Optimization of Pre-Chamber Geometry and Operating Parameters in a Turbulent Jet Ignition Engine

Viktor Dilber, Momir Sjerić *, Rudolf Tomic, Josip Krajnović, Sara Ugrinić and Darko Kozarac

Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Ivanu Lučiča 5, 10002 Zagreb, Croatia; viktor.dilber@fsb.hr (V.D.); rudolf.tomic@fsb.hr (R.T.); josip.krajnovic@fsb.hr (J.K.); sara.ugrinic@fsb.hr (S.U.); darko.kozarac@fsb.hr (D.K.)
* Correspondence: momir.sjeric@fsb.hr; Tel.: +385-1-6168-144

Abstract: A turbulent jet ignition engine enables operation with lean mixtures, decreasing nitrogen oxide (NOx) emissions up to 92%, while the engine efficiency can be increased compared to conventional spark-ignition engines. The geometry of the pre-chamber and engine operating parameters play the most important role in the performance of turbulent jet ignition engines and, therefore, must be optimized. The initial experimental and 3D CFD results of a single-cylinder engine fueled by gasoline were used for the calibration of a 0D/1D simulation model. The 0D/1D simulation model was upgraded to capture the effects of multiple flame propagations, and the evolution of the turbulence level was described by the new K-ε turbulence model, which considers the strong turbulent jets occurring in the main chamber. The optimization of the pre-chamber volume, the orifice diameter, the injected fuel mass in the pre-chamber and the spark timing was made over 9 different operating points covering the variation in engine speed and load with the objective of minimizing the fuel consumption while avoiding knock. Two optimization methods using 0D/1D simulations were presented: an individual optimization method for each operating point and a simultaneous optimization method over 9 operating points. It was found that the optimal pre-chamber volume at each operating point was around 5% of the clearance volume, while the favorable orifice diameters depended on engine load, with optimal values around 2.5 mm and 1.2 mm at stoichiometric mixtures and lean mixtures, respectively. Simultaneous optimization of the pre-chamber geometry for all considered operating points resulted in a pre-chamber volume equal to 5.14% of the clearance volume and an orifice diameter of 1.1 mm.

Keywords: pre-chamber; lean combustion; turbulent jet ignition; 0D/1D model; optimization; efficiency

1. Introduction

Electric mobility represents a long-term solution widely promoted by governments all over the world to satisfy more and more rigorous regulations concerning exhaust gas emissions from internal combustion (IC) engines [1]. Due to the high cost of ownership, long charging times and low driving autonomy of battery electric vehicles (BEV) compared to vehicles powered by conventional IC engines, BEV still have low contribution on the vehicle market [2]. Alternative powertrain systems, such as hybrid electric vehicles (HEV) and advanced combustion systems based on burning ultra-lean mixtures, represents a short-term solution to cover the gap in the transition from conventional IC engines to fully electric drivetrains.

The application of lean burning mixtures can increase engine brake thermal efficiency up to 49%, especially when combined with an electric compressor [3], while reducing raw emissions of nitrogen oxides (NOx) up to 92% [4] compared to conventional IC engines. There are several lean burn combustion concepts that can be adopted in IC engines, such as homogeneous charge compression ignition (HCCI) [5], spark assisted compression ignition (SACI), reactivity-controlled compression ignition (RCCI), jet-controlled
compression ignition (JCCI) [6] and pre-chamber spark-ignited (PCSI) engines. In the last few years, spark-ignited (SI) engines equipped with active or passive pre-chambers have attracted a lot of research work because this concept can easily be integrated into the existing engine architectures of conventional [7] or hybrid powertrains [3]. In such engines, the combustion process is initiated by the discharge of a spark in a small pre-chamber volume, and hot turbulent jets that are formed from the pre-chamber ignite the lean mixture in the main chamber. Hence, engines that use such an ignition concept are usually called turbulent jet ignition (TJI) engines [8]. The geometrical parameters of the pre-chamber, such as the volume and number of pre-chamber nozzles, and its orientation and diameter, affect the lean ignition limit, combustion stability, emissions, and, consequently, engine performance as well [9]. The total number of parameters (operating and geometrical) that affect engine performance is increased compared to conventional SI engines, and the application of numerical simulations can be a useful approach in defining the most favorable parameters that result in the best engine performance.

