

Numerical Simulation and Flame Analysis of Combustion and Knock in a DISI Optically Accessible Research Engine

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ABSTRACT

The increasing limitations in engine emissions and fuel consumption have led researchers to the need to accurately predict combustion and related events in gasoline engines. In particular, knock is one of the most limiting factors for modern SI units, severely hindering thermal efficiency improvements. Modern CFD simulations are becoming an affordable instrument to support experimental practice from the early design to the detailed calibration stage. To this aim, combustion and knock models in RANS formalism provide good time-to-solution trade-off allowing to simulate mean flame front propagation and flame brush geometry, as well as “ensemble average” knock tendency in end-gases. Still, the level of confidence in the use of CFD tools strongly relies on the possibility to validate models and methodologies against experimental measurements.

In the paper, two sets of cycle-resolved flame visualizations are available from a single-cylinder 400 cm³ direct-injection spark-ignition (DISI) unit with optical access. The engine is operated at two spark timings, ranging from knock-safe to light-knock conditions.

On this basis, a numerical analysis is carried out to reproduce flame kernel growth and propagation using the well-known ECFM-3Z combustion model for all the operating conditions. CFD results are compared in terms of enflamed volume and flame morphology against cycle averaged experimental data. In addition, average knock is simulated by means of the in-house built UniMORE Knock Model [1] in terms of knock onset location and phasing.

The agreement between predicted and measured position of the flame front and knock inception location for the two different operating conditions confirms the validity of the adopted models and proves their predictive capability for engine design and optimization.

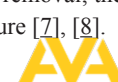
CITATION: Iaccarino, S., Breda, S., D'Adamo, A., Fontanesi, S. et al., "Numerical Simulation and Flame Analysis of Combustion and Knock in a DISI Optically Accessible Research Engine," *SAE Int. J. Engines* 10(2):2017, doi:10.4271/2017-01-0555.

INTRODUCTION

The increasing cost of oil on one side and the need to comply with legislations concerning pollutants and CO₂ emissions on the other one force OEMs to a feverish improvement of the currently available engine technologies. The main challenge in the design phase is nowadays the reduction of fuel consumption while guaranteeing the same performance output; the only way to meet this challenging target is to increase the system chain of efficiencies in the conversion from thermal to mechanical energy.

Nowadays, the trend for gasoline passenger cars is to downsize the engine displacement, while adopting increasingly complex supercharging or turbocharging systems. This allows to achieve the same, or even higher, performance with relatively small engine displacement. Direct injection and variable valve lift and timing are additionally employed to reduce pumping losses and achieve higher combustion efficiency [2][3].

The main limit on performance increase achievable through the use of these technologies lies in the occurrence of abnormal combustion, such as pre-ignition and engine knock [4]. Knock is the consequence of the spontaneous ignition of a portion of unburnt air-fuel mixture before the spark ignited flame front reaches and regularly consumes it. End-gas compression, due to piston motion and expansion of enflamed gases, could lead to unexpected pressure and temperature increase in the unburnt gas region, promoting the occurrence of autoignition. The rapid heat release caused by autoignition chemical reactions may induce a set of high-frequency pressure waves travelling across the combustion chamber, revealed by a metallic knocking sound [5], [6]. Under severe knock condition, high pressure gradients and oscillations from travelling waves could easily damage the solid components facing the combustion chamber, due to metal erosion and/or lubricant film removal; the whole set of events may in turn lead to rapid engine failure [7], [8].



In order to obtain high levels of specific power output and efficiency, modern SI units need to operate as close as possible to knocking conditions, while avoiding the harmful incurrence of knock onset. More difficulties arise considering the stochastic nature of engine flows, causing the cycle-to-cycle variability (CCV) and random cycle-dependent knock occurrence [9,10]

In this scenario, CFD simulation is acquiring more and more importance, since it can help to reduce expensive testing and prototyping enabling a quick comparison among different solutions. Nevertheless, to properly face the current engine development trends, models are continuously evolving and becoming more and more complex. Design tools enabling engineers to easily implement new technologies and solutions with reduced modelling assumptions are needed. With specific reference to SI engines, tools able to describe and predict combustion evolution and fuel autoignition dependency on local thermo-physical conditions are fundamental in the design of modern SI units. Improvements in 3D CFD modelling for spark-combustion and autoignition allow to identify and deepen the understanding of the causes of combustion inefficiencies and autoignition to a level which would not be possible with the experimental approach alone, which is usually confined to laboratory engines [11]. Still, numerical simulations rely on model calibrations and validations which can only be performed through comparison with high-level data acquired on research engines.

