of intake duct or by installing a small orifice on the intake valve (old solution replaced by duct shaping). The helical intake port gives a tangential component to intake flow, the flow is then deflected sideways and downward by cylinder wall, achieving swirl motion. Although there is some decay in the swirl motion due to friction during engine cycle, swirl generated during intake stroke usually persists trough compression, combustion and expansion process. Shape of the intake port influences the axis of swirl motion

Tumble

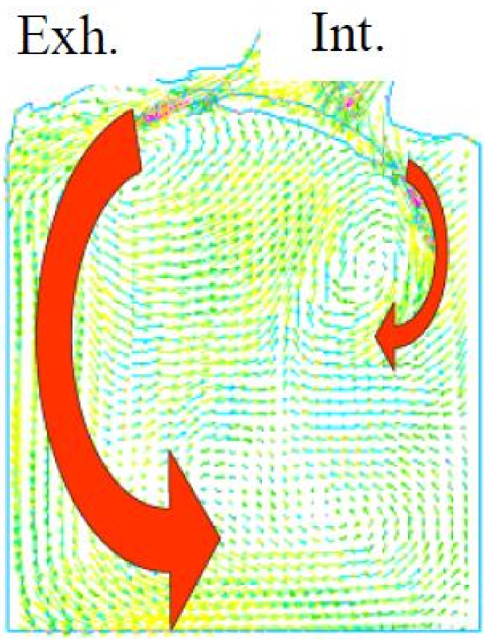


Figure 11: Tumble, Cylinder cross section [11]

Rotation motion about an axis that is perpendicular to that of the cylinder. Tumble is generated during intake and then amplified during compression stroke. Towards the TDC tumble is converted into turbulence energy at small scales. It is obtained through intake duct shaping.

Squish

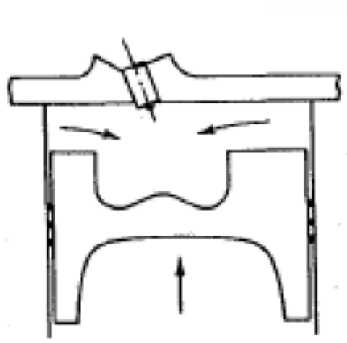


Figure 12: Squish [11]

Radially inward gas motion that occurs towards the end of the compression stroke thanks to the generation of different local compression ratios. During compression stroke air is forced to the center of the cylinder, while during the expansion stroke the gases are dragged towards the cylinder walls. Squish is maximal at TDC when tother cylinder motions are limited.

These three motions coexist inside the combustion chamber, in diesel engine the priority is given to swirl and squish motion.

Parameters playing significant role in creating the fuel vapor are the pressure with which the fuel is injected, injector geometry and ignition advance. Intake duct design to achieve high intensity impacts negatively the volumetric efficiency of the engine, but it allows for lower air-fuel ratio equivalence factor – lambda.

3. Simulation software - GT Suite

This chapter introduces and explains the operating of a CFD simulation software used during the entire thesis work. The main equations, physical laws and discretization methods used by the software will be highlighted.
The 1-D simulation codes used for the analysis of the internal combustion engines have become wildly used in predicting the most of the parameters that define the performance of the engines, namely volumetric efficiency, BSFC, mean effective pressure and the influence that injection parameters and engine geometry may have on a combustion process. GT-Suite allows to carry out the theoretical experiments to investigate the combustion process, acoustics, thermal properties, electric and electromagnetic systems and mechanical characteristics of the automotive subsystems. The use of a built-in libraries enables to obtain information about quantities that are difficult to measure experimentally and consequently reduce the costs and time needed associated with experimental testing.

GT-Power is a library present within the GT-Suite focused on the analysis of the performance of internal combustion engines, both spark and compression ignition. Software provides the possibility to simulate stationary and transient conditions. During the recent years the modules of the software were elaborated allowing for faster operation, as well as more accurate predictions of exhaust emissions. [8]

3.1 Fluid dynamics governing equations

The flow model is based on the solutions of the Navier-Stokes equations: conservation of mass, momentum and energy equations.
The entire engine system is modeled within the software with use of specific templates, blocks and reference object which represent the physicality of the components, their length, volume, surface roughness and other parameters necessary to describe the object completely.
The whole system is discretized into many volumes and these volumes are connected by boundaries. Scalar variables (temperature, pressure, density, etc) are assumed to be uniform over each volume and are calculated in the centroid, while vector variables (mass flux, velocity, mass fraction fluxes etc.) are calculated for each boundary. This type of discretization is called "staggered grid".

GT-Power solves following fluid dynamics equations:

- Continuity
- Energy
- Enthalpy
- Momentum

The flow solution is carried out by integrating this equations in both time and space. This integration can be done using explicit, implicit or quasit-steady method. In this paper the most common used was explicit.

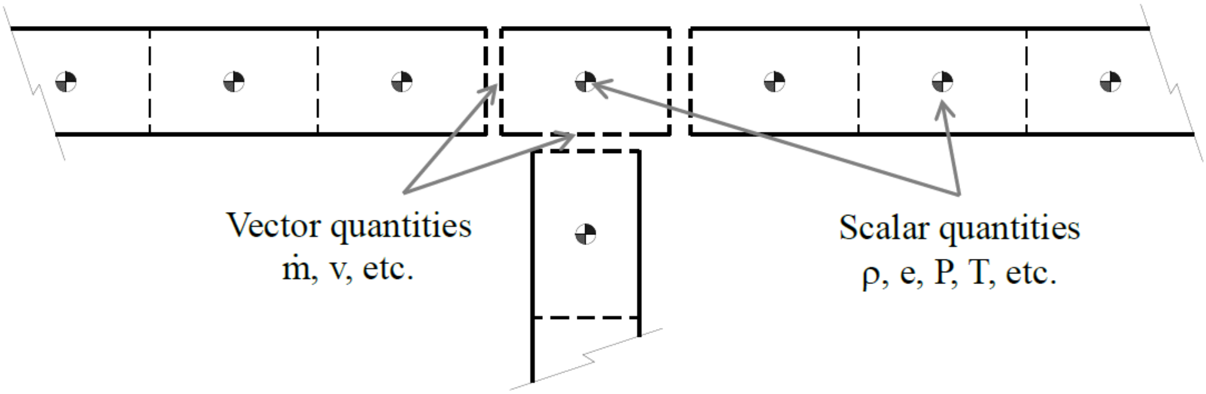


Figure 13: GT-Suite, Staggered grid [9]

The solution is calculated for each time-step, based on the information related to the previous time-step using the conservation of mass, moment and energy as well as information from the volume's neighbors. For the solution to be stable it need to satisfy the Courant condition. Courant number is a characteristic number that defines the relationship between the discretization's length and time step. As such an adequate time-step and length of discretization are required.

Discretization is an action of dividing the large volumes into smaller section to improve model's accuracy. Larger discretization length will result in faster simulation run-time but at possible cost of the solution's accuracy. Finer discretization may provide more accurate solution but the trade-off would be computational time. The goal should be to find a best accuracy with good computational time.

3.2 GT-Power structure

GT-Power uses an object-oriented structure. User is presented with graphical tree interface, in which the following are distinguished:

- Templates: Types of predefined elements in which attributes need to be define to create an object
- Objects: Elements deriving from the template, which attributes have been defined
- Parts: copy of the object placed on the project map. Projects map represent the virtual worksheet where the desired model/system is built.

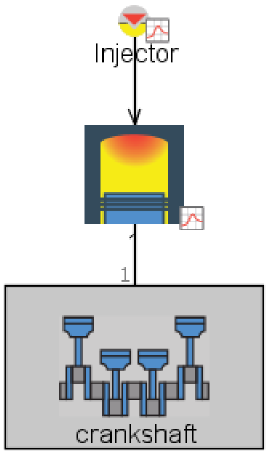


Figure 14: Mono-cylinder DI model

To build a GT-Power model it is necessary to import the templates from the Template library. There are three types of templates:

- Components which allow to model physical entities, such as pipes, cylinders, crankshaft, turbine.
- Connections are elements used to connect two or more objects: injectors, intake and exhaust valves, orifices.
- References that represent the set of data entered within certain objects: angle profiles, wall temperature maps, fuel composition. [8]

3.3 Combustion models

Fundamental aspect of correct modelling of the internal combustion engine, within GT-Power simulation environment, is the correct definition of the combustion process. Within the "EngCylinder" template it is possible to define all the parameters that characterize the combustion process. Setting these parameters correctly allows for a accurate prediction of engine performance. Combustion process analysis provides the information about the air-fuel interactions and the products of the combustion. Before presenting which combustion models are available in GT-Power a introduction to the terminology used by a code is needed:

- **Combustion** – transfer of a defined amount of unburned fuel mass and air from the unburned zone to a burned zone.
- **Unburned zone** – characteristics of the area where the fresh charge is present
- **Burned zone** – characteristics of the are where the burned gases are present.

- **Burn rate** – instantaneous rate of fuel consumption within the cylinder combustion process, it is a rate at which the fuel and air molecules are transferred from the unburned zone to the burned zone. As it will be pointed out in later the burn rate can be imposed or predicted.
- **Heat Release Rate** – instantaneous rate at which energy stored in the fuel molecules is release in the cylinder as thermal energy. Heat release lags the burn rate as some of the energy contained in fuel will not be release until later. Energy released per mass of fuel changes with equivalence ratio and temperature, which causes the difference between burn rate and heat release rate
- **Apparent Burn Rate** – Burn rate than is imposed in the simulation in a non-predictive model to reproduce the pressure trace. It can be used both in forward and reverse run.
- **Apparent Heat Release Rate** – calculated instantaneous rate of thermal energy release based on measurements of cylinder pressure. Instantaneous chemical composition in the cylinder is difficult to measure which makes it impossible to measure the actual Heat Release rate. Due to simplifying assumptions Apparent heat release rate and the actual heat release rate will differ.
- **Forward Run Combustion calculation** – in the forward run the burn rate is an input and cylinder pressure is the output. Fuel is transferred from unburned to burned zone as specified by burn rate.
- **Reverse Run Combustion calculation** – in the reverse run cylinder pressure is the input and apparent heat release rate is the output. Apparent heat release rate is then used in a forward run to reproduce the cylinder pressure.
- **Predictive combustion** – Burn rate is predicted from the inputs, such as pressure, temperature, equivalence ratio, residual fraction etc. and then applied in the forward rim
- **Non-predictive combustion** – Burn rate is imposed as a simulation input. Fuel and air will burn at the prescribe rate, ignoring the cylinder pressure or residual fraction.

When simulating the engine the primary decision is on the combustion model: predictive, non-predictive or semi-predictive. This will depend on the type of simulation to be carried out and the objective of the simulation.

As mentioned earlier in a non-predictive combustion burn rate is imposed as a function of crank angle. Regardless of the conditions inside the cylinder this prescribed burn rate will be followed as long there is enough fuel to satisfy the burn rate. Non-predictive models are fast, but limited.

It can be used to study the phenomena that has little effect on the burn rate, for example the influence of intake manifold runner length on the volumetric efficiency.
A semi-predictive or predictive model should be used when studying the variable that has direct and significant impact on burn rate, so that the burn rate can respond accordingly to the change made to that variable, for example study of injection timing and profile in a diesel engine.
Theoretically predictive combustion models are right choice for all simulations, but as time is an important resource in the engineering world, it is not always worth it to run a predictive simulation that requires more computational power and above all requires calibration to provide accurate data. [8]

3.3.1 Non-predictive combustion models

When referring to non-predictive combustion models, the following can be distinguished within GT-Power software:

- Imposed Combustion Profile ('EngCylCombProfile'): Imposes the combustion burn rate in a function of crank angle. This template is typically used when pressure signal inside the cylinder is available from the experimental tests and burn rate is calculated through a reverse run.
- Direct Injection Diesel Wiebe Model ('EngCylCombDIWiebe'): Imposes a burn rate and emissions in a compression ignition engine with a single direct injection. Using three term Wiebe function it is possible to approximate the typical shape of a DI compression ignition. This model provides reasonable burn rate when there are no data about the in-cylinder pressure
- MultiWiebie Diesel Model ('EngCylCombMultiWiebe'): Imposes a burn rate using multiple Wiebe functions. The main use of this model is to approximate the fuel injection with multiple injection events. [8]

3.3.2 Predictive combustion models

Predictive combustion models should be used when the purpose of the analysis is to study the parameters that directly affect the burn rate. Within The GT-Power there are:

- Spark Ignition Turbulent Flame Model ('EngCylCombSITurb'): Predicts combustion burn rate, emissions and knock model for spark ignition engines for the homogenous charge. The model takes into account combustion chamber geometry, position of the spark plugs, ignition timing, fuel properties

- Direct-Injection Diesel Jet Model (‘EngCylCombDIJet’): predictive combustion model for modeling combustion rate and emissions in direct injection diesel engines within single or multiple injection events. One of the first compression ignition models, which has been replaced by DI Pulse, which offers greater accuracy and faster computational time.
- Direct-injection Diesel Multi-Pulse Model (‘EngCylCombDIPulse’): predictive model able to predict burn rate and associated emissions faster than beforementioned Jet Model. It is wildly used during this thesis work. The model tracks the fuel as it is injected, evaporates, mixes with air and burns. It requires accurate injection profiles. The Di Pulse model must be calibrated to achieve good precision, which is one of the subjects of this thesis. [8]

4. Burn Rate Calculations

As previously described calculation of the burn rate from experimentally measured cylinder pressure is referred to as a reverse run, while in forward run the burn rate is the input and cylinder pressure is the output. Both forward and reverse run use the same energy equations.

Combustion in GT-Power is modeled with two-zone approach, the burned and unburned zone (with exception of DI Pulse, which will be described later). At the start of injection in compression ignition engine cylinder is divided in said two zones. All the cylinder's content (including residual gases from EGR) starts in unburned zone. With each time step certain amount of fuel-air mixture transferred from burned to unburned zone. This amount is defined as burn rate, which can be either calculated or prescribed (reverse or forward run). At each time step chemical equilibrium calculation is carried out for the entire burned zone, obtaining the concentration of the products of combustion species. Then when the new composition of the burned zone has been obtained, the internal energy of each species is calculated. Summation of all these species' energies gives the energy of the whole burned zone. Solving the energy equations for burned and unburned zone, the pressure and temperature of these two zones is calculated.

Within the software library there are two approaches available to calculate the apparent burn rate from the measured cylinder pressure.

- **Cylinder Pressure Only, Analysis (CPOA)**
- **Three Pressure Analysis (TPA)**

During this thesis work the first method (CPOA) was used due to the lack of experimental data necessary to perform TPA. TPA requires data from experimental activity that were not measured in the test bench activity, such as the pressure at the intake and exhaust port pressure and temperature. GT also refers to CPOA as Closed Volume Analysis. [8]

4.1 Cylinder pressure only analysis (CPOA) overview

Fundamental input to perform CPOA is the cylinder pressure, it can be either ensemble average of many cycles or a single cycle. Apart from that few basic cycle average results are required such as volumetric efficiency or residual ratio, as well as cylinder geometry and injection events data. Simple model consisting of cylinder, crank train and injector should be built.

The model runs two cycle, but essentially the first cycle is repeated in order to reach the convergence of the solution. Simulation requires the cylinder geometry, found in the 'Engine Crank Train' template, volumetric efficiency, trapping ratio, residual gas fraction, cylinder wall temperatures and heat transfer object found in the 'Engine Cylinder' template and injection events timing and profiles found in Injector template. Initial conditions represent the conditions inside the cylinder at Intake Valve Closure (IVC), hence the second name of this model, closed volume analysis. Cylinder pressure data should be entered in the Measured Cylinder Pressure Analysis Object called 'EngBurnRate'. Finally the Cylinder Pressure Analysis Mode must be set to 'Analysis, Closed Volume (CPOA)'.

The calculations are based on the following methodology:

1. First attempt at calculation of a combustion burn rate at the beginning of a cycle making some assumptions about the heat transfer inside the cylinder (Woschni).
2. The burn rate calculated in the previous point is applied in a forward run to calculate the actual heat transfer.
3. Burn rate is calculated once again, using the actual heat transfer from step two.
4. The final burn rate calculated at step three is applied during the second forward run to provide a comparison between measured and simulated results.

As it was mentioned before, this method if fast and requires reduced number of experimental data – mainly measured instantaneous pressure data. The main disadvantage of this approach is requirement to estimate some of the parameters that are difficult to acquire during the experimental activity (trapping ratio and residual fraction). Estimation of these parameters is not required in TPA as there are calculated independently during the simulation. TPA do requires additional experimental data, such as intake and exhaust pressure and temperature, as it was states before. [8]

4.2 Burn Rate Input Data Consistency Checks

When calculating the burn rate from cylinder pressure there is always some percentage of error. There may be errors in experimental data or other quantities measured or estimated and included as input into the analysis. Some of the estimated values and assumptions are a simplification of reality. All the potential error's sources add up to a cumulative error, which will almost never be zero and will indicate the difference between simulated and measured data. It all means that the fuel available in the cylinder will not be an exact match to predicted fuel burn. GT-Power handles this problem by adjusting the fuel energy multiplier (LHV multiplier). It corrects the amount of energy released during combustion, to target combustion efficiency or burned fuel fraction with respect to the experimental data. LHV multiplier may indicate the existence of a cumulative error, but does not provide the source of an error. GT-Power documentation provides a number of possible checks to verify the input data, those that are relevant to CPOA will be listed hereafter.

- Reasonable IMEP – IMEP (integrated mean effective pressure) calculated by integrating the cylinder pressure profile should be greater than BMEP (brake mean effective pressure) calculated from the brake torque measurement by an FMEP (friction mean effective pressure)
- Cumulative Burn During Compression (or Compression Heat Release): During the compression stroke up until the start of combustion there should be no fuel burning. Non-zero value calculated during this period indicates inconsistency in the input data. If the compression heat release is greater than 2% of total fuel, an error is marked and consistency check is failed.
- Compression slope – The slope of the measured LogP vs. LogV curve during the compression stroke starting from IVC until the start of combustion should be approximately constant and close to the polytropic coefficient of the gas trapped inside cylinder. In the direct injection compression ignition engines, polytropic coefficient should be near the ratio of specific heats of air, so 1.4 at 300K and it decreases to 1.33 at 1000K.
- Fraction of fuel injected late: If there is insufficient amount of fuel in the cylinder during the combustion to carry out the predicted burn rate, that amount of fuel is tracked and integrated over cycle. The value should be zero and consistency check fails when fraction of the fuel exceeds 0.002.

- Large LHV change required: LHV multiplier provides a cumulative error in the burn rate calculation. LHV multiplier should be 1 and if the indicated value deviates from 1 by more than 5% the error is flagged. [8]

4.3 DI Pulse

The DI Pulse predictive model was extensively used during this thesis work. It is a innovative multi-zone combustion model developed entirely by Gamma Technologies and able to predict the combustion process for direct injection compression ignition engine with single and multiple injections per cycle.

DI Pulse discretizes the cylinder content into three thermodynamic zones, each having their own temperature and composition.

- Main Unburned Zone (MUZ) contains all the mass present in the cylinder at IVC.
- Spray Unburned Zone (SUZ) contains all the mass of fuel injected during the injection event and entrained gases.
- Spray Burned Zone (SBZ) contains combustion products.