The influence of pre-chamber design on the mass transfer between the passive pre-chamber and main chamber was investigated numerically using 3D CFD simulations [7]. In that study, it was found that a favorable charge of the pre-chamber can be achieved during the compression stroke, while better scavenging from residual gases could be achieved during the expansion stroke by the addition of chambers near the pre-chamber nozzles. The efficiency and raw emissions from passive PCSI engines fueled by natural gas were investigated in [10] by using the strategy of cooled exhaust gas recirculation (EGR). The application of EGR decreased the indicated efficiency and NOx emissions, while CO emissions slightly increased. The compromise solution between a minor drop in indicated efficiency (around 1%) and a significant reduction of NOx emissions (up to 50% compared to operation without EGR) can be achieved with the operation of 10% cooled EGR. The experimental evaluation of advantages from combustion in an un-scavenged TJI engine fueled by natural gas was made in [11]. It was confirmed that TJI demonstrates more stable combustion compared to conventional SI combustion when the spark timing and excess air ratio are modified. In addition, the study confirms that EGR decreases NOx emissions, while lean mixtures decrease exhaust temperatures, which reduces the conversion efficiency of the three-way catalyst. The usage of a passive pre-chamber extends the knock limit significantly when compared to a conventional SI engine, which can be even further extended with an active pre-chamber [12]. A 3D CFD analysis of a passive PC design for a two-stroke engine was published in [13]. Two variants of pre-chambers, which have the same volume but different numbers of nozzles (6 or 8 nozzles), were analyzed. It was found that the PC with 8 nozzles resulted in better air-fuel mixture homogeneity and lowered residual gas fractions due to a more favorable ratio between PC volume and height.

The integration of an active PC on a rapid compression-expansion machine was made, and the analysis of flame development was performed with zero-dimensional turbulence and flame speed model [14]. Different air excess ratios in the PC were investigated, and it was found that modification of the air excess ratio from 0.9 to 1.1 reduced flame speed by 40%, indicating the importance of controlling the air-to-fuel ratio in the PC. The influence of injection parameters and different PC geometries on a TJI engine’s efficiency and emissions were investigated experimentally in [4]. Several different PC volumes and numbers of nozzles were studied with variations in injection timings. It was concluded that injection timing in the PC around the bottom dead center was the most favorable in terms of reduced emissions and higher efficiency, while the best efficiency was achieved with the smallest PC volume, which had one central nozzle and an MC air excess ratio of 1.5. At such operating conditions, the reduction of NOx emissions was 92% compared to the stoichiometric mixture, and it could be even higher (up to 99%) with the additional dilution of the mixture. An active PC can significantly extend the dilution of the mixture compared to an un-fueled PC [15], where the injected PC fuel is critical for combustion stability [16]. Numerical simulations with detailed chemical kinetics were
adopted to evaluate the effect of different temperatures in the active PC of a TJI engine [17]. For initial PC temperatures above 1200 K, auto-ignition and supersonic flow in the PC can occur, which indicates that temperature conditions in the PC should also be controlled to achieve stable combustion and engine durability. An optical engine equipped with an active PC fueled by natural gas was used in [18] to investigate different excess air ratios in the MC on combustion properties. The optical images confirmed that a local rich mixture is formed around the PC location in the MC because a small amount of mixture flows out during the initial combustion stage in the PC. It was also found that flames propagate to the MC asymmetrically, especially if the PC mixture is not completely mixed or because of intense turbulence caused by fuel injection and stochastic ignition, causing jets to emerge from the pre-chamber at different times. The optical diagnosis of PC jets and combustion in the MC was made in [19], where two rows of orifices were applied. Experimental results showed that the upper orifices have much weaker jets than lower orifices, which indicates the importance of the orifice location. The flame images from the optical images also confirm that the ultra-lean mixture has unburned zones located around orifices and between two adjacent jet flames that become larger as the excess air ratio becomes higher. The influence of three different orifice diameters on a constant PC volume with 6 orifices in an active TJI engine fueled by natural gas on engine performance was experimentally investigated in [20]. It was shown that the best gross indicated efficiency of 44% can be achieved with an MC air excess ratio equal to 2.0 and an orifice diameter of 1.6 mm, while the lowest NOx emissions were achieved with an orifice diameter of 1.4 mm.

The literature overview indicates that pre-chamber geometries in TJI engines are usually designed by a trial and error method, where several pre-chamber designs are investigated experimentally, and then TJI engine performance is compared [9,21]. Since the pre-chamber geometry includes several parameters, such as volume, neck diameter, orifice diameter, orifice number and orientation, several pre-chamber variants used within the trial and error method cannot guarantee that the most favorable design is really found. Notably, 3D CFD simulations can be a useful tool to investigate specific local phenomena, i.e., the distribution of the air excess ratio and/or residual gases in the pre-chamber. Due to the relatively high computational time and the large number of pre-chamber variants that should be investigated, 3D CFD simulations are also not an appropriate solution for finding the most favorable pre-chamber geometry [21]. Therefore, in this study, a validated 0D/1D simulation model was used to optimize pre-chamber geometry and operating parameters.

The upgraded 0D/1D simulation model of an experimental single-cylinder engine was validated with initial experimental combustion results and 3D CFD results of cold flow. After that, the optimization of the pre-chamber geometry (volume, neck and orifice diameter) and operating parameters (PC injected fuel mass and spark timing) was performed in two different ways over 9 operating points that represented different engine speeds and loads. Within the first step, the optimization of pre-chamber geometry and operating parameters was made individually for each operating point, resulting in optimal pre-chamber geometry for individual operating points. Such an approach is applicable to engines that have a naturally restricted operating range, i.e., the drive of the electric generator, which requires constant engine speed. In the second step, the optimization of pre-chamber geometry and operating parameters was performed simultaneously for all operating points considered within the analysis, and the optimization result is the compromise solution for the defined operating area of the engine, which, on average, provides the most favorable performance. Such an approach for the definition of pre-chamber geometry can be applied on TJI engines that will be operated in a wide range of engine operating conditions, i.e., for vehicle powertrains.