A rigorous approach to model the autoignition process in a mixture of air and fuel is to take into account all the chemical reactions leading to spontaneous ignition onset. The accuracy of such approach is limited by the robustness of the chemical model itself and by numerical approximations, especially regarding temporal discretization. Beside accuracy, the enormous CPU cost makes this approach practically unaffordable for complex geometries and actual fuels, whose chemical representation would require thousands of intermediate species and therefore transport equations. In addition, this approach considers the computational cell as a laminar chemical reactor, which is intrinsically not correct when the simulation is performed on highly turbulent flows, since any interaction between turbulent flow and flame development is neglected. Such disadvantages enhance the need of a different modelling strategy.

Another consolidated approach consists in associating an autoignition (AI) delay time at each fluid cell to indicate unburnt gases reaction rate. Basically two kinds of approaches can be distinguished in the generation of the AI delay. In the first, these are calculated as function of physical conditions inside the cell through empirical correlations. An extensive research campaign in this direction has been carried out by Douaud and Ezyat in [12] and by other authors in [13]. The CPU-efficiency of this strategy is guaranteed by the simple algebraic expression which is solved for each cell at each time-step in order to calculate the reaction rate. Nevertheless, the accuracy of the chemical reactivity estimation is usually good on a limited range of physical conditions.

An alternative way is to calculate AI delays again using a detailed chemical approach, specifically assigned to a complex-chemistry solver. These simulations are carried out just once prior to the CFD run and their results in terms of autoignition delays are tabulated in a dedicated database (look-up table), which can be accessed by the

CFD solver during the engine simulation. Since chemicals calculations have to be solved in advance, it is possible to create tables spanning wide range of physical conditions, thus overcoming the need of an algebraic fitting and still preserving the accuracy of the chemical scheme. To maintain a good level of CPU-efficiency a good strategy of table interrogation and interpolation is needed.

The present paper describes a numerical study of an experimental optically accessible research engine available at the Istituto Motori of CNR. In particular, the engine is equipped with a currently produced engine head and the optical access to the combustion chamber is guaranteed by a flat transparent piston [11]. 1D and 3D CFD simulations are performed in a RANS framework with the objective of confirming and motivating the outcomes and results of the aforementioned experimental campaign on combustion and knock. At first, knock safe operating condition is explored through simulation and flame morphology analysis is carried out to validate numerical results against acquired visualizations. Secondly, a light knocking condition is simulated with the aim of representing the trend in combustion evolution and knock onset outcome from experimental evidence. Finally, knock analysis is deepened to study the influence of secondary flames due to knock on the main spark-ignited flame front evolution, again in comparison with optical results.

EXPERIMENTAL SETUP AND PROCEDURE

Measurements were performed with commercial RON 95 gasoline on the described unit, whose main specifications are listed in Table 1. The cylinder head of a commercial power unit was coupled to a cylinder block that features an elongated piston. A combustion chamber overview is shown in Figure 1. This design [14] allowed optical accessibility through an 18 mm thick quartz window fitted in the piston crown. Two uninterrupted Teflon-bronze rings ensured sealing and along with a slotted graphite ring allowed oil-less lubrication on the upper part of the engine.

Spray pattern was governed by injector positioning and phasing of fuel delivery. Side mounting, nozzle orientation and injection timing resulted in fuel impingement mostly on the piston crown, with part of the six jets also hitting the cylinder liner (Figure 2). This meant that charge stratification during combustion was dictated mainly by the non-evaporated fraction that ended up on the piston [15].

In-cylinder pressure was measured with an accuracy of ± 1 % using a flush-installed piezo-electric sensor; acquisitions were performed during 200 consecutive cycles for every condition, with sets of 100 cycles each that featured correlated optical data.

Table 1. Single cylinder SI engine characteristics.