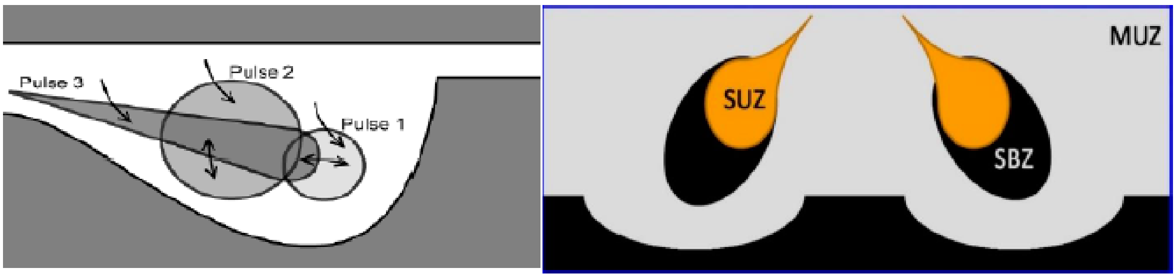


Figure 15: DI Pulse combustion background [10]

The idea of the model is to track the fuel as it is injected, evaporates and mixes with surrounding gas and finally burns. DI Pulse can be applied to single or multiple injection events where each injection is defined as an injection pulse, which is then tracked separately from all the other pulses.

The DI Pulse model contains several submodels that simulate the physical processes that occur during injection and combustion. Inside the 'EngCylCombDIPulse' template there are four attributes' multipliers that should be used for model calibration.

- Entrainment – when spray enters the combustion chamber it slows down as surrounding gases, both burned and unburned, are entrained into the pulse. The penetration of the jet, mixing between surrounding air, residual gases and fuel air mixture from the previous injections, is determined applying the conservation of momentum and can be modified using *Entrainment Rate Multiplier* (C_{ent})

$$S = \begin{cases} u_{inj}t\left[1-\frac{1}{16}\left(\frac{t}{t_b}\right)^8\right] & \frac{t}{t_b}\leq 1 \\ u_{inj}t\frac{15}{16}\left(\frac{t}{t_b}\right)^{0.5} & \frac{t}{t_b}\geq 1 \end{cases} \qquad t_b = 4.351\sqrt{\frac{2\rho_l}{\rho_g}}\frac{d_n}{C_d u_{inj}} \qquad u_{inj} = C_d\sqrt{\frac{2\Delta P}{\rho_l}} = \frac{\dot{m_{inj}}}{A_n\rho_l}$$

$$\frac{d_m}{d_t} = -C_{ent}\frac{m_{inj}u_{inj}}{u^2}\frac{d_u}{d_t} \qquad u = \frac{dS}{dt} \qquad m\,u = m_{inj}u_{inj}$$

t	=	Time	An	=	Injector nozzle area
tb	=	Breakup time	dn	=	Injector nozzle diameter
u	=	Velocity	Cd	=	Injector nozzle discharge coefficient
u_{inj}	=	Velocity at injector nozzle	ρ_l	=	Liquid fuel density
S	=	Spray tip length	ρ_g	=	Gaseous fuel density
m_{inj}	=	Injection mass flow rate	ΔP	=	Pressure drop across injector nozzle

- Ignition – In each pulse a mixture undergoes an ignition delay (time interval between start of injection and start of combustion) . Ignition delay is modeled with an Arrhenius expression and can be modified with *Ignition Delay Multiplier* (C_{ign}) The ignition delay is calculated separately for each pulse based on the conditions within the pulse. It accounts for the pulse-to-pulse interactions as well as entrainment and evaporation within the pulse.

$$\tau_{ign} = C_{ign}\rho^{-1.5}\exp\left(\frac{3500}{T}\right)[O_2]^{-0.5}$$

Ignition occurs when $\int_{t_0}^{t_{ign}}\frac{1}{\tau_{ign}}dt = 1$

τ_{ign}	=	Ignition delay	T	=	Pulse temperature
$[O_2]$	=	Oxygen concentration	ρ	=	Pulse gas density

- Premixed Combustion – after the ignition delay premixed burn phase starts. Fuel accumulated during ignition delay ignites spontaneously. The rate of this combustion is kinetically limited and can be modified with *Premixed Combustion Rate Multiplier* (C_{pm})

$$\frac{dm_{pm}}{dt} = C_{pm}\, m_{pm} k \left(t - t_{ign}\right)^2 f([O_2])$$

t	$=$	*Time*	k	$=$	*Turbulent kinetic Energy*
t_{ign}	$=$	*Time at ignition*	$[O_2]$	$=$	*Oxygen concentration*
m_{pm}	$=$	*Premixed mass*			

- Diffusion Combustion – After pulse ignition, the remaining unmixed fuel and entrained gas continue to mix and burn in a diffusion phase. *Diffusion Combustion Multiplier* Rate (C_{df}) can modify that rate of combustion.

$$\frac{dm}{dt} = C_{df}\, m \frac{\sqrt{k}}{\sqrt[3]{V_{cyl}}} f([O_2])$$

k	$=$	Turbulent kinetic energy	V_{cyl}	$=$	Cylinder volume

In the advanced options of the DI Pulse template there are three additional parameters which can be used during the calibration process.

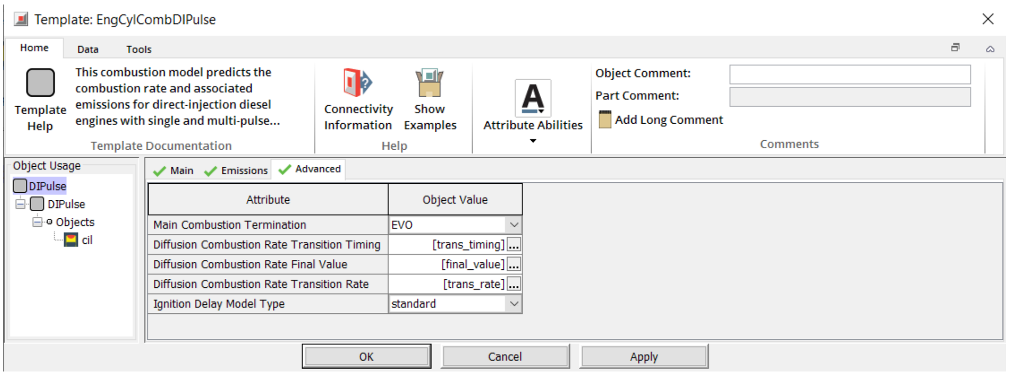


Figure 16: Diffusion combustion advanced parameters

- Diffusion Combustion Rate Transition Timing which defines the time at which the diffusion combustion rate begins to decrease
- Diffusion Combustion Rate Final Value which defines the final value of the multiplier applied to the diffusion combustion burn rate
- Diffusion Combustion Rate Transition Rate which defines the rate at which diffusion combustion rate is reduced.

If the accuracy of the results is unsatisfactory there are two more parameters which can influence the burn rate.

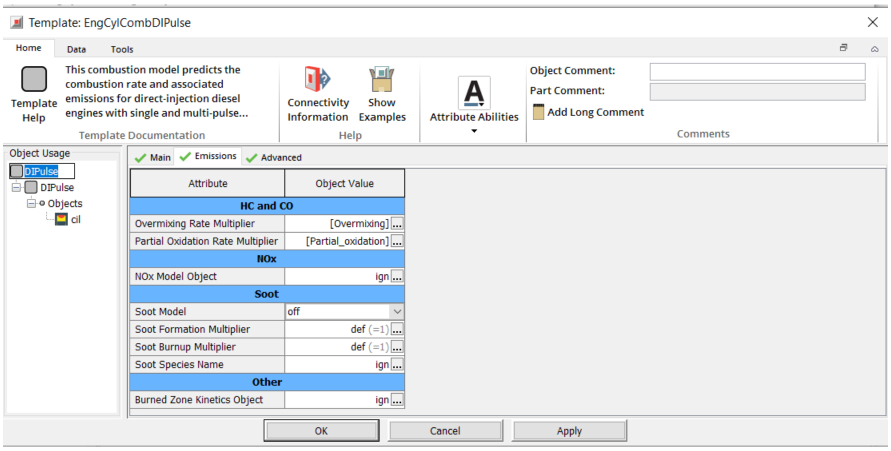


Figure 17: Over and under-mixing parameters

- Overmixing Rate Multiplier which is a multiplier to a rate at which the fuel is overmixed beyond the lean limit.
- Partial Oxidation Rate which is a multiplier to the rate at which overmixed and undermixed fuel is partially oxidized to CO, H2, H20, N2 and SO2 [8]

4.4 Calibration procedure for DI Pulse

The calibration of a DI Pulse predictive combustion model consist of identifying a single set of parameters described in the previous chapter, suggested four multipliers, and as it is the case in this paper additional three specifying the diffusion combustion and two describing over and undermixing. These parameters allow to control each step of the combustion process.

Coefficients that will be calibrated modify the empirical formulas that constitute the model. They allow to readjust the one-dimensional predictive combustion model to the characteristic of the combustion process that exist in the engine under test.

The calibration of a predictive model is performed on a simplified single-cylinder model, similar to what is recommended for CPOA, which allows to reduce the computation time. DI Pulse model takes as a reference the results obtained during Closed Volume Analysis, which highlights the importance of the non-predictive model. The set of parameters that GT-Power optimizer tool searches for during the calibration phase is such to ensure that the burn-rate generated by the predictive model is as close as possible to the burn rate obtained from the non-predictive model through the reverse run calculation. In mathematical terms this translates into minimizing the value of 'EngCylinder' result called "Improved Burn Rate RMS Error (Meas vs Pred)" averaged over all cases. [8]

$$Improved\ Burn\ Rate\ RMS\ Error = \frac{\sqrt{\int_{t_0}^{t_f}(LHV_{pred}\ BR_{pred} - BR_{meas})^2 dt}}{t_f - t_0}$$

BR_{pred}	Combustion burn rate calculated from predicted pressure
BR_{meas}	Combustion burn rate calculated from measured pressure
t_f	Time at the end of integration (Time at which 90% burn point is reached)
t_0	Time at the beginning of integration

4.5 Experimental data required for calibration

To properly calibrate the DI Pulse predictive model the experimental data of the engine are required.

- Set of operating points spread well distributed over entire engine map. It is important to select operating points that correspond to different combustion process developments, operating points with different levels of EGR, engine rotational speed, load and injection events.
- Cylinder pressure traces with maximum increment of 0.5 degrees.
- Detailed injection rate profiles
- Injected fuel mass and start of injection for each injection event.
- Flow of air and fuel
- EGR rate
- Engine out emissions

Calibration of the predictive model

To calibrate the predictive combustion model subsequent steps need to be followed.

- Analysis of the experimental pressure signal in order to calculate measured burn-rate and compare the simulated cylinder pressures with measured ones.
- Set up a predictive combustion model in order to calculate the predicted burn rate and cylinder pressure
- Compare the simulated results with the predicted for burn rate and cylinder pressure.
- Identify the best set of calibration parameters that satisfy the response's target.
- Validate the predictive model paying close attention to the operating points that were left out of DI Pulse calibration procedure.

Within the 'EngCylinder' template the Cylinder Pressure Analysis Mode needs to be switched to 'Calibration, Closed Volume (M+P)' in order to calibrate the model. In this module the software will provide the comparison of predicted and simulated burn rate, as well as comparison between predicted, simulated and measured cylinder pressure.

The four main parameters used for a calibration activity have recommended minimum and maximum values as indicated in the table. To identify the best set of coefficients that approximate the simulated burn rate in the best way, the "Improved Burn Rate RMS Error" should be tracked response with its objective set to minimize. [8]

Parameter	Min	Max
Entrainment Rate multiplier	0.95	2.8
Ignition Delay Multiplier	0.3	1.7
Premixed Combustion Rate Multiplier	0.05	2.5
Diffusion Combustion Rate Multiplier	0.40	1.4

Table 1:Upper and Lower limit of Entrainment, Ignition delay, Premixed and Diffusion combustion for the optimization

Within the optimizer the values of the variables assigned to the next iteration are based on the results obtained from the previous iteration. Parameters reaching convergence are one of the criterion that indicate good solution. The Genetic Algorithm is recommended for the designs with multiple factors and medium to high complexity. The population size should increase with the number of parameters. The Case Handling must be set to "Case Sweep and Cross-Case Studies" as the calibrated parameters have to be the same for all the operating points rather than change independently. Final optimizer settings for the first step calibration are present in the figure.

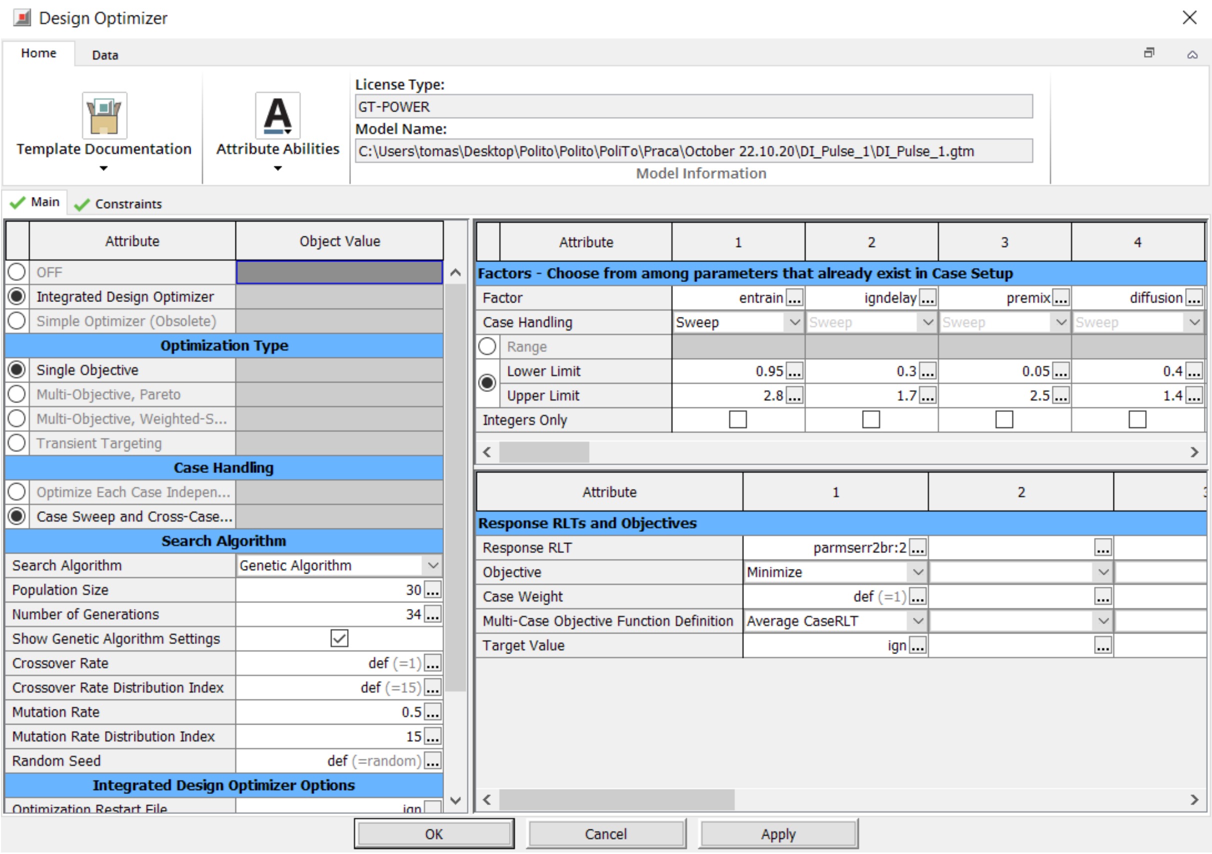


Figure 18: Optimizer setup

5. Cylinder Pressure Only Analysis

The aim of the first part of the thesis was to set up a non-predictive combustion model using the experimental data-set to calculate the burn rates that would represent the combustion process in the most accurate way and be subsequently used as targets for a DI Pulse predictive model analysis.

5.1 Experimental and technical data

Geometry and performance characteristics of the investigated engine

Engine type	DI Turbocharged Diesel EURO6
Displacement	1598 cm3
Bore x stroke	79.7 mm x 80.1 mm
Compression ratio	16:1
Turbocharger	Single-stage with VGT
Fuel injection system	Common Rail
Maximum power	100kW @ 4000rpm
Maximum torque	320Nm @ 2000rpm

Table 2: Engine technical data

In order to achieve precise correlation between the physical model of the engine at the simulated engine model in GT-Power, an adequate set of experimental data must implemented in the CPOA model. A map of experimental data was provided for 41 operating points representing different loads, engine speeds and EGR levels. Each operating point provides:

- Instantaneous cylinder pressure signal for 4 cylinders acquired for 100 cycles.
- Average values of characteristics such as: BMEP, cooling and oil temperatures, mass flow rate of fuel.
- Injection strategy: number of injection events per cycle, energizing and dwell time, rail pressure, start of injection.

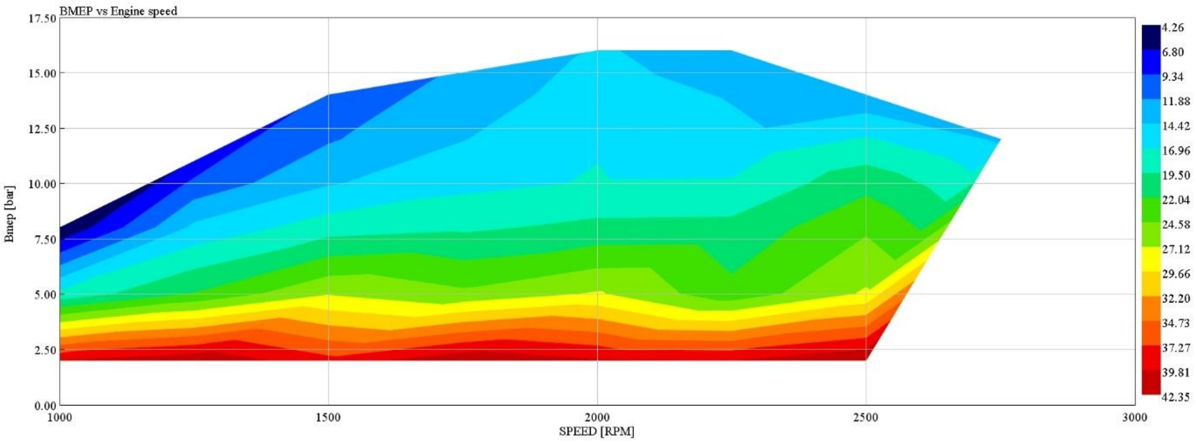


Figure 19: EGR as a fuction of BMEP and Engine Speed

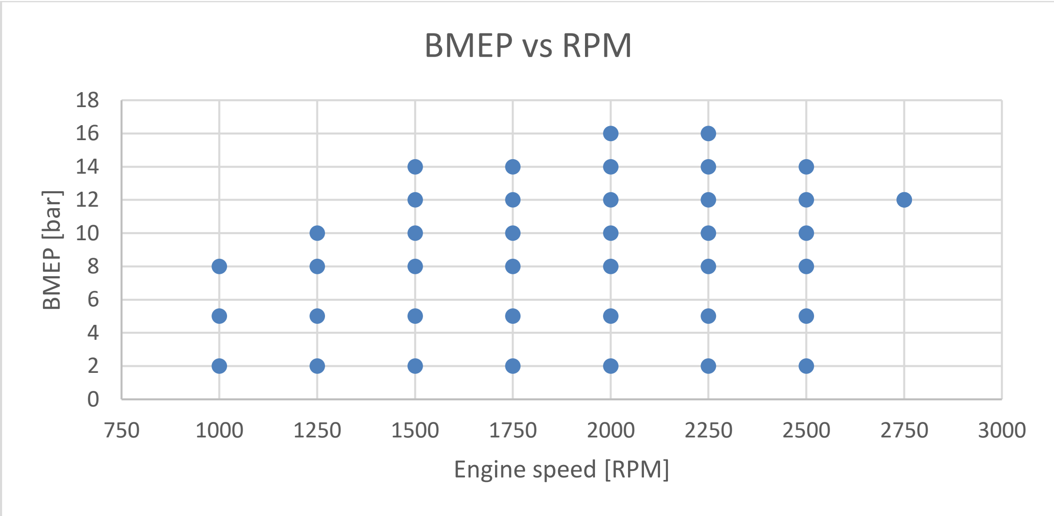


Figure 20: BMEP vs Engine speed for 41 operating points

5.2 Closed Volume Analysis

CPOA was used to calculate the burn rate from the measured cylinder pressures, as there were not enough data for the TPA analysis. Typically the model used for CPOA is simplified 1 cylinder model, in this paper 4 cylinder model was used, for no other reason than simplification of the data acquisition. If 1 cylinder model were to be used, the simulation would need to be repeated for each of the 4 cylinders separately or 4 times more cases would need to be run for each investigated calibration parameter. Having 4 cylinder simulated in one simulation makes the post processing analysis more convenient.