Displacement	399 cm ³
Bore	79 mm
Stroke	81.3 mm
Compression Ratio	10:1
Injection pressure	100 bar

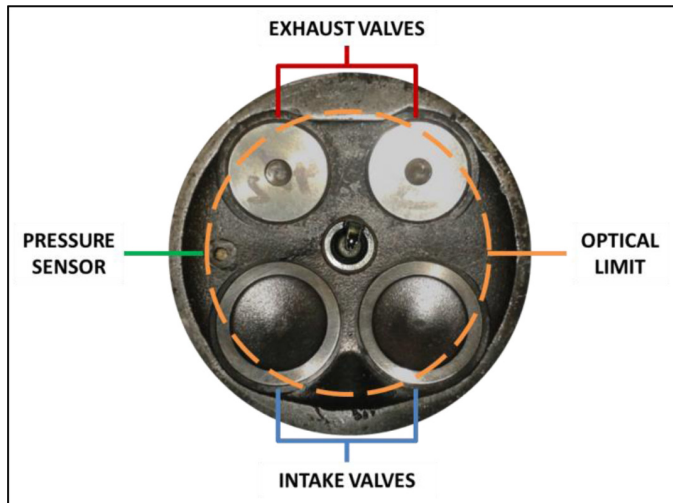


Figure 1. Bottom view of the combustion chamber.

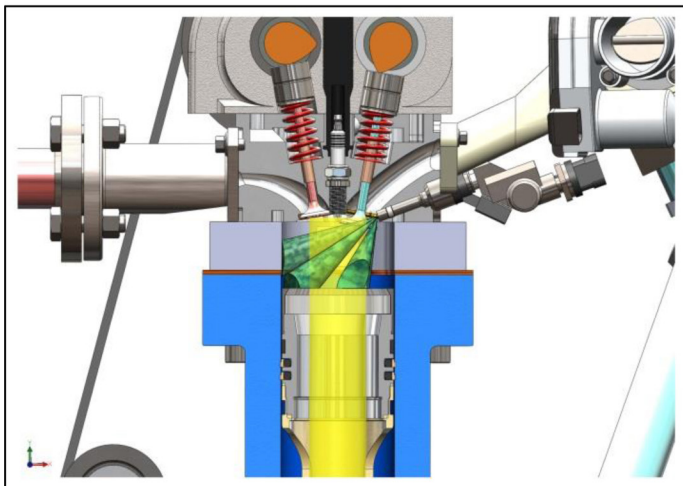
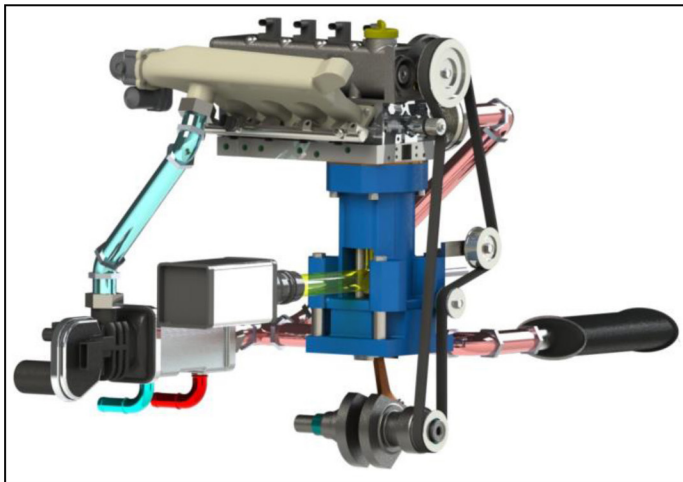


Figure 2. Experimental apparatus for the optically accessible engine (top) and illustration of spray pattern with respect to the piston crown (bottom).

Thermodynamic data was analyzed using a simplified approach based on the first law, with mass fraction burned (MFB) values calculated through the procedure developed by Rassweiler & Withrow [16]; a low pass filter set at 5 kHz was used for this analysis in order to capture only the frequencies specific for normal combustion

phenomena. For knocking cycles, the intensity of this phenomenon was quantified through the maximum amplitude of pressure oscillations (MAPO), after applying a high-pass filter set at 5 kHz; this parameter was calculated as $MAPO = \max(|\text{filtered}|_{\text{ignitionEVO}})$ in the crank angle interval ranging from ignition to exhaust valves opening. Given that the sampling frequency was 60 kHz, the 5-30 kHz range can be considered more than sufficient for identifying knock specific oscillations. The threshold for distinguishing between normal and knocking cycles was chosen based on the motored peak pressure (around 27-28 bar). A value of 5% was imposed as the limit that distinguishes between normal and knocking cycles, and traces with MAPO over 10% of the motored peak pressure were considered as heavy knocking events. The same procedure was applied in an experimental study aimed at correlating knock and secondary flames induced by pre-ignition phenomena [17]. Although the purpose of the aforementioned work was different compared to this one, the overall concept is the same, with the aim of gaining more detailed information on normal and abnormal combustion development compared to the acquisition of thermodynamic parameters only.