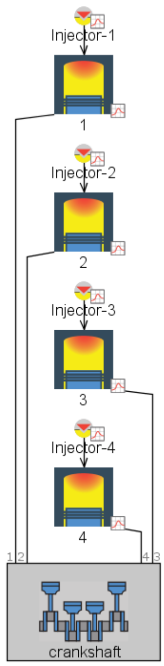


Figure 21: 4 cylinder model

Input data used in the analysis are summarized below:

1. Measured pressure cycle: Pressure signals were provided in the IFile format. To get access to that data a simple Matlab function developed by catool (combustion analysis tool) was used. The pressure cycle that were provided consisted of pressure traces acquired over 100 consecutive cycles. These 100 cycles could be directly implemented in GT-Power as it has the function of calculating the ensemble average and using it as the input for the analysis. The drawback of that solution is the computational time, as the pressure data input increases by the factor of 100. Instead the average of the 100 cycles was calculated separately in Matlab environment, saved as txt file and referenced in the case setup for the CPOA analysis.
2. Volumetric efficiency: Volumetric efficiency was not provided directly but the experimental data present within the map allowed for it to be calculated, given the engine RPM, air mass flow rate, air temperature and pressure and engine geometry
3. Residual gas fraction: Residual gas at IVC was estimated calculating the EGR level, knowing the oxygen concentration at the intake and exhaust, and increasing it by 4% as suggested in the GT manual.
4. Air trapping ratio: ratio of air trapped in the cylinder to the air delivered to the cylinder. This value is typically 1.
5. Wall temperatures inside the cylinder: Head, Piston and Cylinder temperature were initially set to a constant value over the scope of all operating cycle. During the calibration of CPOA the wall temperature map for this components was used.
6. Cylinder geometry: Cylinder geometry data were provided with the engine and as such they were implemented in the cylinder geometry object in the crank train template.
7. Injection events: for each operating conditions there are data providing the Start of injection, amount of fuel injected into the cylinder, energizing and dwell time of the solenoid and rail pressure. During the calibration process the amount of fuel injected into the cylinder was recalculated considering the mass of fuel rate measured during the experimental activity. [8]

5.2.1 CPOA model validation

During the model validation process Overall Convection Multiplier was extensively used. This multiplier is used for the convective heat transfer to achieve better correlation between simulated and experimental data. In each step of the validation corrective actions were taken to represent the final model with high degree of accuracy.

5.2.2 CPOA evaluation.

Since the CPOA runs only 2 cycles the wall temperature solver cannot be activated. As a first attempt the in-cylinder chamber's surface temperature of head, piston and cylinder could be considered constant for all operating points. In this paper a temperature map for the in-cylinder surfaces was acquired and implemented as a reference object in the 'Cylinder Wall Temperatures' template. More accurate in-cylinder surface temperature allows for better heat transfer representation.

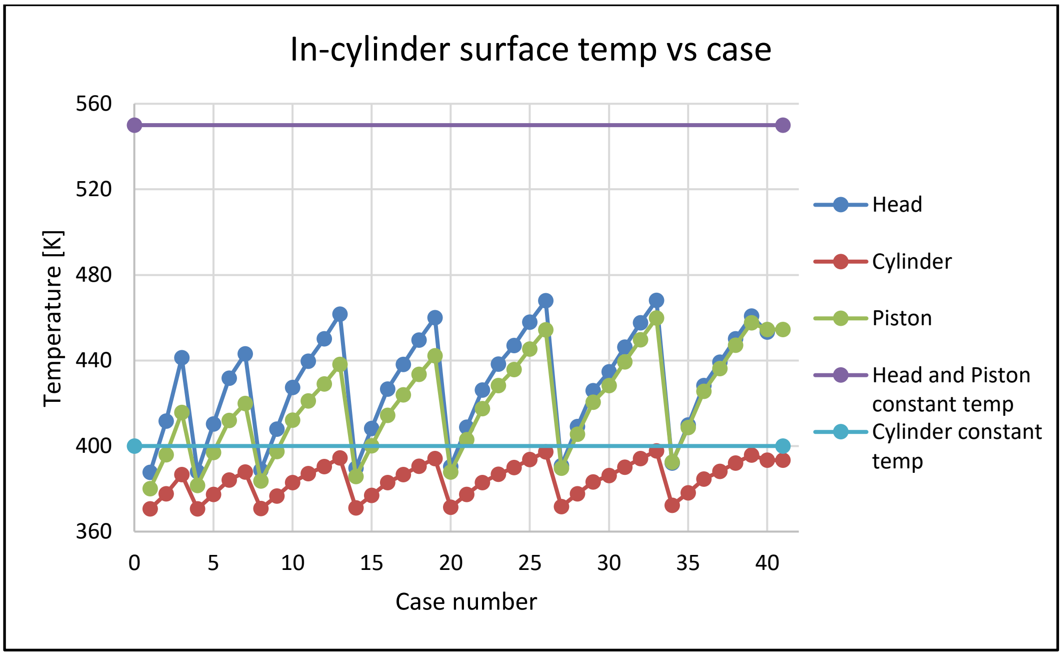


Figure 22: In-cylinder surface temperature in the function case number

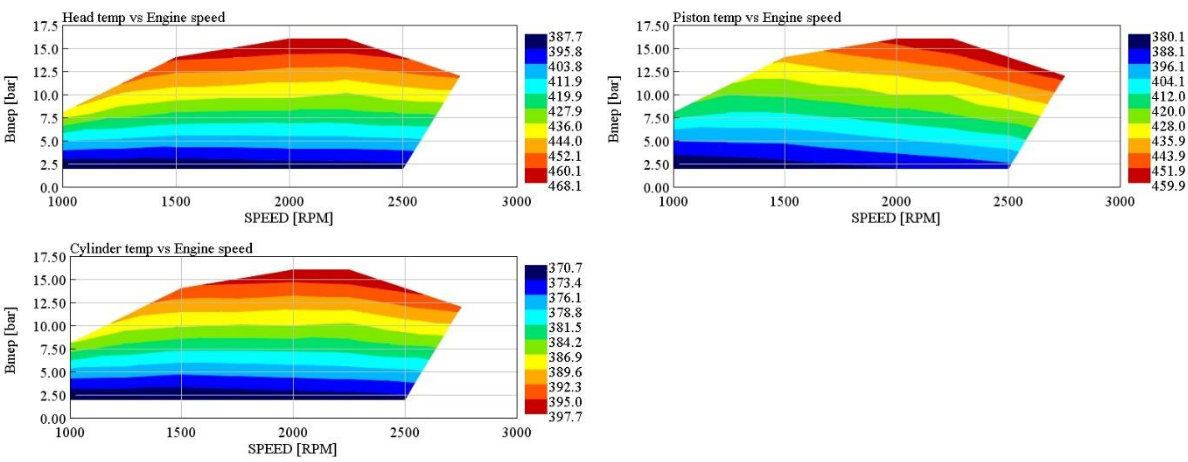


Figure 23: Head, Piston and Cylinder temperature map

Nominal compression ratio of the engine equals 16:1. The compression ratio can be a subject to a change due to the tolerances and accuracies with which the engine has been manufactured and assembled. As the engine is operated its components are subject to wear: cylinder linear, piston rings, piston crown etc. The compression ratio of the engine can be checked easily during the motored cycle at the test bench, cycle during which the engine is powered by an external source, without power stroke (fuel injection). The data was not available hence 3 different compression ratios were compared in the CPOA simulation model and LogP vs LogV compared to identify the compression ratio which overlap the compression curve most accurately.

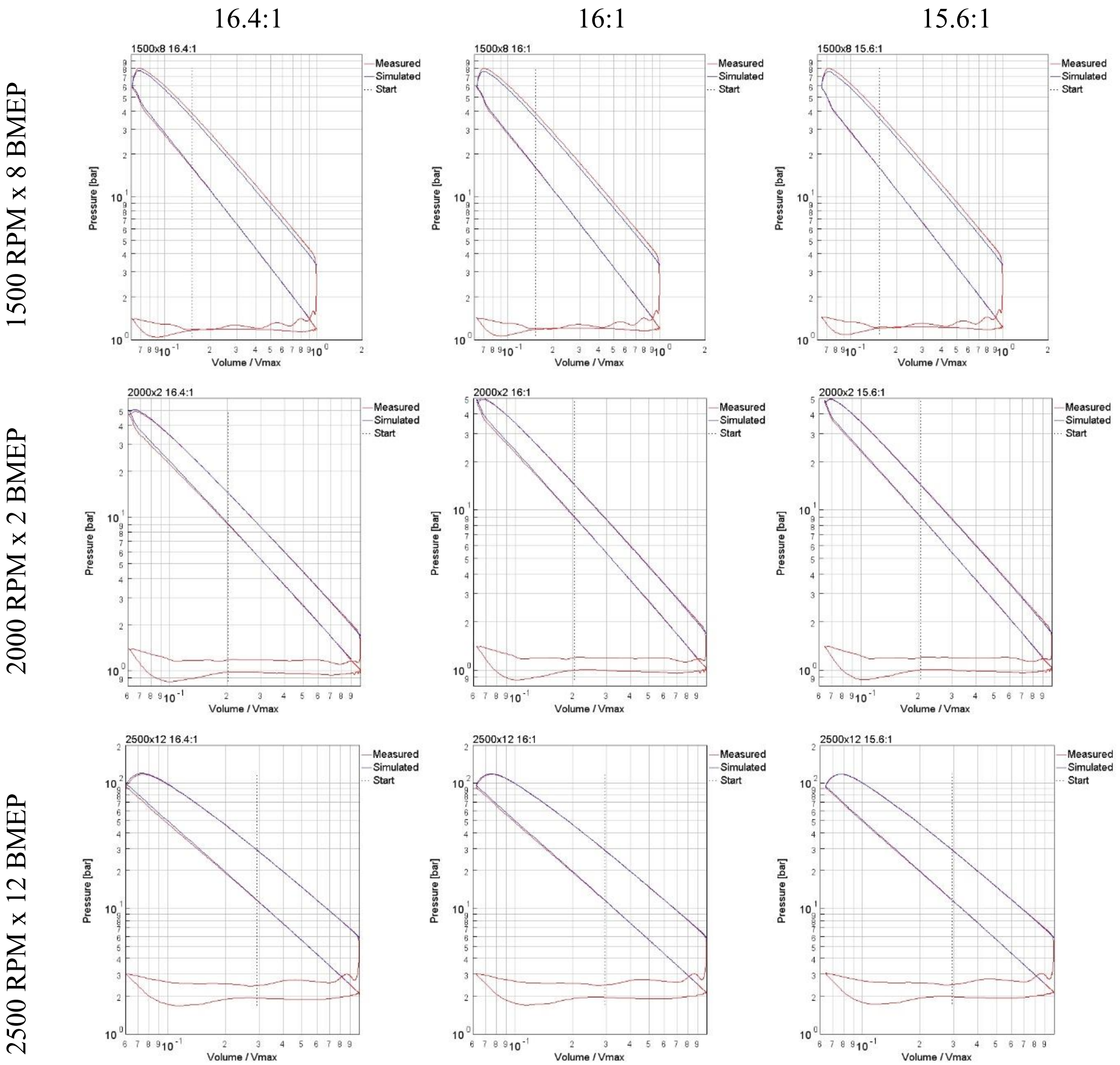


Figure 24: LogP vs LogV diagram for 3 operating points and 3 different compression ratios

Analysis of the compression ratios reveal that the greatest match was achieved for the CR = 15.6:1. This compression ratio was then used for the reminder of the analysis of CPOA and consequently DI Pulse.

Engine map provides mass of the fuel injected during each of the injection event, these values are calculated according to the formulas encoded in the ECU. The correctness of these calculations can be checked by comparison with fuel mass flow rate, which was monitored during the engine test bench activity and recorded in the engine map as well.

Taking the engine speed [RPM] and fuel mass flow rate [kg/h] fuel injected into the cylinder during one cycle [mg/cycle] can be calculated.

$$m_{inj} = \frac{\dot{m}_f}{60\left(\frac{Eng_{speed}}{4 \cdot 2}\right)} 10^6$$

m_{inj}	=	Mass of fuel injected into the cylinder during one cycle [mg/cycle]
Eng_{speed}	=	Engine speed [RPM]
$\dot{m}_f$	=	Fuel mass flow rate [kg/h]

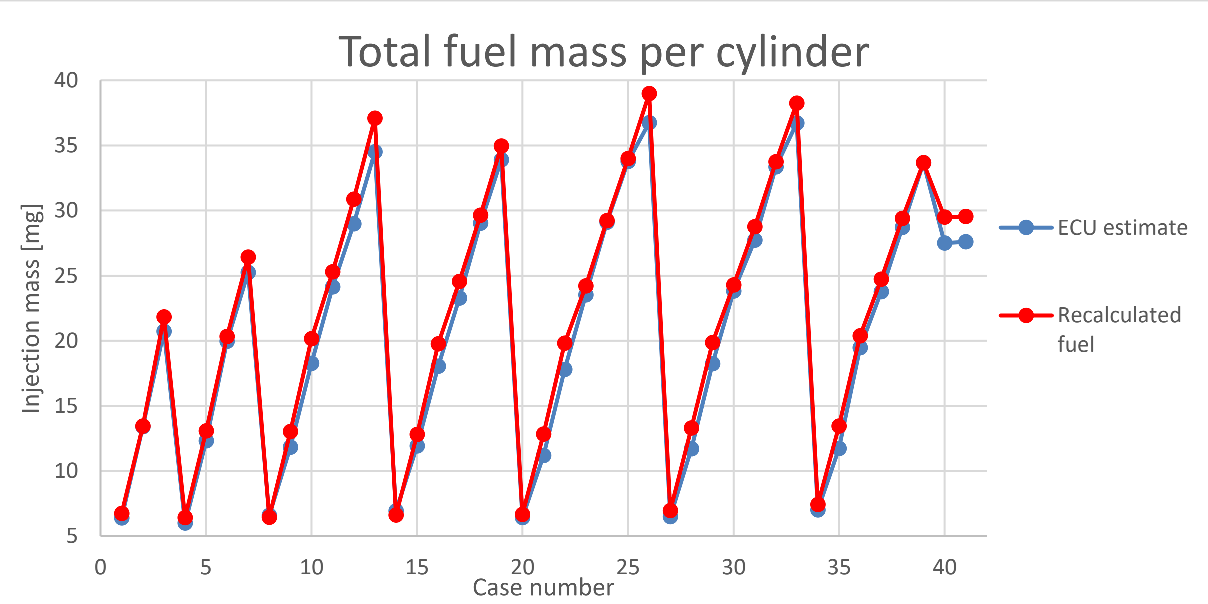


Figure 25: Mass of fuel injected to the cylinder, recalculated vs ECU estimate

By simple mass fraction comparison of the fuel injected in each pulse according to the ECU estimate with new recalculated fuel the new recalculated fuel injected during each of the injection event can be calculated.

$$R_{1recal} = \frac{R_{1ECU}}{m_{inj,ECU}} m_{inj}$$

R_{1recal}	=	Recalculated mass of fuel, inj R1	m_{inj}	=	Recalculated mass of fuel, total
R_{1ECU}	=	Estimated mass of fuel, inj R1	$m_{inj,ECU}$	=	Estimated mass of fuel, total