Coolant and lubricant temperature was monitored and maintained at 330 K using a thermal conditioning unit. Engine speed was set at 2000 rpm, while fuel injection is initiated 300 CAD bTDC with an injection pressure equal to 100 bar. Spark timing was swept in a relatively narrow range, at 12 and 15 CAD bTDC, with the first right at the knock limit, and the second under light-knocking conditions. It should be noted that crank angle references are made with respect to the TDC at the end of compression. Finally, the investigated condition was 0.5 bar boosted and the Air to Fuel Ratio (AFR) was close to stoichiometry.

Cycle-resolved digital imaging of the combustion process was carried out by an 8-bit CMOS camera with a 512x512-pixel sensor, 16x16 μm pixel size and 9 V/lux-second sensitivity at 550nm; the camera was coupled with 50-mm focus lens. Flame visualization was performed in full chip configuration at 5000 frames per second, corresponding to an acquisition interval of 2.4 CAD at 2000 rpm. The exposure time was fixed at 200 μs . For each engine condition, 100 sequences were acquired.

Macroscopic parameters related to flame morphology in the early stages of combustion were evaluated via image processing developed by Vision Assistant of National Instruments and detailed in [11]. The fundamental step of the procedure was the application of an automatic routine to binarize the images. Successively, the enflamed area and coordinates of the luminous center of mass were calculated. The areas were normalized to the equivalent circle with the engine bore as diameter. Then, the routine detected the flame boundaries by fixing the edge threshold equal to 1 and comparing the intensity value at each pixel with the intensities of its neighboring pixels. Finally, the numerical procedure evaluated the local curvature from the flame front by selecting a 5x5 pixel region of interest (or kernel) [18]. The curvature represents the inverse radius of the circle inscribed by a cubic b-spline at each edge point. In order to obtain a mean value of the curvature the average of the absolute values was calculated and then divided by the total number of points of the flame contour related to each image.

3D CFD SIMULATIONS

The 3D CFD analyses presented in this paper are carried out by means of a customized version of STAR-CD v4.22, licensed by SIEMENS.

The 3D domain covers the combustion chamber and the intake/exhaust ports. Thanks to geometrical and physical symmetry of the problem, only half of the domain is simulated, to reduce computational times. All the analyses are carried out in a RANS framework, adopting as closure model the k- ϵ RNG for compressible flows.

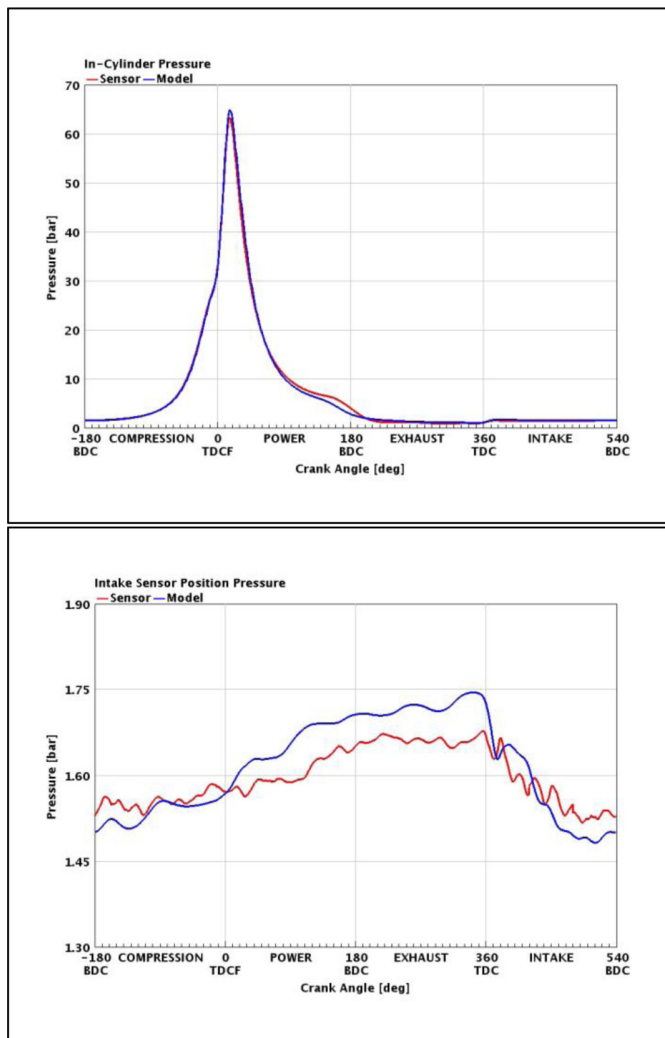


Figure 3. Comparison between measured ensemble average (red) and simulated (blue) pressures inside the cylinder (top) and in the intake manifold (bottom).

A purposely developed 1D engine model is used to simulate the whole engine test bench layout, from the intake air conditioning system to the exhaust chimney discharging burnt gases into the atmosphere. Intake conditions for this model carefully match those of the air conditioning system feeding the engine and replicating the presence of the turbocharger unit. Exhaust boundary conditions are imposed as measured ambient pressure and temperature. The model has been calibrated against experiments for a motored naturally aspirated operating point. Then, in order to calibrate the model in

firing conditions as well, a heat release rate profile is calculated from the ensemble average of the measured pressure traces using a standalone pressure analysis procedure.

As visible in Figure 3, the 1D model is reliable enough to generate boundary conditions for the 3D simulations. In particular, in the top part of Figure 3, the red and blue lines represent the ensemble average experimental pressure trace inside the cylinder over 200 consecutive experimental cycles and the numerical one, respectively. In the bottom part, the same comparison is reported for a fast response pressure sensor placed inside the intake manifold.

Instantaneous time-varying pressure and temperature profiles at the intake and exhaust ports are then extracted from the 1D model and applied at the 3D domain boundaries.

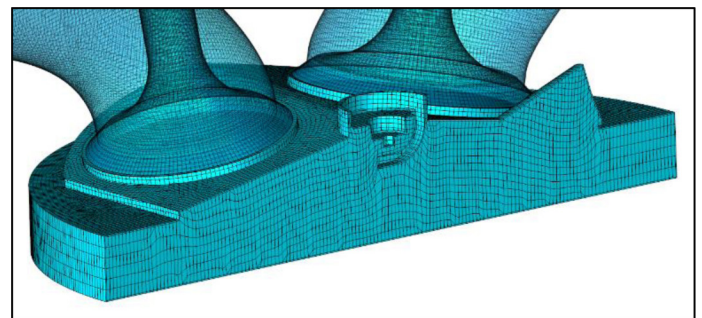


Figure 4. 3D computational domain and grid.

A close-up view of the computational mesh used in the 3D simulations is reported in Figure 4 for the TDC piston position. As visible, the regions around the spark plug and the injector are carefully meshed in order to preserve the consistency with the experiments. The grid counts around 800'000 cells at TDC and 1'830'000 cells at BDC.

Spray, Combustion and Knock Modelling

The liquid spray is modeled using a Lagrangian approach, where the fuel atomization is replaced by a distribution of numerical parcels whose size is represented by a purposely-calibrated Rosin-Rammler function and whose velocity is derived in relation to the nozzle diameter by means of a prescribed experimental instantaneous mass flow rate. The effective nozzle diameter, used to estimate the spray characteristics at the nozzle exit, is evaluated using the Kuensberg 1D model [19]. Secondary break-up and droplet-droplet interaction are accounted for using a dedicated method described in [20]. In this simulation, combustion is modeled with ECFM-3Z [21] model, which has been widely used in previous publications by the authors [22, 23] and which has demonstrated the capability to simulate partially premixed as well as autoigniting combustion events. Regarding spark ignition, it is modeled with the Imposed Stretch Ignition Model (ISSIM) [24, 25], which represents an Eulerian approach to the modelling of spark ignition and initial flame kernel growth. In this model, an electrical circuit model is used to initialize a first amount of burnt gas mass deposited at the spark. Then, the kernel growth rate is ruled by the flame surface density equation in

the same formalism as that used in the ECFM combustion model family, conveniently modified to take into account the influence of the spark glow.