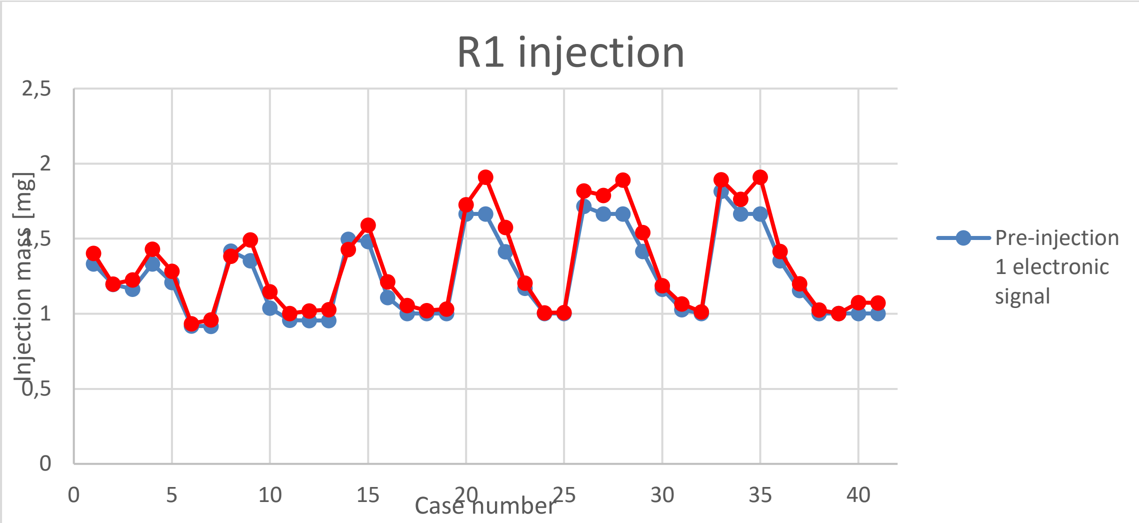


Figure 26: Pre-injection 1 - fuel mass injection

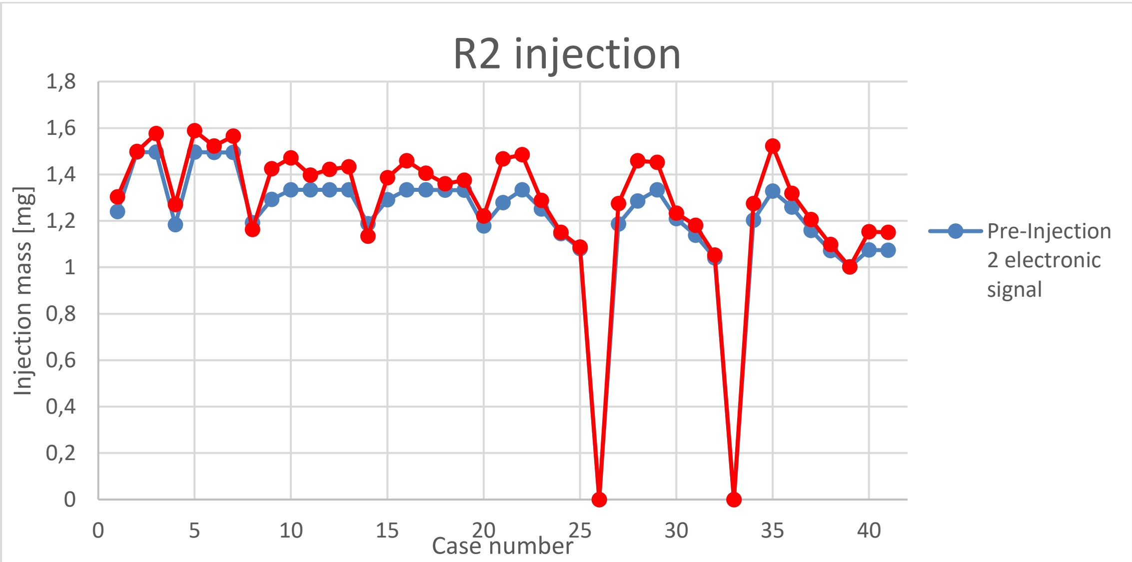


Figure 27: Pre-injection 2 - fuel mass injection

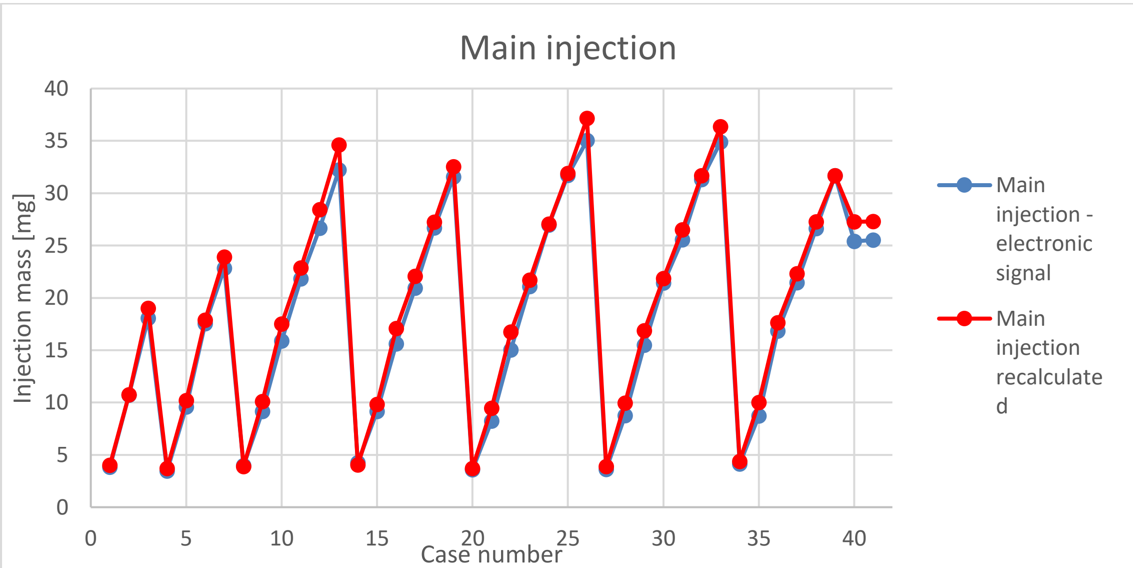


Figure 28: Main injection mass of injection

After modifying the CPOA model with the updated data the LHV multiplier, Compression Heat Release (CHR) and Consistency Check were investigated for three different values of Overall Convection Multiplier (OCM)

As previously described the LHV multiplier provides the estimate of the cumulative error. In order to pass the consistency check LHV multiplier needs to be within 5% of 1. 5% error margin is indicated in the figures with yellow horizontal dashed line, while the purple vertical line indicate change of an engine speed.

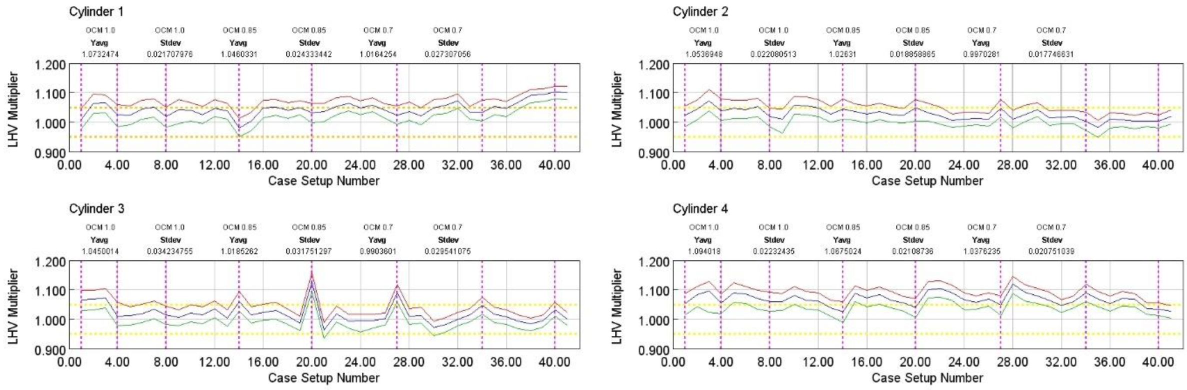


Figure 29: LHV multiplier for 4 cylinders and 3 different values of Overall Convection Multiplier

Compression Heat Release indicates amount of integrated energy release during compression, before the combustion begins, divided by the total fuel energy. There should be no energy release during this part of the cycle, hence an error of 0.002 is set. Exceeding the error indicates inconsistency in the input data. Error line is indicated with yellow horizontal dashed line.

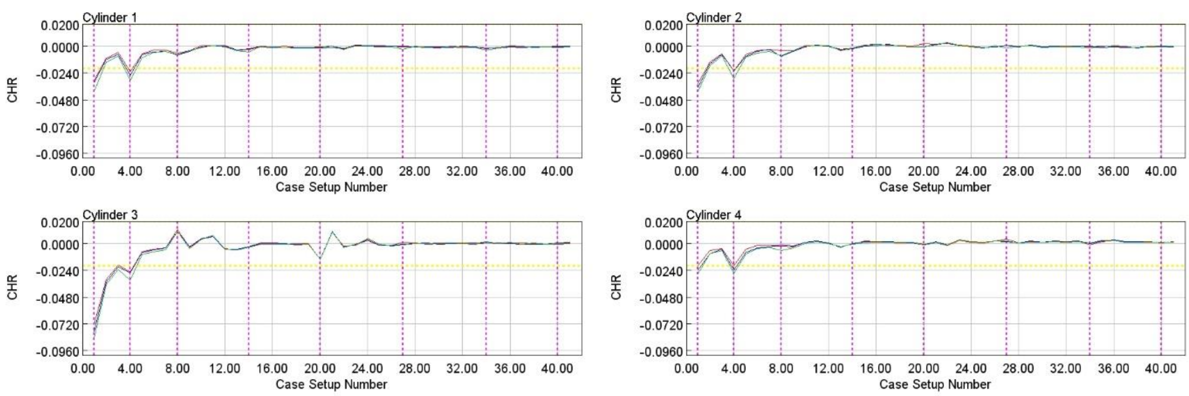


Figure 30: Compression Heat Release for 4 cylinders

The consistency check will be set to 0 if any of the consistency check (described in the previous part of the thesis) indicate a potential error.

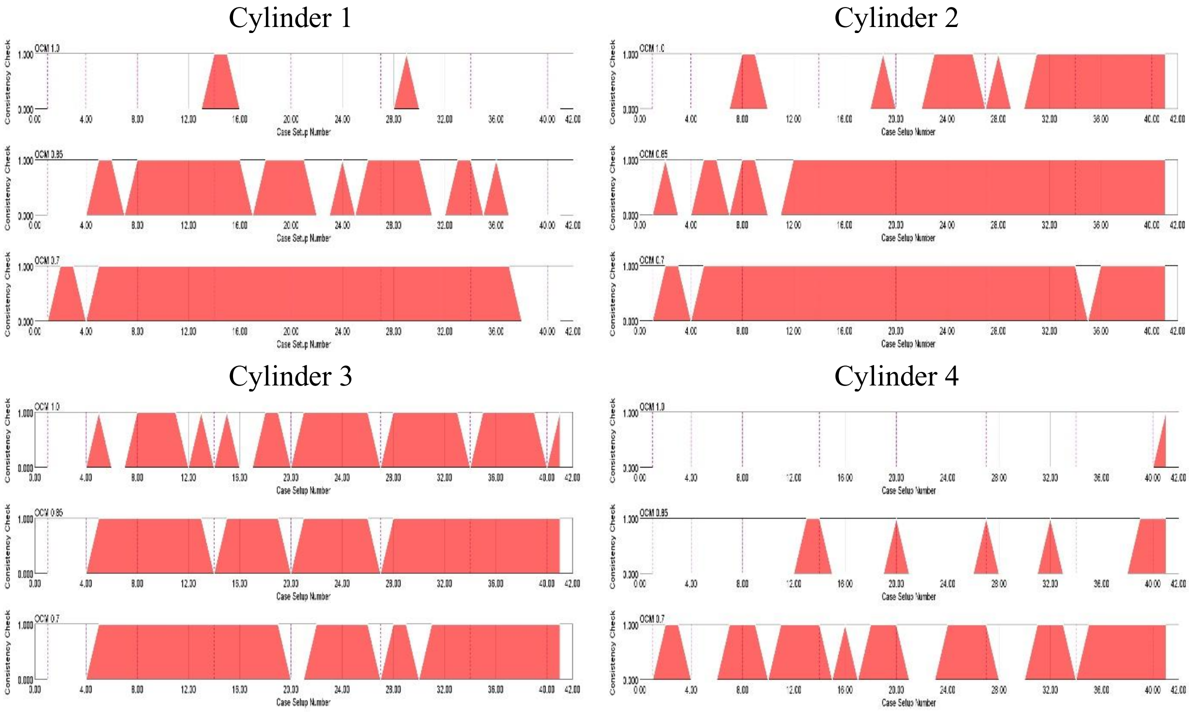


Figure 31: Consistency Check for 4 cylinders and different levels of Overall Convection Multiplier

CPOA analysis was performed for 4 cylinders, DI Pulse requires 1. Therefore after the analysis of CPOA is finished the assessment of results is required to choose the cylinder most suitable for the predictive model calibration.

1. Cylinder 1 does not reach the Consistency Check at high engine speed and loads due to error margin exceeding LHV multiplier results.
2. Cylinder 2 presents the best results as it reaches the consistency check for 38 out 41 operating points if the right overall convection multiplier it set thanks to the consistent LHV multiplier and compression heat release.
3. Cylinder 3 does not reach the Consistency Check at low engine speeds due to the CHR exceeding the error margin. The results of the compression heat release for cylinder 3 may indicate the problem with the data acquisition system during the test bench activity which is clearly visible at the low engine speed.
4. Cylinder 4 does not reach the Consistency Check due to the LHV Multiplier being too high for majority of the cases that were investigated, and only excessive Overall Convection Multiplier reduction could bring LHV to the desired level.

5.3 Cylinder selection for the DI Pulse model

Based on the comparison of the LHV, CHR and Consistency Check for each cylinder presented above cylinder 2 was chosen to be used in the DI Pulse predictive model. One more simulation is run and analyzed in order to choose the suitable overall convection multiplier.

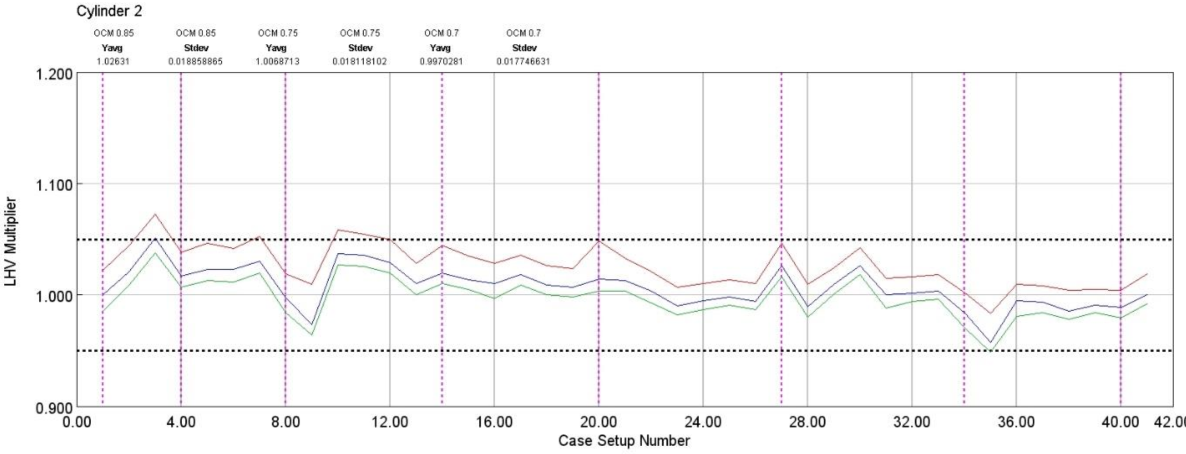


Figure 32: LHV multiplier for final model of CPOA

And the corresponding Consistency Check

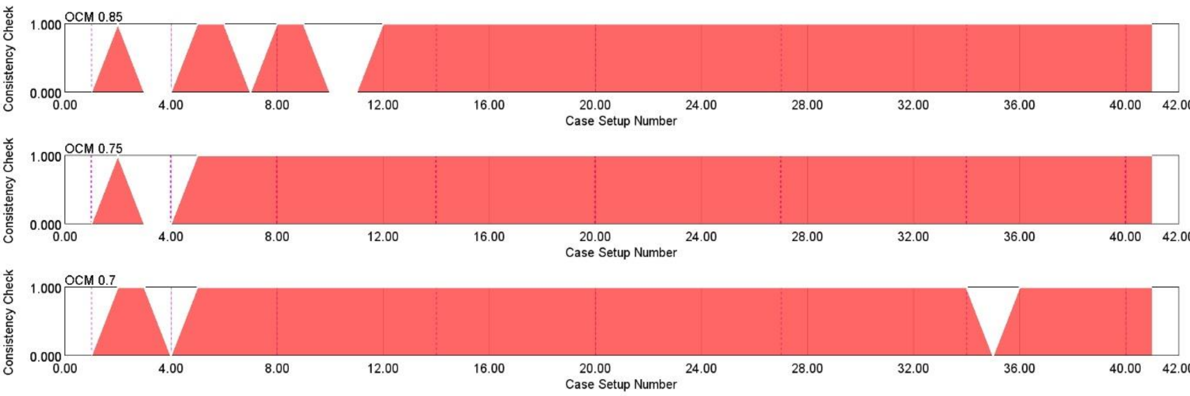
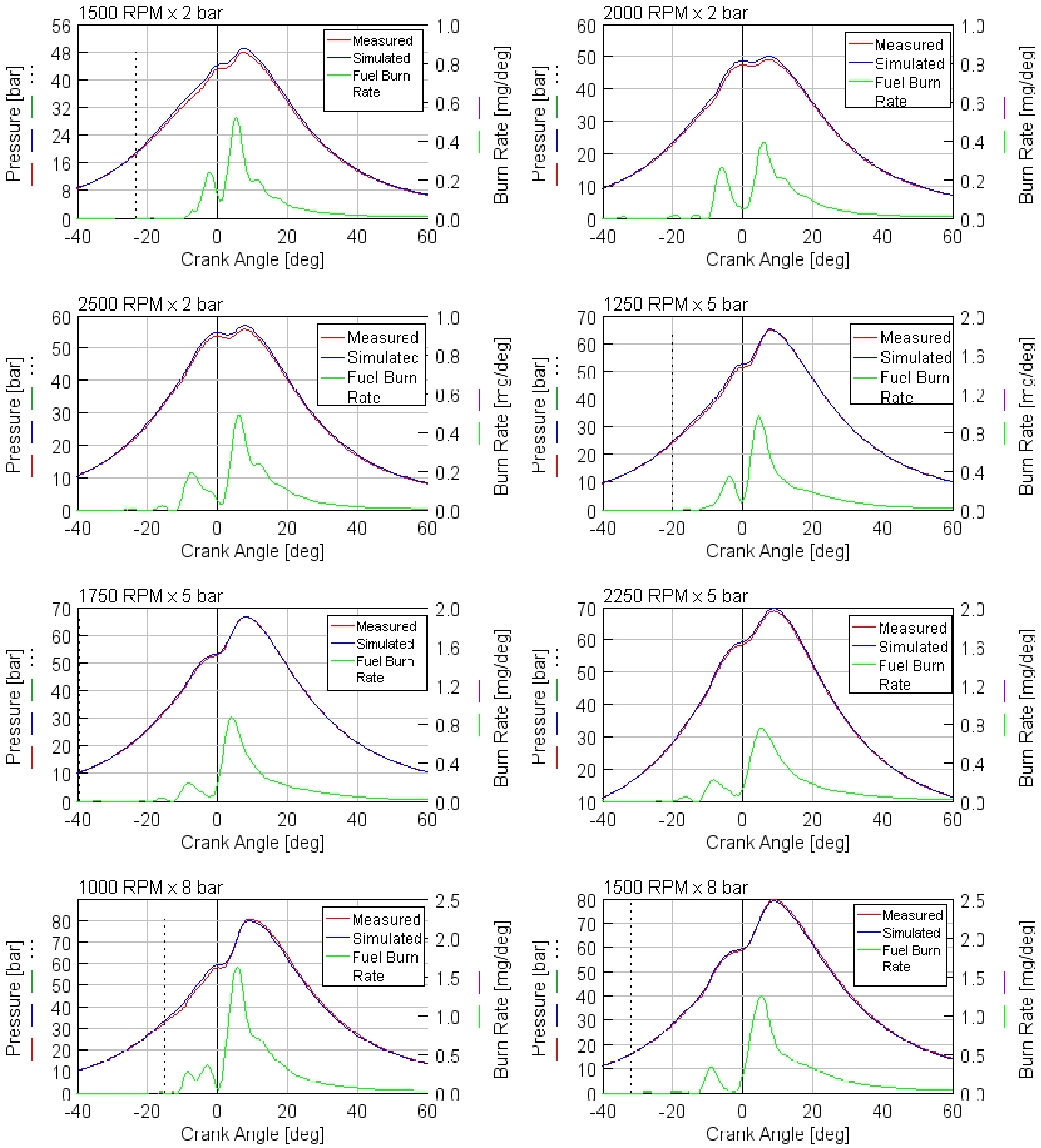


Figure 33: Consistency Check for final model of CPOA

Based on the results presented in the forms of LHV and Consistency Check figures, Overall Convection Multiplier equal to 0.75 was chosen for the DI Pulse.

As for the operating points that didn't pass the consistency check:

- operating point in case 1 and 4 were excluded from the calibration of predictive combustion model due to the CHR error considerably exceeding set limit,
- operating point in case 3 was considered valid for the predictive model as the reason that it didn't pass the Consistency Check was LHV multiplier error. While 5% is the error margin set by GT-Suite, operating point in case 3 exceeded upper error limit of 1.05 by 0.0009, which considering limited number of operating points available considered satisfactory.