As for knock and wall heat transfer modelling, an in-house procedure developed and validated by the authors and described in detail in [23, 26] is adopted. The knock model consists of a variation of the synthetic Lafossas et al. model [27] based on an extended tabulation of autoignition delays for the adopted fuel. The calculations of AI delay tables are carried out through use of 0D chemical solver preliminary to CFD runs, based on a constant pressure reactor model. The independent variation of the physical variables driving end-gas reaction rate (namely; pressure, temperature, air-to-fuel ratio and EGR dilution) are independently varied at discrete steps, resulting in approx. simulated states 100'000. This database is queried by the CFD code for each fluid cell, for which a multi-linear interpolating procedure is carried out to calculate an interpolated AI delay time. The look-up table is fuel-tailored and it provides chemically-accurate AI times without solving any chemical reaction during the CFD run. The mechanism used for the Gasoline surrogate blend is the 143-species TRF (Toluene Reference Fuel) by Andrae et al. [28], based on a blend of n-Heptane/Toluene/iso-Octane suggested by the fuel supplier to reproduce the autoignition quality of the real fuel. The adopted modelling framework allows to relevantly preserve the computational efficiency of a 2-species model [2929] on one hand by improving the calculation accuracy of AI delay with respect to empirical correlations, on the other hand without solving transport equations for any intermediate chemical species considered in the mechanism.

RESULTS

As a starting point, results are presented for flame development for the first operating condition, i.e. 12 CAD bTDC spark advance. This condition is a knock-safe operating point in the experiments. Then, a spark sweep has been operated on the 3D model in order to simulate the 15 CAD bTDC spark advance. In this second condition, after a brief analysis of the flame development, the focus is shifted towards knock tendency.

Spark Advance 12 CAD

The validation of the 3D CFD simulation has been performed against the ensemble average of 200 consecutive cycles acquired at the test bench. In a RANS framework, three consecutive cycles have been simulated with the aim of avoiding incomplete convergence.

The results are reported in Figure 5, where the ensemble average of the experimental cycle is highlighted to ease the comparison against the simulated RANS cycle. As it can be seen, the simulated cycle well represents the behavior of the engine in terms of both in-cylinder pressure peak magnitude and phasing.

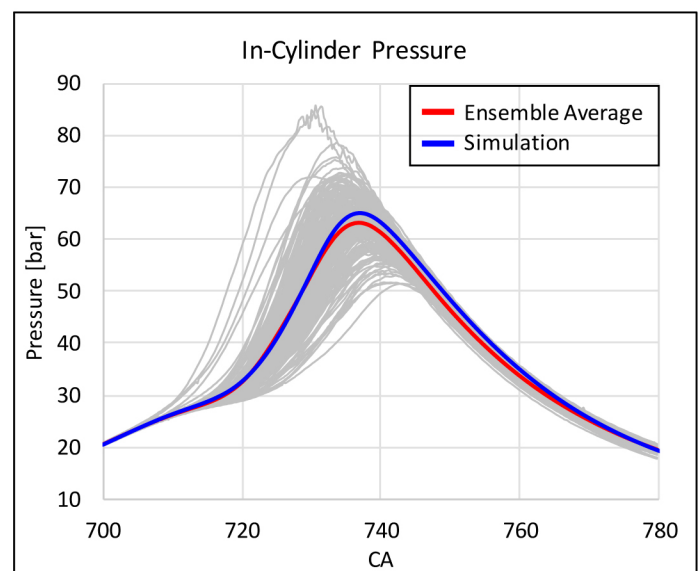
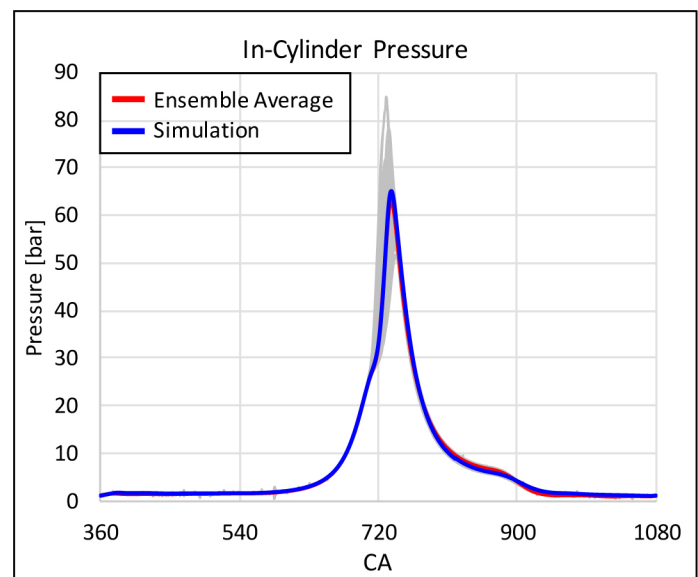


Figure 5. In-cylinder pressure: comparison between experimental data and CFD analysis (top) and combustion phase detail (bottom) for the SA12 condition.

Anyway, since this engine shows a high degree of cycle to cycle variability (CCV), a direct comparison of simulation and experiment is not trivial. In Figure 6 (top), the probability density function (PDF) of the Indicated Mean Effective Pressure (IMEP) for the measured cycles is presented, showing that 63.5% of cycles fall in a range of ± 0.5 bar of the simulated IMEP. As for the crank angle at which 50% of the gas mass fraction is burnt (MFB50%), 51.5% of the experimental cycles has a deviation of ± 1.5 CA around the simulated value. This is shown in Figure 6 (bottom).

Moreover, an increasing trend of the IMEP and maximum pressure level inside the cylinder during the recorded 200 consecutive cycles, justified by the increasing thermal status of the engine, which is in mild temperature condition at the beginning of the acquisition in order to avoid overheating of the unlubricated sealing rings of the piston. Nonetheless, IMEP variability evaluated through the

coefficient of variation (COV), can be considered as representative of a steady-state condition, given that it was around 2% for all investigated points.

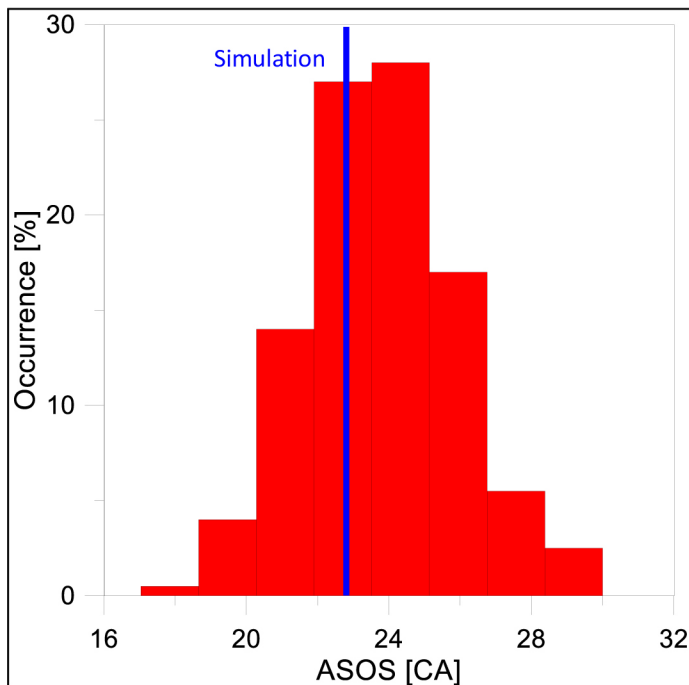
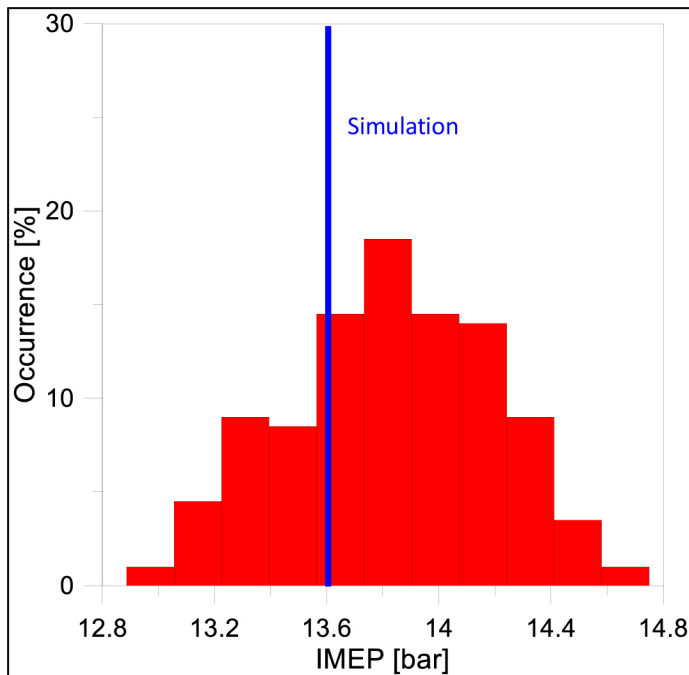