1500 RPM x 2 bar
2000 RPM x 2 bar
2500 RPM x 2 bar
1250 RPM x 5 bar
1750 RPM x 5 bar
2250 RPM x 5 bar
1000 RPM x 8 bar
1500 RPM x 8 bar
Measured
Simulated
Fuel Burn Rate
Pressure [bar]
Burn Rate [mg/deg]
Crank Angle [deg]

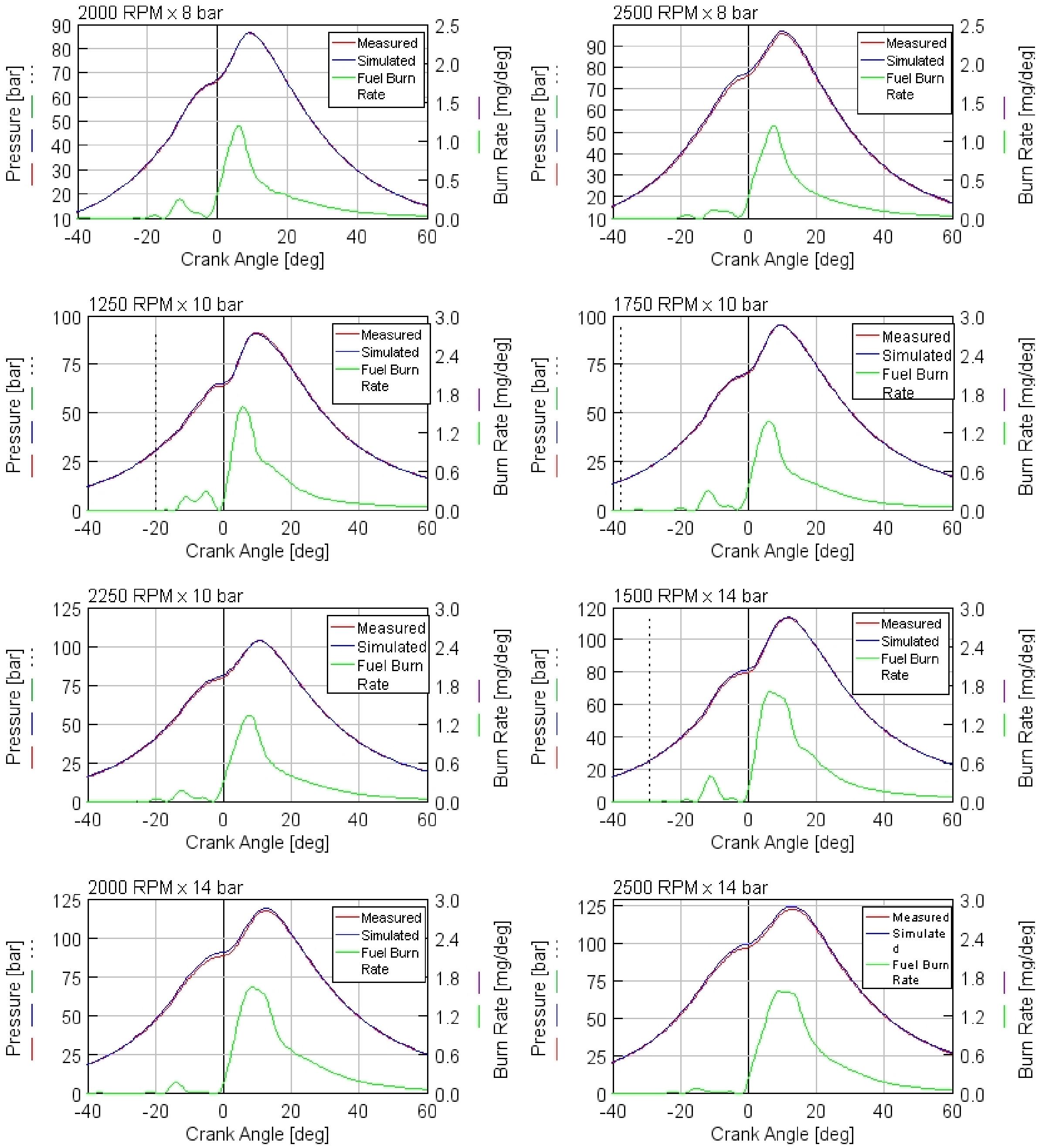


Figure 34: Figures of simulated and measured cylinder pressure, and burn rate as results of CPOA analysis

The simulated model represents the measured cylinder pressure with a very good approximation. Burn rate characteristics are satisfying. To sum up:

1. Engine temperature map replaced constant values of in-cylinder surfaces temperature.
2. Compression ratio was reduced to 15.6
3. Fuel injected into the cylinder during the injection event was recalculated, taking into account more accurate measuring device.

6. DI Pulse

After completing the validation of the CPOA model, the next step is to calibrate the DI Pulse predicted model.

A detailed calibration procedure was carried out in order to identify the best set of coefficients that would allow to obtain good results over the whole engine map provided. Calibration procedure was performed using the build in Design Optimizer.

After reaching satisfactory results in terms of quality of combustion the NOx emissions predictive model based on the extended Zeldovich mechanism was added in order to match the experimental and predicted NOx emissions.

After each calibration procedure validation of the results was performed by running the simulation with calibrated parameters and investigating the operating points that had no direct impact on the DI Pulse calibration. [8]

As it was explained in the previous chapters the predictive models use semi-empirical equations that are the basis of the combustion model. These formulas can be modified by varying the multiplication parameters. Goal of the calibration is to minimize the error between the predicted burn rate and burn rate obtained during the reverse run in CPOA analysis.

6.1 Operating points

Engine map consist of 41 operating points, out of which 39 passed the consistency check and were allowed as inputs for the predictive model. Using 39 points for the predictive model is unnecessary, as it prolongs the optimization process and makes the validation impossible, as there would be no points to validate. For the purpose of calibration 22 operating points were chosen, these operating points cover the entire engine map.

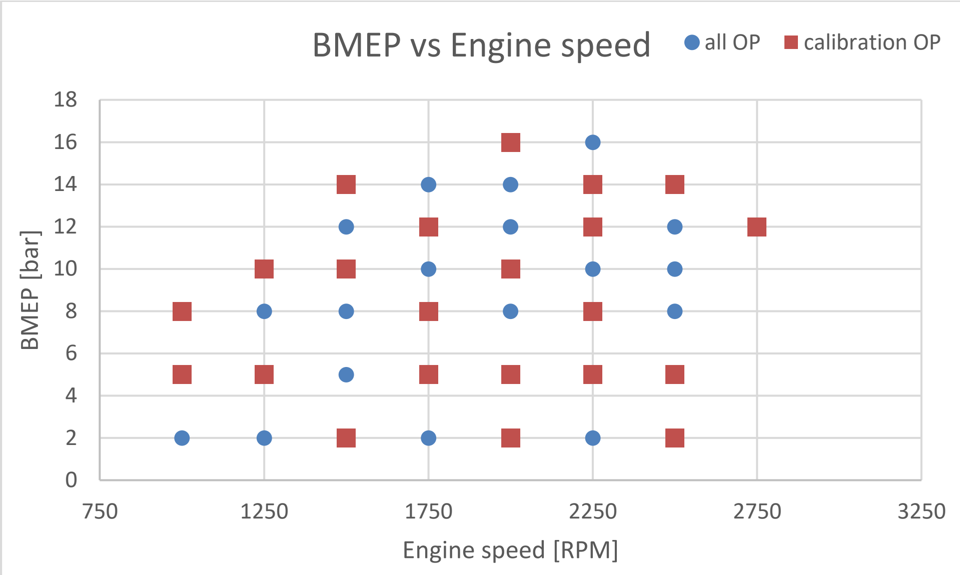


Figure 35: Operating points used for DI Pulse analysis represented on BMEP vs RPM map

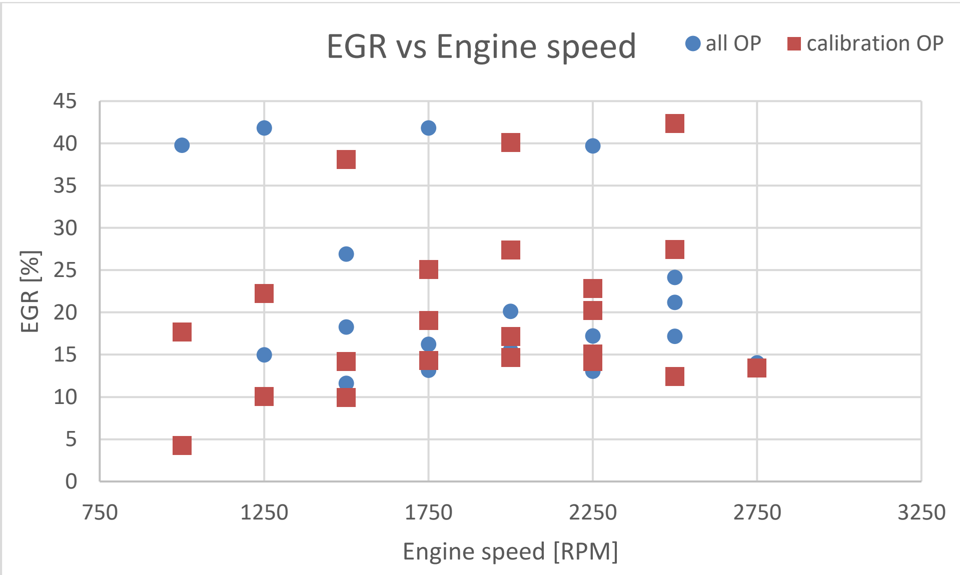


Figure 36: Operating points used for DI Pulse analysis represented on EGR vs RPM map

6.2 DI Pulse calibrations

During the calibrations process number of calibrations were performed, each using different set of parameters to be optimized and different objectives to pursue in order to find the best solution.

Optimization type was either Single or Multi-objective, and the objectives itself were:

- Improved Burn Rate RMS Error – to minimize the error between predicted and reverse run simulated burn rate
- Pressure RMS Error – to minimize the error between predicted and measured peak pressure

- IMEP % Error – IMEP difference between the mean effective pressure predicted and measured.

Total of 9 calibration parameters were used during the optimization:

- Entrainment Rate Multiplier
- Ignition Delay Multiplier
- Premixed Combustion Rate Multiplier
- Diffusion Combustion Rate Multiplier
- Diffusion Combustion Rate Transition Timing
- Diffusion Combustion Rate Final Value
- Diffusion Combustion Rate Transition Rate
- Overmixing Rate Multiplier
- Partial Oxidation Rate Multiplier

Performed calibration procedures were examined and compared with one another to understand which combination of parameters allowed to obtain best results in prediction of all the parameters related to the combustion process. Improved Burn Rate RMS Error and Pressure RMS Error can be also evaluated visually observing the difference between predicted and simulated profiles.

To evaluate the results of the calibration validation of the new parameters will be performed and presented in the figures. The quantities that will be evaluated and their suggested maximum error are presented in the table:

Parameter	Unit	Error limit
Improved Burn Rate RMS Error	RMS	0.0054
IMEP % Error During Combustion	%	±5%
Maximum pressure	Bar	±5
Mass fraction burned 50%	Degree	±2
Burn Duration 10-75	degree	±2

Table 3: Results investigated after validation and their error limits [8]

6.3 Calibration 1: minimizing the Improved Burn Rate RMS Error using 4 calibration parameters

First optimization was carried out using 4 parameters as suggested by GT-Suite manual. The set of coefficients related to that optimization is found in the table, together with the objective, which is averaged over set of 22 operating points (points that were used for the calibration analysis).

Calibration 1 Optimized parameters	
Entrainment Rate Multiplier	2.338
Ignition Delay Multiplier	0.337
Premixed Combustion Rate Multiplier	0.050
Diffusion Combustion Rate Multiplier	0.804
Improved Burn Rate RMS Error	0.00383

Table 4: Calibration 1 optimized results

After the optimization, the parameters values obtained through the optimization were used to run a validation simulation, where all the operating points (41) provided were used.

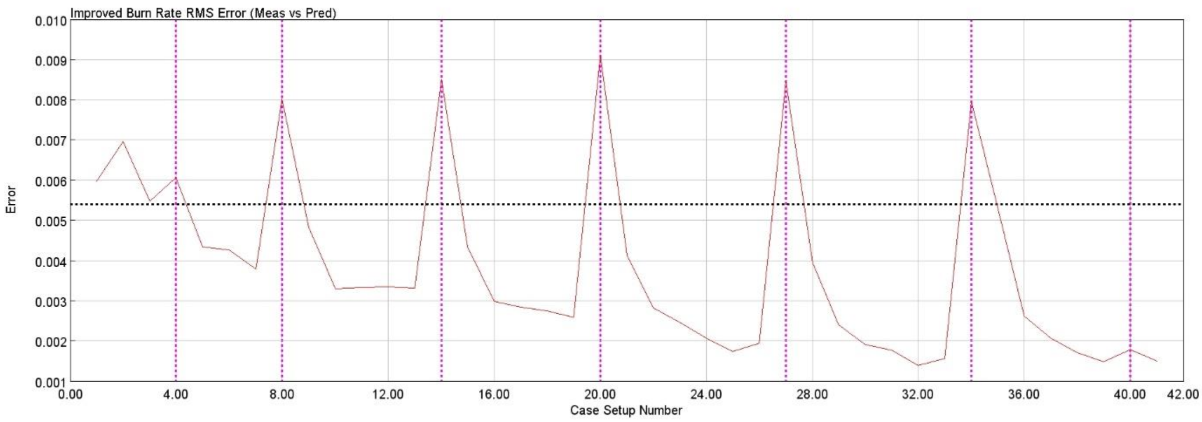


Figure 37: Improved Burn Rate RMS Error for the 1st calibration

Improved Burn Rate RMS Error shows good first approximation results. Most of the operating points are below the error limit. The most noticeable elements of the figure are spikes corresponding to the lowest BMEP for a given engine speed.

The comparison of measured and predicted data for IMEP, Maximum pressure, Crank angle at 50% Burned (MFB50) and Burn duration 10-75 are represented in the figures underneath.

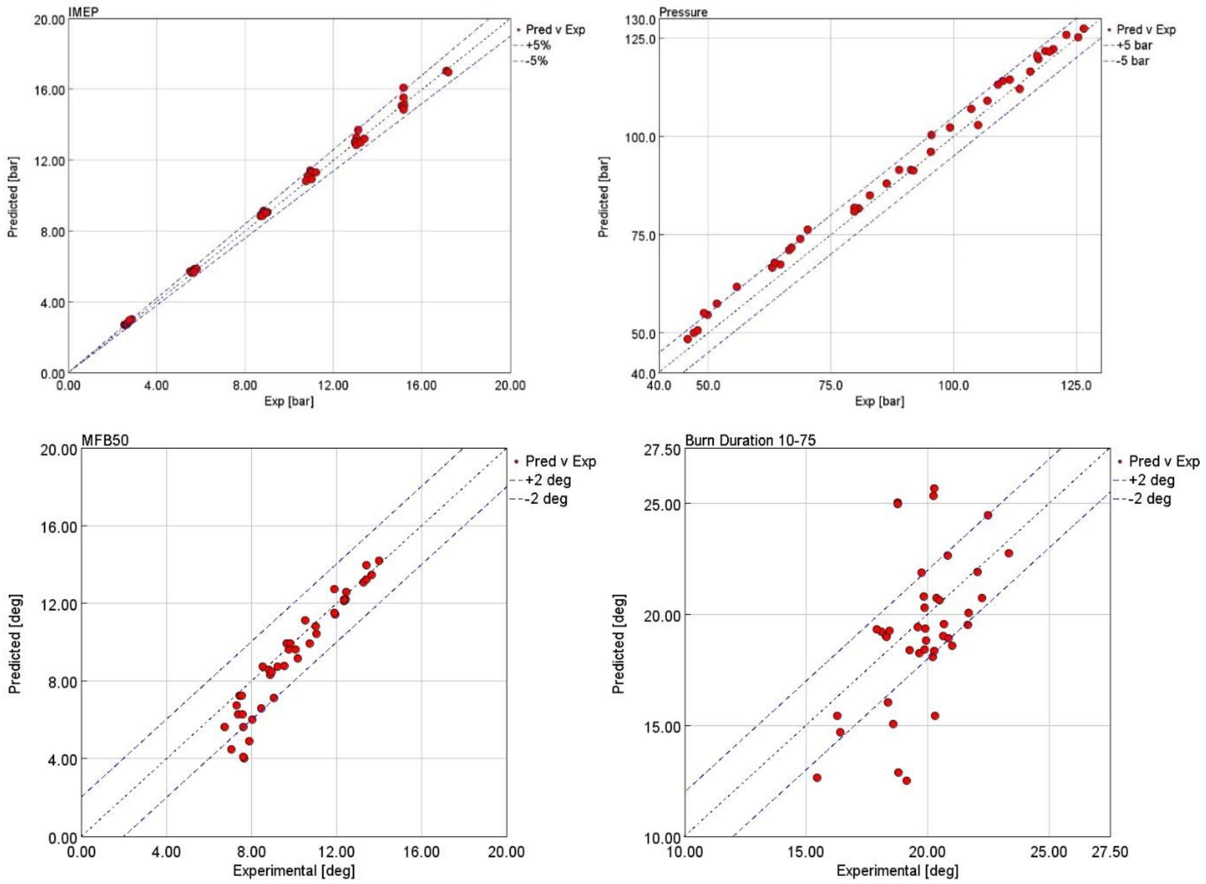


Figure 38: IMEP, maximum pressure, MFB50 and Burn duration 10-75. Predicted vs experimental data for the 1st calibration

Parameter	Unit	Error limit	Validation average error
Improved Burn Rate RMS Error	RMS	0.0054	0.0038
IMEP % Error During Combustion	%	±5%	1.55
Maximum pressure	Bar	±5	2.90
Mass fraction burned 50%	Degree	±2	0.89
Burn Duration 10-75	degree	±2	2.12

Table 5: Calibration 1, average errors indicated

To choose the current optimization parameters it is not enough to look at the average data and plots of the parameters such as MFB50%, Burn duration, improved RMS Error. It is important analyze the figures that present the instantaneous cylinder pressure and burn rates. In the figures below there are 3 sets of pressures:

- Measured in red (from experimental data)
- Simulated in blue (from CPOA)
- Predicted in green (from DI Pulse calibration)

As well as 2 sets of Burn rates

- Simulated in bright green (CPOA) and predicted in purple (DI Pulse calibration)

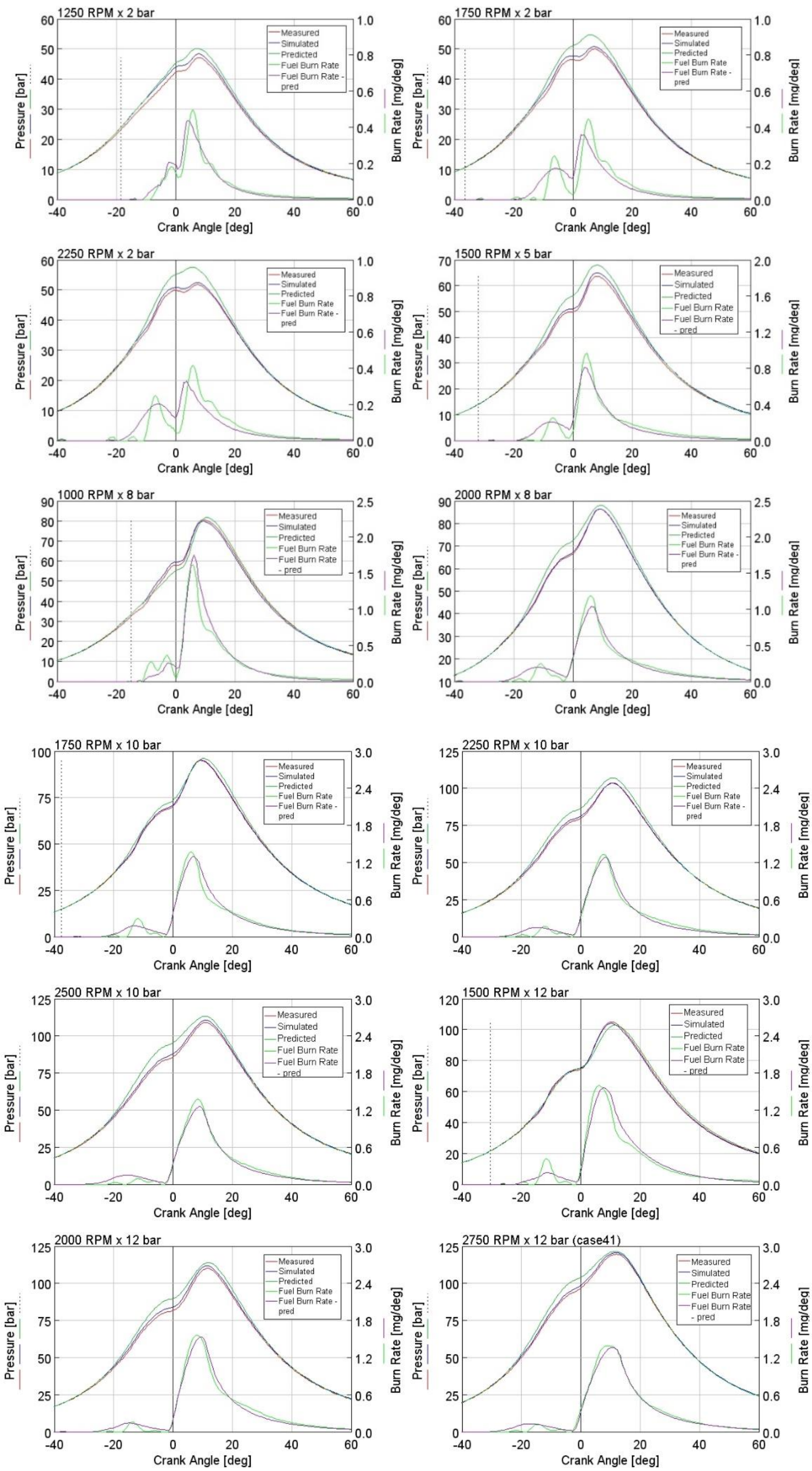


Figure 39: Predicted and Measured cylinder pressure and burn rate as a function of crank angle

Predicted pressure and burn rate curves presented in the figure above were generally able to capture the trend of simulated curves. Calibrated model has however visible difficulties with accurate prediction of the pressure trace and initial part of the burn rate.

6.4 Calibration 2: minimizing the Improved Burn Rate RMS Error using 7 calibration parameters

Trying to address the problems pointed out in the calibration 1, 3 new Diffusion Combustion focused parameters were added to calibration 2, keeping the objective the same as in the first calibration.

The resulting from the optimization parameters' values are listed in the table.

Calibration 2 Optimized parameters	
Entrainment Rate Multiplier	2.093
Ignition Delay Multiplier	0.357
Premixed Combustion Rate Multiplier	0.056
Diffusion Combustion Rate Multiplier	0.856
Diffusion Combustion Rate Transition Timing	0.347
Diffusion Combustion Rate Final Value	0.385
Diffusion Combustion Rate Transition Rate	10.704
Improved Burn Rate RMS Error	0.00357

Table 6: Calibration 2 optimized parameters

Increasing number of parameters allowed to lower the Improved Burn Rate RMS Error, especially in the middle load ranges for the lower engine speed portion of the map.

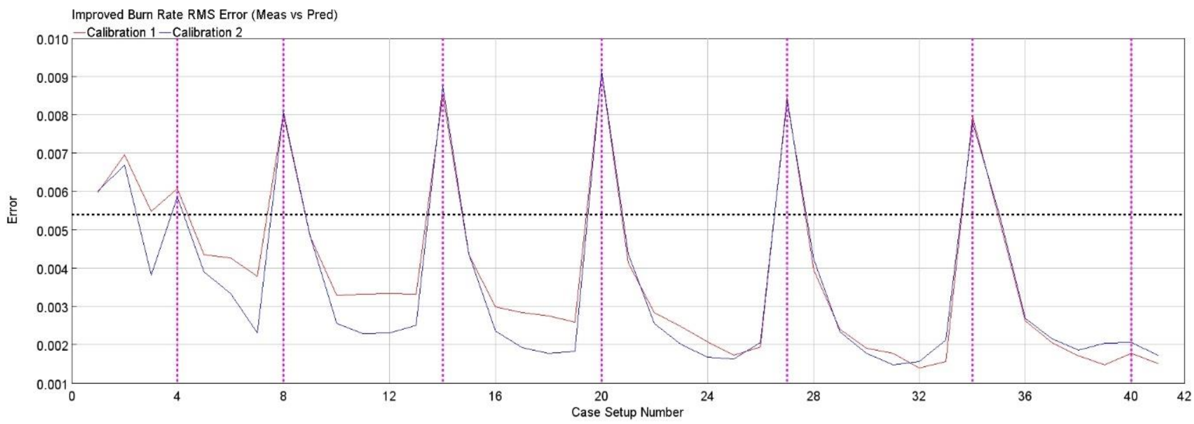


Figure 40: Improved Burn Rate RMS Error, comparison of calibration 1 and 2

In the figures below a comparison of calibration 1 and 2 is presented. 3 additional parameters used in this calibration brought the experimental and predictive IMEP closer together, which can be also observed looking at the average error of the validation in the table below. The other results mostly remained in the same error rage.

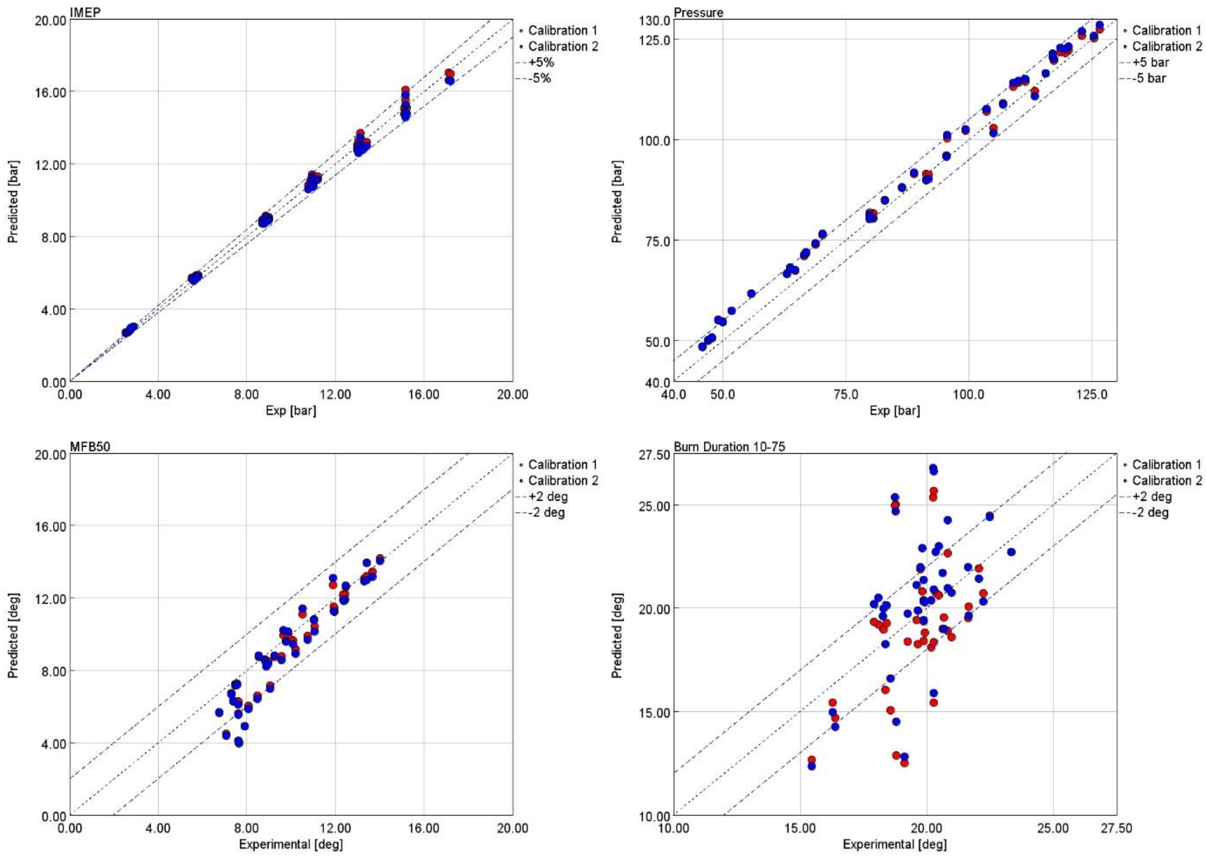


Figure 41:IMEP, maximum pressure, MFB50 and Burn duration 10-75. Predicted vs experimental, comparison of 1st and 2nd calibration

Parameter	Unit	Error limit	Validation average error
Improved Burn Rate RMS Error	RMS	0.0054	0.0036
IMEP % Error During Combustion	%	±5%	0.21
Maximum pressure	Bar	±5	3.26
Mass fraction burned 50%	Degree	±2	1.02
Burn Duration 10-75	degree	±2	2.16

Table 7: Calibration 2, average results errors

The pressure and burn rate plots presented below confirm lack of significant influence of these parameters at the model in this form. Predicted cylinder pressure and burn rate look almost indistinguishable when comparing calibration 1 and 2 together.

For what concerns the plots below, calibration 1 is on the left hand side and calibration 2 on the right hand side

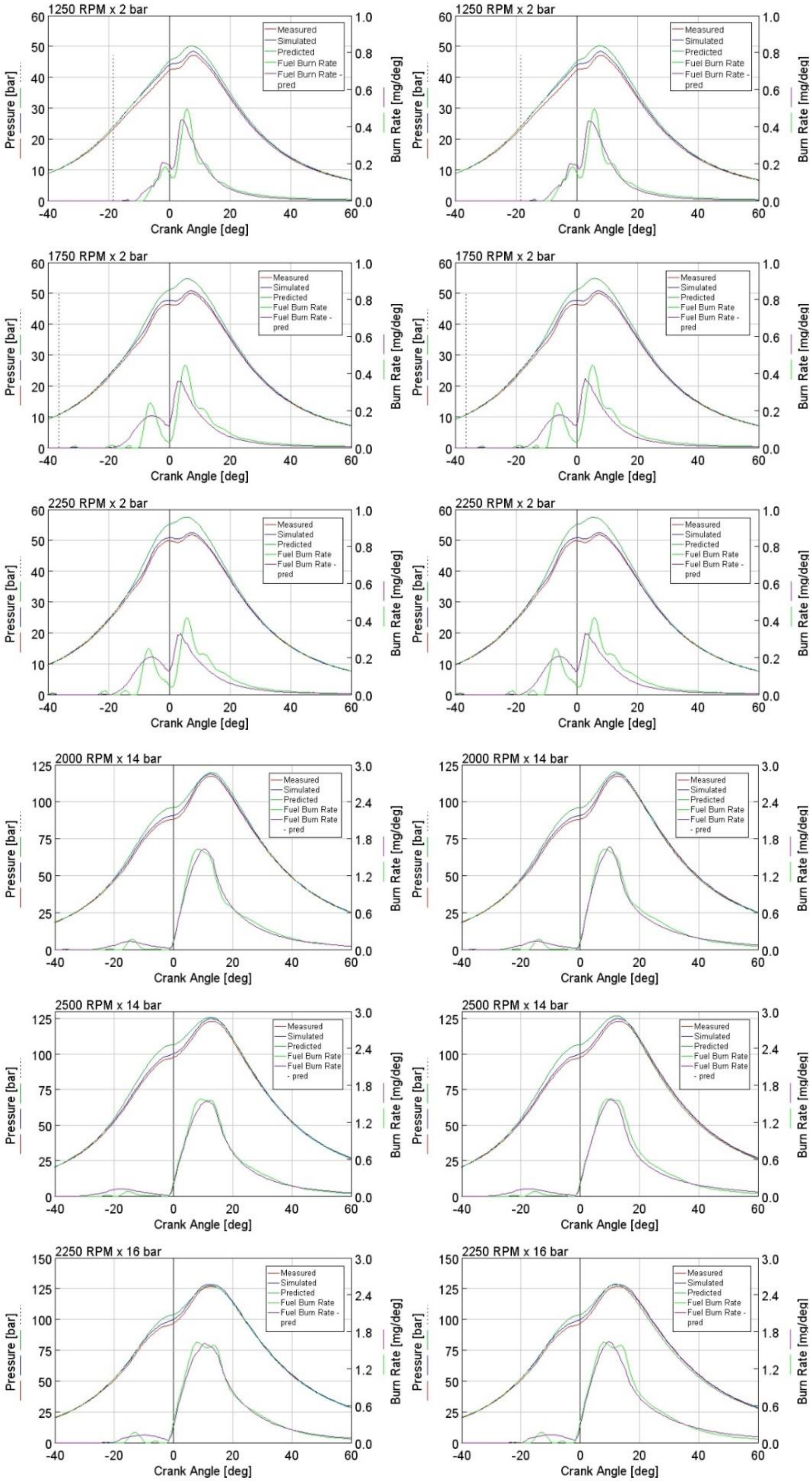


Figure 42: Predicted and Measured cylinder pressure and burn rate as a function of crank angle. Left hand side: calibration 1, right hand side: calibration 2.

6.5 Calibration 3: minimizing the Improved Burn Rate RMS Error and Pressure RMS Error using 7 calibration parameters

Setting two parameters as the objective of optimizer the multi-objective, Pareto optimization type is activated. In this setup optimizer searches for parameters that can satisfy both objectives at once. Points that can do that are referred to as optimal designs or Pareto points, while the rest of solution is non-optimal. When the Pareto points create a concave function, knee point of that function is usually a good start for the validation analysis.

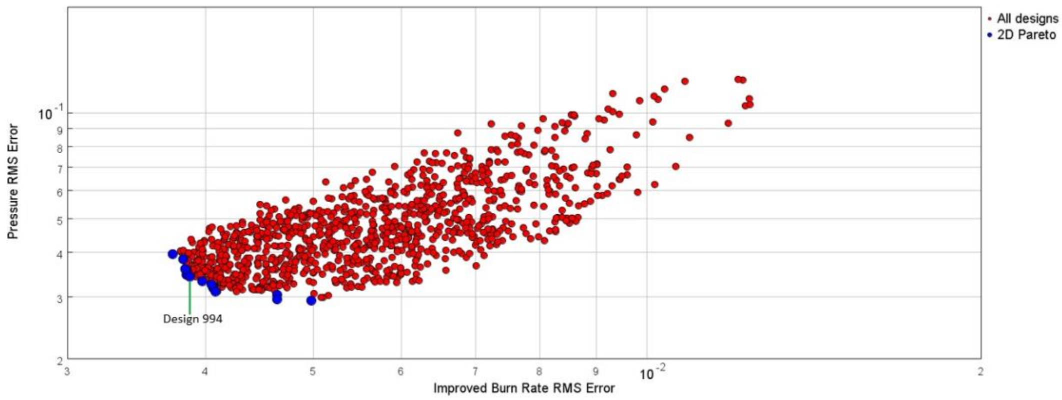


Figure 43: The results of the multi-objective optimization with 7 parameters Calibration 3. Pareto points

The selected design optimized parameters are listed in the table.

Calibration 3 Optimized parameters	
Entrainment Rate Multiplier	1.835
Ignition Delay Multiplier	0.308
Premixed Combustion Rate Multiplier	0.030
Diffusion Combustion Rate Multiplier	0.865
Diffusion Combustion Rate Transition Timing	0.337
Diffusion Combustion Rate Final Value	0.385
Diffusion Combustion Rate Transition Rate	10.701
Improved Burn Rate RMS Error	0.00370
Pressure RMS Error	0.03265

Table 8: Calibration 3 optimized results

As it can be expected, trying to target 2 objectives while using the same 7 parameters as in calibration 2, will impacts the Improved Burn Rate RMS error negatively. Looking at the figure it might seem as all the progress of calibration 2 reversed to calibration 1 in terms of Improved Burn Rate RMS Error.

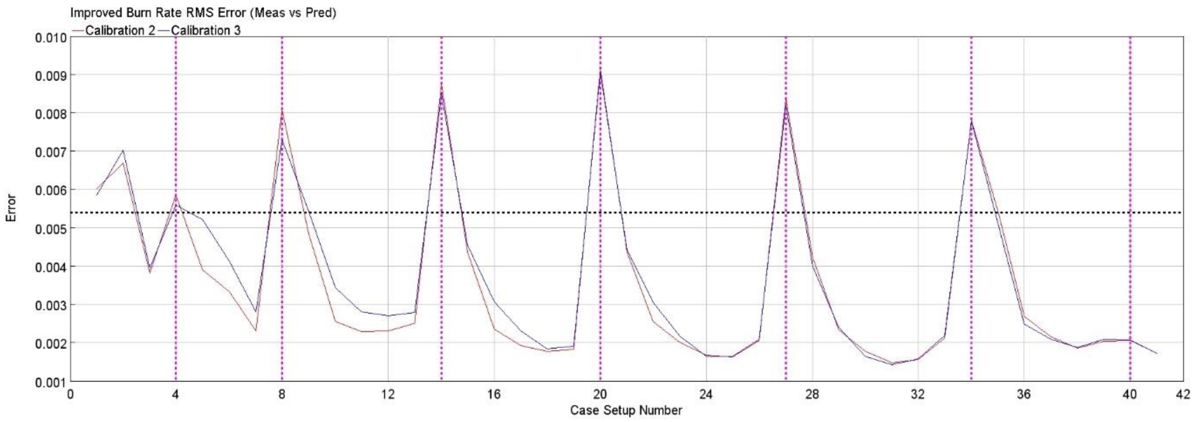


Figure 44: Improved Burn Rate RMS Error, comparison of calibration 2 and 3

Pressure RMS Error set to target minimalization was specifically chosen in order to match the measured and predicted cylinder pressure. The influence of this objective at the maximum pressure results can be seen in the figure below. Reducing the pressure error between measured and predicted data improves the MFB50 and burn duration as well.