Figure 6. IMEP (top) and CAD@50%MFB (bottom) probability density function of experimental acquisition and CFD value.

Once the agreement of heat release rate has been found with calculations, a deeper analysis of the development of the enflamed area has been performed thanks to the optical access of the engine. Beside the aforementioned methodology of thresholding of the experimental optical data, on the CFD side the enflamed area has been considered as the surface surrounding the gas volume where the combustion progress variable of ECFM model exceeds a threshold

value of 0.1: this variable is defined as the mass fraction of fuel burnt in the computational cell and ranges from 0 to 1 for unburnt and fully burnt gases, respectively. Cells of the computational domain where the progress variable is lower than 0.1 (i.e. less than 10% of fuel burned) are considered not yet properly enflamed, while cells in which its value is higher than 0.1 are considered part of the enflamed region. Sensitivity analysis for the choice of the threshold value was preliminarily carried out, revealing low impact of the chosen value on the enflamed volume for values between 0.05 and 0.5. Regardless the specific choice, such method leads to a binarization of the flame images similar to the one performed on the optical acquired cycles.

It is important to point out that the CMOS camera images represent an integration through the optical path of the emitted light towards the camera sensor (along the cylinder axis). This means that the measured surface is not the actual enflamed one, but the footprint of the enflamed volume on the piston face. For consistency reasons, a similar procedure has been carried out in CFD to flatten the flame front surface as seen from the piston crown.

Experimental and simulated areas are then calculated from binarized images using the same process, which counts the enflamed pixels and normalizes the value using the cylinder bore.

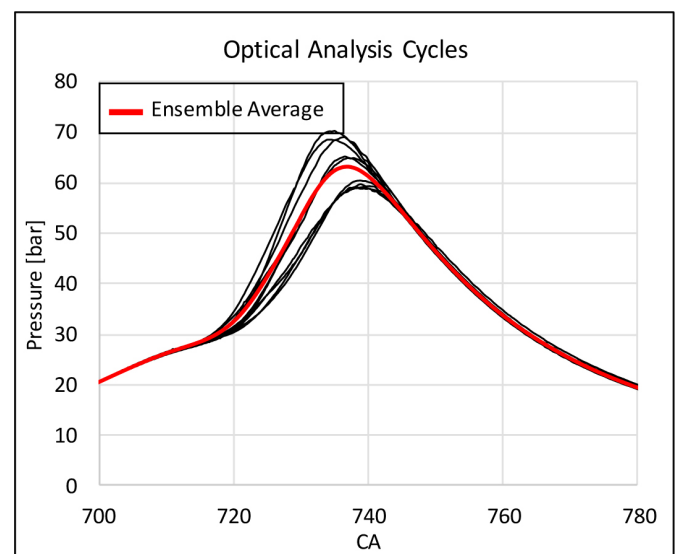


Figure 7. In-cylinder pressure trace for the cycles chosen for the optical flame analysis.

To ensure consistency with the adopted RANS framework, the procedure has been performed selecting 10 experimental cycles, plotted in Figure 7, representing faster-than-average, slower-than-average and close-to-average cycles.

Results of the comparison between simulated and experimental normalized ensemble averaged area are presented in Figure 8. In this figure, the dotted/dashed black line represents the optical window limit, which is 75% of the piston bore. This justifies the different slope between simulation and experiments once the flame approaches the optical limit. While CFD has its flame freely developing towards