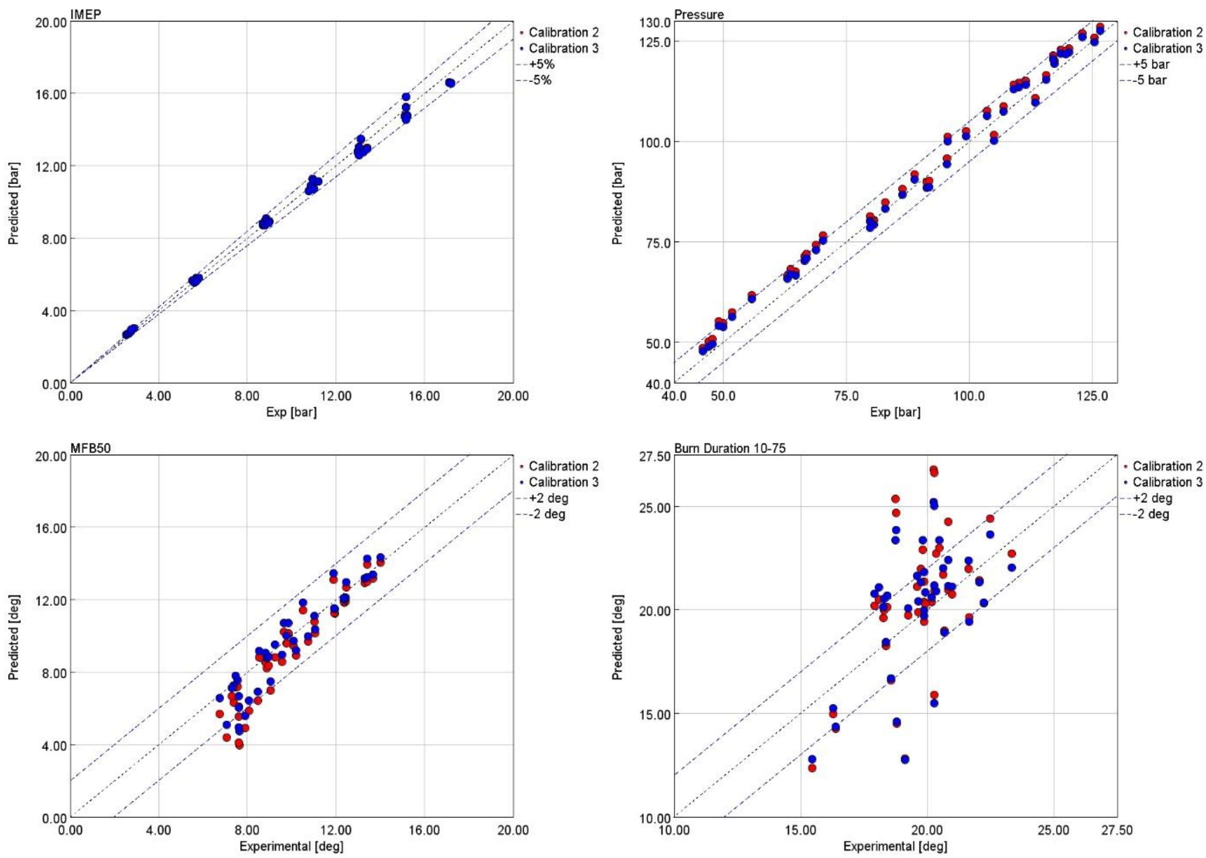


Figure 45:IMEP, maximum pressure, MFB50 and Burn duration 10-75. Predicted vs experimental data, comparison of 2nd and 3rd calibration

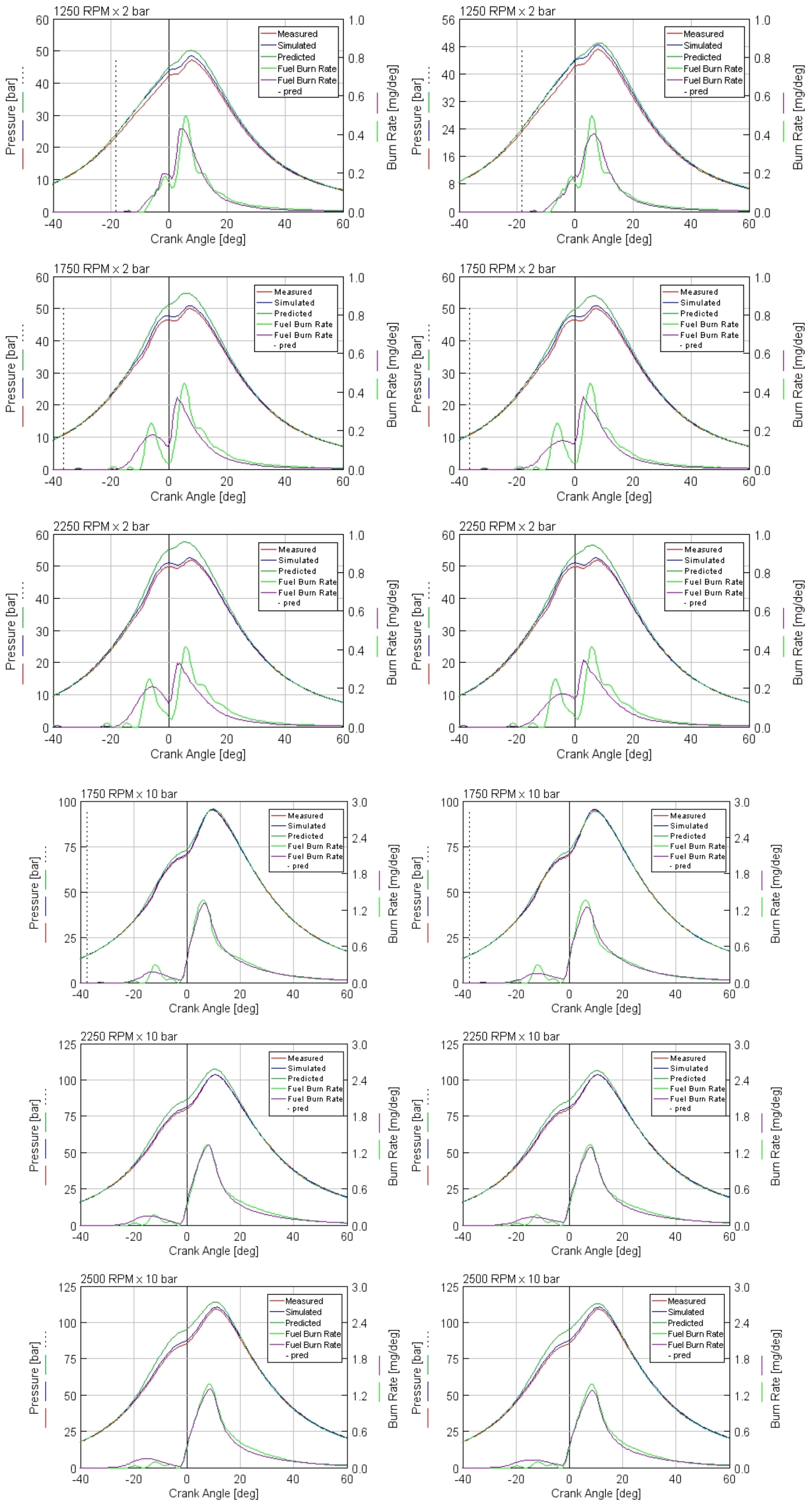


Figure 46: Predicted and Measured cylinder pressure and burn rate as a function of crank angle. Left hand side: calibration 2, right hand side: calibration 3

Parameter	Unit	Error limit	Validation average error
Improved Burn Rate RMS Error	RMS	0.0054	0.0037
IMEP % Error During Combustion	%	±5%	0.16
Maximum pressure	Bar	±5	2.61
Mass fraction burned 50%	Degree	±2	0.79
Burn Duration 10-75	degree	±2	2.06

Table 9: Calibration 3, average results errors

6.6 Calibration 4: minimizing the Improved Burn Rate RMS Error and Pressure RMS Error using 9 calibration parameters

Three calibration actions performed so far did not improve significantly the predicted cylinder pressure or burn rate. To improve on these results, two more calibration parameters were incorporated into the model, for a total of 9. Similarly to the previous calibration an multi-objective optimization was run and the knee point of the Pareto curve was chosen for the validation of the parameters.

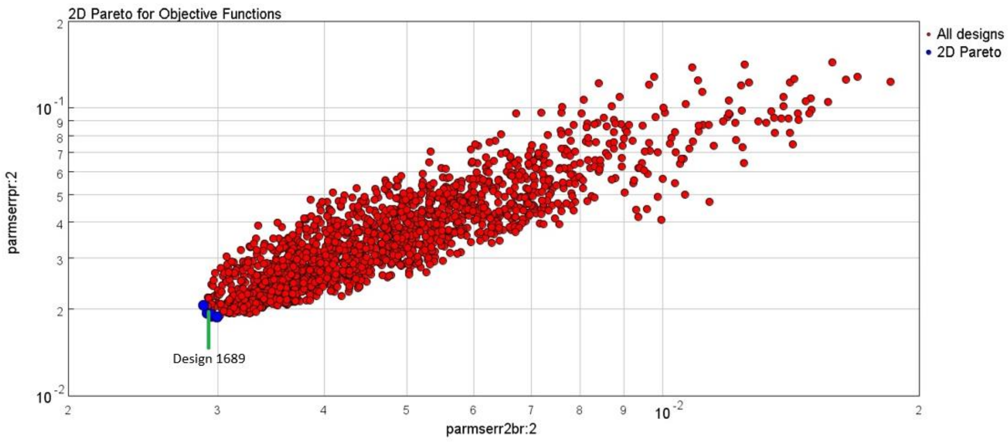


Figure 47: The results of the multi-objective optimization with 9 parameters Calibration 4. Pareto points

Calibration 4 Optimized parameters	
Entrainment Rate Multiplier	2.189
Ignition Delay Multiplier	0.547
Premixed Combustion Rate Multiplier	0.400
Diffusion Combustion Rate Multiplier	0.811
Diffusion Combustion Rate Transition Timing	0.341
Diffusion Combustion Rate Final Value	0.342
Diffusion Combustion Rate Transition Rate	8.045
Overmixing Rate Multiplier	2.518
Partial Oxidation Rate Multiplier	2.761
Improved Burn Rate RMS Error	0.00274
Pressure RMS Error	0.01880

Table 10: Calibration 4 optimized parameters

Introduction of Partial oxidation and overmixing rate multiplier into the model improved all the results that were investigated in this part of thesis. Improved Burn Rate RMS Error is know below its error limit for majority of the operating points and the spikes that indicated the lowest BMEP for a given engine speed were reduced more than twofold.

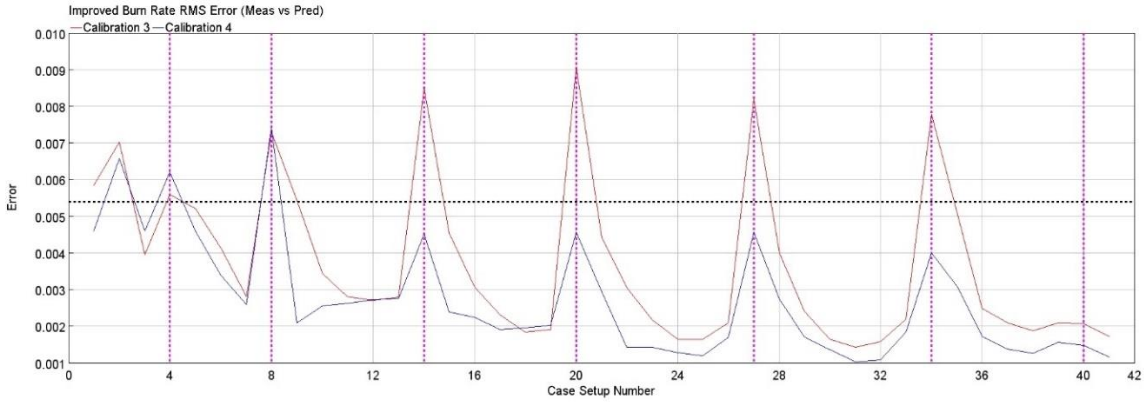


Figure 48: Improved Burn Rate RMS Error, comparison of calibration 3 and 4

Predicted maximum pressure and MFB50 are now completely within their respective error margins. Predicted burn duration improved significantly all although not all operating points managed to achieve 2 degrees error margin, the average error of the burn duration 10-75 for the first time is within the limit error, as it ca be seen in the table below.

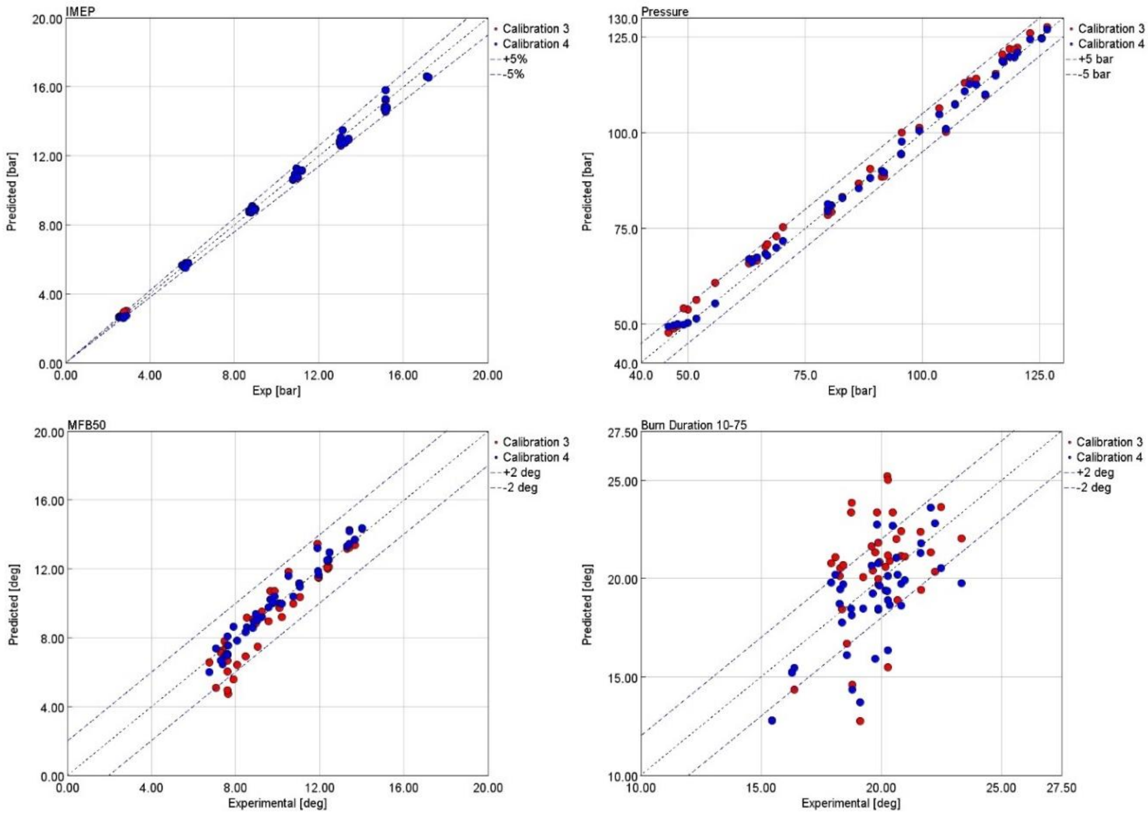
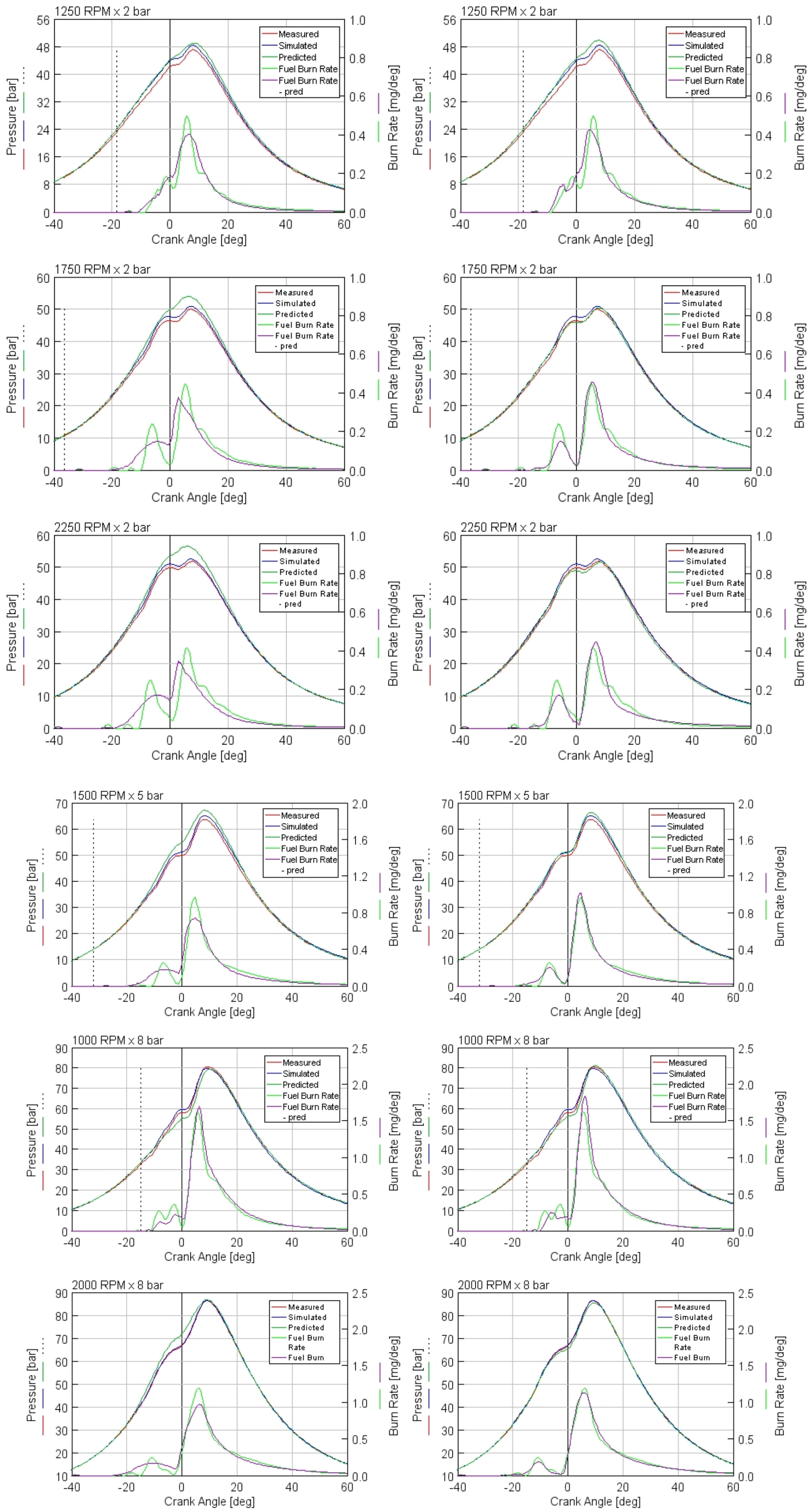
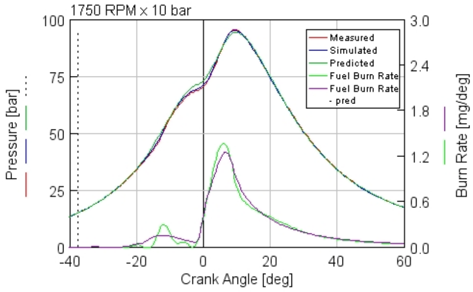
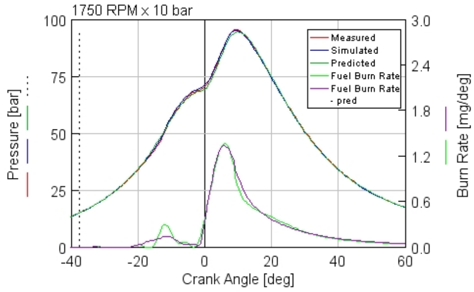


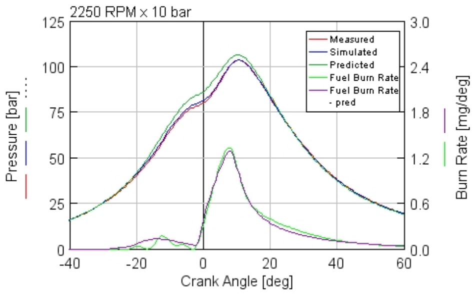
Figure 49:IMEP, maximum pressure, MFB50 and Burn duration 10-75. Predicted vs experimental data, comparison of 3rd and 4th calibration

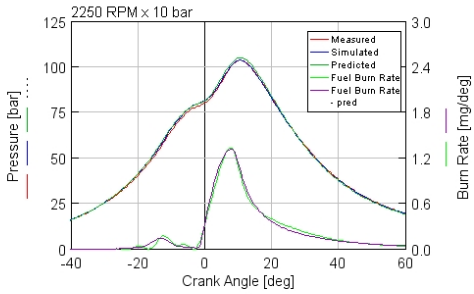


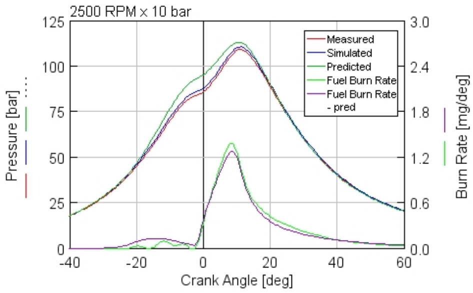
1250 RPM x 2 bar
1250 RPM x 2 bar
1750 RPM x 2 bar
1750 RPM x 2 bar
2250 RPM x 2 bar
2250 RPM x 2 bar
1500 RPM x 5 bar
1500 RPM x 5 bar
1000 RPM x 8 bar
1000 RPM x 8 bar
2000 RPM x 8 bar
2000 RPM x 8 bar
Measured
Simulated
Predicted
Fuel Burn Rate
Fuel Burn Rate - pred
Pressure [bar]
Burn Rate [mg/deg]
Crank Angle [deg]

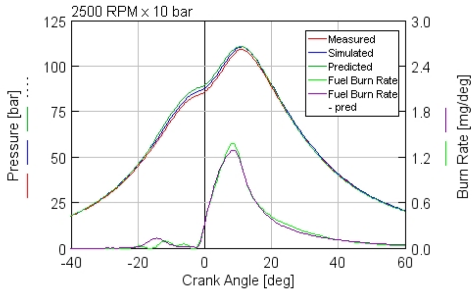

1750 RPM x 10 bar
Measured
Simulated
Predicted
Fuel Burn Rate
Fuel Burn Rate - pred
Pressure [bar]
Burn Rate [mg/deg]
Crank Angle [deg]

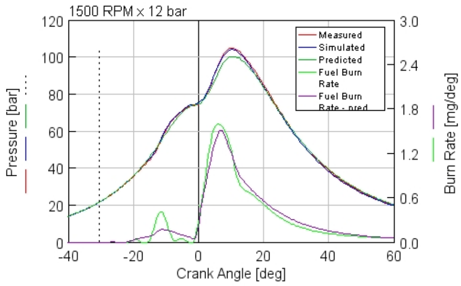

1750 RPM x 10 bar
Measured
Simulated
Predicted
Fuel Burn Rate
Fuel Burn Rate - pred
Pressure [bar]
Burn Rate [mg/deg]
Crank Angle [deg]

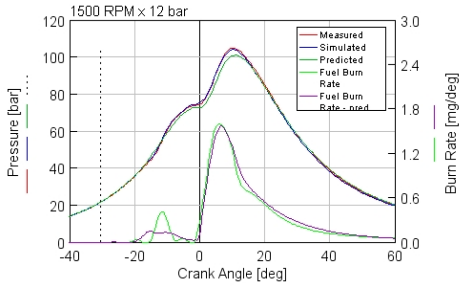

2250 RPM x 10 bar
Measured
Simulated
Predicted
Fuel Burn Rate
Fuel Burn Rate - pred
Pressure [bar]
Burn Rate [mg/deg]
Crank Angle [deg]

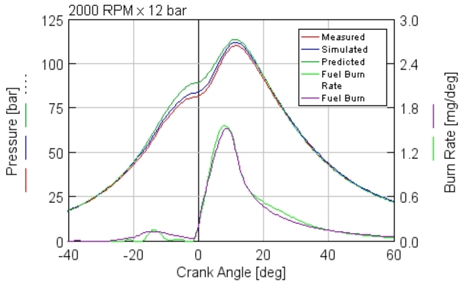

2250 RPM x 10 bar
Measured
Simulated
Predicted
Fuel Burn Rate
Fuel Burn Rate - pred
Pressure [bar]
Burn Rate [mg/deg]
Crank Angle [deg]

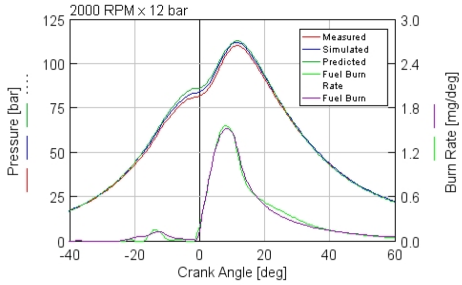

2500 RPM x 10 bar
Measured
Simulated
Predicted
Fuel Burn Rate
Fuel Burn Rate - pred
Pressure [bar]
Burn Rate [mg/deg]
Crank Angle [deg]

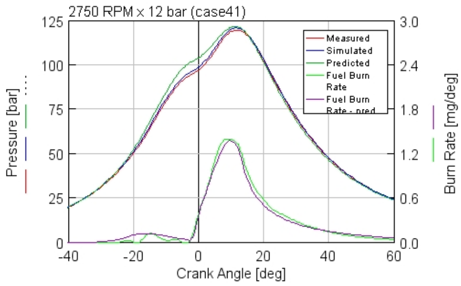

2500 RPM x 10 bar
Measured
Simulated
Predicted
Fuel Burn Rate
Fuel Burn Rate - pred
Pressure [bar]
Burn Rate [mg/deg]
Crank Angle [deg]

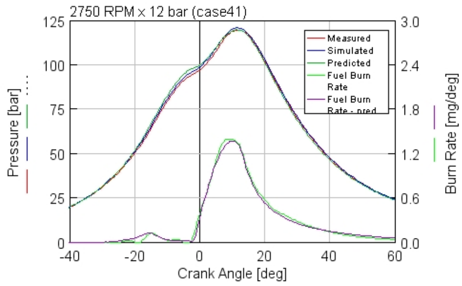

1500 RPM x 12 bar
Measured
Simulated
Predicted
Fuel Burn Rate
Fuel Burn Rate - pred
Pressure [bar]
Burn Rate [mg/deg]
Crank Angle [deg]


1500 RPM x 12 bar
Measured
Simulated
Predicted
Fuel Burn Rate
Fuel Burn Rate - pred
Pressure [bar]
Burn Rate [mg/deg]
Crank Angle [deg]


2000 RPM x 12 bar
Measured
Simulated
Predicted
Fuel Burn Rate
Fuel Burn
Pressure [bar]
Burn Rate [mg/deg]
Crank Angle [deg]


2000 RPM x 12 bar
Measured
Simulated
Predicted
Fuel Burn Rate
Fuel Burn
Pressure [bar]
Burn Rate [mg/deg]
Crank Angle [deg]


2750 RPM x 12 bar (case41)
Measured
Simulated
Predicted
Fuel Burn Rate
Fuel Burn Rate - pred
Pressure [bar]
Burn Rate [mg/deg]
Crank Angle [deg]


2750 RPM x 12 bar (case41)
Measured
Simulated
Predicted
Fuel Burn Rate
Fuel Burn Rate - pred
Pressure [bar]
Burn Rate [mg/deg]
Crank Angle [deg]

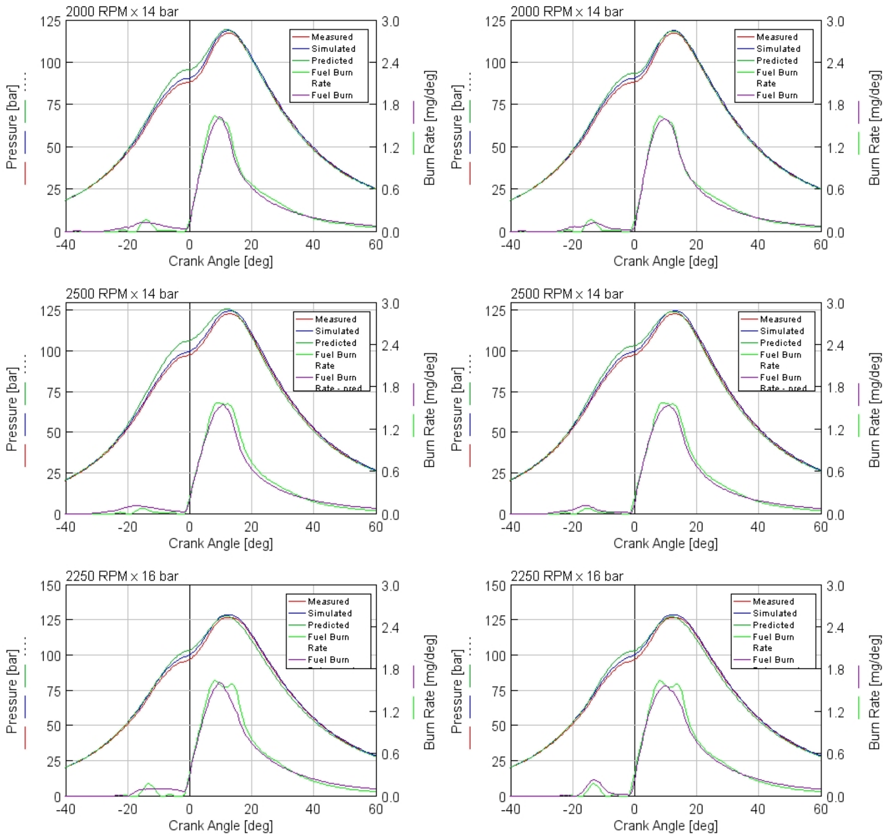


Figure 50: Predicted and Measured cylinder pressure and burn rate as a function of crank angle. Left hand side: calibration 3, right hand side: calibration 4

Looking at figure 50, the 4th calibration of a DI pulse is extremely successful at predicting the cylinder pressure. As for a burn rate a visible improvement can be seen for the following operating points:

- 1750 rpm and 2250 rpm x 2 bar and 1500 rpm x 5 BMEP, where predicted burn rate managed to predict the simulated burn rate.

Parameter	Unit	Error limit	Validation average error
Improved Burn Rate RMS Error	RMS	0.0054	0.0027
IMEP % Error During Combustion	%	±5%	-0.91
Maximum pressure	Bar	±5	1.43
Mass fraction burned 50%	Degree	±2	0.36
Burn Duration 10-75	degree	±2	1.53

Table 11: Calibration 4, average results errors

4th calibration procedure provided the most accurate results. Validation average errors from the table above are all within the limit specified by GT manual. IMEP, Maximum pressure and MFB50 have all the operating points within the error limit and the burn duration results are good enough to move to the NO_x emission model.

6.7 NOx emissions

GT combustion models include the capability to calculate NO_x concentrations, calling an 'EngCylNOx' reference object. The NO_x emissions are calculated using the Extended Zeldovich mechanism. This model is very sensitive to the trapped cylinder mass, air-fuel ratio and combustion rate, hence NO_x emissions should be simulated after achieving satisfactory results with a DI Pulse predictive model.

In Diesel engine NO_x split is usually

- 70-90% NO,
- 30-10% NO_2

NO forms as a by-product of the combustion process, because of the oxidation in high temperature and then NO_2 forms from NO. There are 3 main chemical reactions that are important in the Zeldovich mechanism.

$$\mathrm{O} + \mathrm{N}_2 \rightarrow NO + N$$

$$\mathrm{N} + \mathrm{N}_2 \rightarrow NO + O$$

$$\mathrm{N} + \mathrm{OH} \rightarrow NO + N$$

Inside the 'EngCylNOx' object there are coefficients that are used to calculate rate of reactions listed above. There are 6 parameters total, which are used to predict the NO_x concentration.

- NOx Calibration Multiplier
- N2 Oxidation Rate multiplier
- N2 Oxidation Activation Energy Multiplier
- N Oxidation Rate Multiplier
- N Oxidation Activation Energy Multiplier
- OH Reduction Rate Multiplier

These parameters are set in the Design Optimizer for a single-objective optimization, which objective is to minimize the difference between the experimentally measured NO_x and 'NO_x at EVO'. Two set of optimizations were performed for NO_x emissions model. One that includes all 6 parameters and the second one for 2 parameters which showed the highest sensitivity, and are highlighted in the table below. **[8] [3]**

Multiplier	Parameter's range
NOx Calibration Multiplier	0.1 ÷ 2
N2 Oxidation Activation Energy Multiplier	0.3 ÷ 1.1

Table 12: Upper and lower limits of NOx influencing parameters

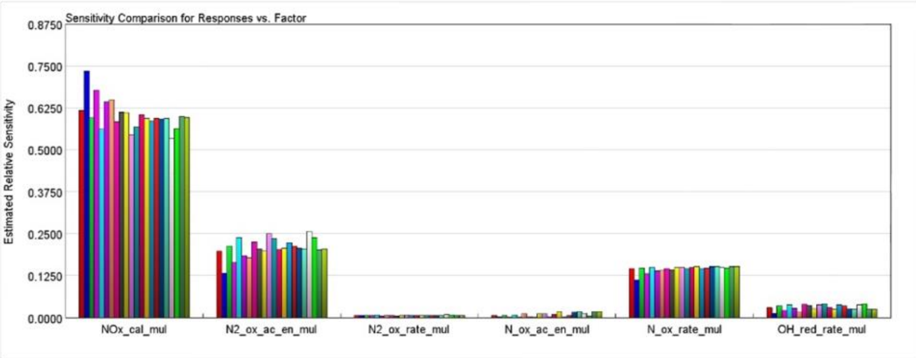


Figure 51: NOx optimization parameters, sensitivity.

The calibrated parameters are:

Parameter	6 parameters optimization	2 parameters optimization
NOx Calibration Multiplier	0.154	0.167
N2 Oxidation Rate multiplier	0.117	def
N2 Oxidation Activation Energy Multiplier	0.670	0.309
N Oxidation Rate Multiplier	0.965	def
N Oxidation Activation Energy Multiplier	0.3712	def
OH Reduction Rate Multiplier	1.458	def

Table 13: NOx emissions optimized coefficients

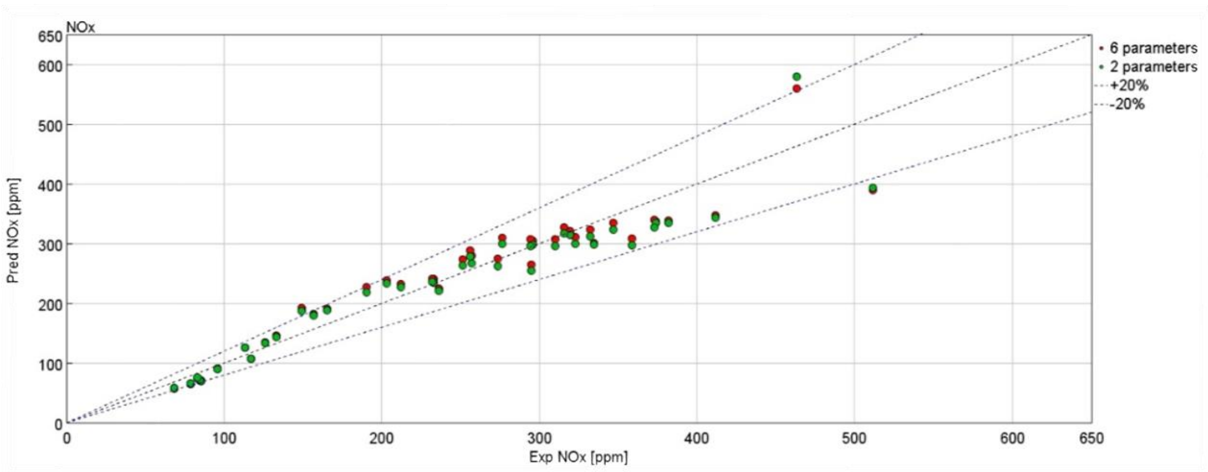


Figure 52: NOx validation, comparison of 2 and 6 parameters model

There are 3 out of 41 cases that are outside of the 20% range:

- 1000 RPM x 8BMEP,
- 1250 RPM x 10 BMEP,
- 2500 RPM x 8BMEP.

7. Conclusions

In this thesis, the predictive capabilities of a predictive combustion model have been evaluated for a 1.6L light-duty diesel engine. The analysis focused on replicating the measured conditions during the CPOA, combustion process during DI Pulse and NO_x emissions calibration.

The Cylinder Pressure Only Analysis (CPOA) was performed to obtain the burn rate from the experimental cylinder pressure signals through the reverse run. The experimental data and engine geometry were the subject of investigation. In order to match measured and simulated cylinder pressures during the non-predictive run several calibration steps were performed. The in-cylinder surface temperature was adjusted for every operating point that was investigated, the compression ratio was reduced to match the compression slope in more accurate way, fuel injected mass estimated by the ECU was recalculated using the fuel mass flow rate measured during the test bench activity and the Overall Convection Multiplier's influence on the cumulative error was tested. Total of 39 out of 41 operating points passed the consistency check for cylinder 2, and the experimental and simulated results matched well. 1 cylinder model was subsequently used in DI Pulse predictive model analysis.

For the calibration of the DI Pulse model 22 operating points distributed on the engine map (both in terms of BMEP and EGR) were selected. 4 calibrations were performed, increasing the number of parameters to be optimized with each subsequent step. Single-objective optimization was used at first and then switched to multiple-objective to target the cylinder pressure differences between simulated and predicted results. All the investigated results (IMEP during combustion, Maximum Pressure, MFB50 and Burn Duration 10-75) showed a significant improvement at the end of calibration process, and passed their respective error limits. Predicted and simulated pressure show the same characteristic and overlap for the majority of operating points, predicted burn rate deals very well with the main burn rate spike, however it has problems trying to predict the initial burn rate.

NO_x emissions model was optimized using 6 and 2 parameters respectively. 92% of the predicted NO_x emissions fall within 20% error of the measured data, the RMS error of the NO_x emissions equals 10.05 The further analysis of NO_x predictive model is recommended, perhaps with bigger set of experimental data.

Computational simulations are powerful tools which can significantly impact the engine development phase, as well provide an estimate when new systems and/or solutions are to be investigated on the calibrated engine.

The recommended future work on the model includes the soot calibration and investigating the ‘virtual test bench’ capabilities of the model, which can be achieved by loading different blend of diesel fuel into the model and comparing the predictive results with measured ones, as experimental activity concerning this engine and different fuel blends was carried out on this engine.

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