2. Research Methods
The presented research data in this study include experimental and numerical results. The combustion results of the experimental TJI engine were used for the calibration of an upgraded 0D/1D simulation model. Before that, the verification of the newly integrated $k$-$\varepsilon$ turbulence model was made using 3D CFD results of in-cylinder flow. Once the 0D/1D simulation model was calibrated, the optimization of the pre-chamber geometry and operating parameters was performed using a genetic algorithm. In the following sections, descriptions of the experimental setup and numerical models are given with emphasis on new components and features required for the operation and simulation of TJI combustion.

2.1. Experimental Setup

The measurement of engine operation was made on the experimental setup at the Laboratory of IC Engines and Motor Vehicles of the Faculty of Mechanical Engineering and Naval Architecture at the University of Zagreb. The experimental setup was developed and upgraded over several years. The base of the setup is a modified single-cylinder engine Hatz 1D81 connected to an AC dynamometer and equipped with multiple measurement devices. The schematic layout of the experimental setup is given in Figure 1, and details of the setup and the measurement equipment can be found in [22].

![Layout of experimental setup](image)

Figure 1. Layout of experimental setup.

To perform the experiments required for this work, the existing research engine was significantly modified, and additional systems were added to the experimental setup. The modifications include a decrease in the compression ratio (from the original 20.5 to 12.8) and the new ignition and fuel injection system (low and high pressure). Although its original geometry suits the compression ignition combustion regime, the selected Hatz 1D81Z engine has a robust and simple design, and due to the air cooling system, it can be easily modified and upgraded for different investigation purposes and different combustion modes. One intake and exhaust valve ensure enough free space on the cylinder head to easily mount the main chamber pressure sensor (AVL GH14DK) and active pre-chamber ignition system used in this study. A Maximator S100 pump driven by compressed air was added to the experimental setup for obtaining the high-pressure fuel injection in the PC, while a pressurized fuel tank and standard passenger car port fuel injection were used for providing fuel for the main combustion chamber. The main data of the experimental engine after modification are specified in Table 1.

Table 1. Specifications of 1-cylinder research engine.
The most significant part of the modified experimental engine was the developed pre-chamber (PC) ignition system (14), representing the modular design with a possible variation of the PC volume from 3.4% to 5.4% of clearance volume. More details about the developed PC ignition system are given in the next chapter.

Pre-Chamber Design

All pre-chamber components and their respective positions are shown in Figure 2. The PC system consisted of a housing and orifice cap that formed the ignition chamber. The PC housing contained a Borg-Warner low-flow injector for direct gasoline injection, an NGK EPR10ES spark plug with an M8 thread and an AVL GH14DK pressure sensor.

Figure 2. Components of the developed pre-chamber ignition system.

The orifice cap was held in position by a positioning pin and a locking nut, and its position must be unambiguous because the PC system was mounted into the cylinder head at an angle of 20° to the cylinder axes (Figure 3), with orifice holes being asymmetrical in relation to the main PC axis so that the TJI jets were symmetrical to the piston bowl.
Figure 3. Pre-chamber position in cylinder head.

The PC ignition system was defined by the shape of the orifice cap and was formed by the inner contour of the orifice cap and adjacent housing surfaces. The sealing of the ignition chamber was achieved by the locking nut clamping force and locking nut thread surface.

The PC system was held in place by a bolted PC system housing clamp, and the main combustion chamber was sealed by a copper washer (Figure 3). The pre-chamber volume, orifice dimensions and arrangement greatly affect combustion efficiency. The designed pre-chamber system offered the possibility to change the pre-chamber volume, orifice diameter, the number of orifices and orifice angle by changing the orifice cap. The design of the PC system was governed by the constraints imposed by the research engine combustion chamber design, cylinder head layout and manufacturing possibilities at disposal. The target was to keep the main parameters of the ignition chamber of the PC system within the limits suggested in the literature [9,23]. The dimensions of the initial orifice cap are listed in Table 2.

Table 2. Specification of the initial pre-chamber geometry.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orifice diameter ((d_{orf}))</td>
<td>1.3 mm</td>
</tr>
<tr>
<td>Number of orifices ((n))</td>
<td>6</td>
</tr>
<tr>
<td>Orifice angle ((\gamma))</td>
<td>140°</td>
</tr>
<tr>
<td>Neck diameter ((d_{nc}))</td>
<td>7 mm</td>
</tr>
<tr>
<td>Pre-chamber volume ((V_{pc}))</td>
<td>2400 mm³</td>
</tr>
<tr>
<td>Volume ratio (\frac{V_{pc}}{V_{cit}})</td>
<td>4.2%</td>
</tr>
<tr>
<td>Cross-section area (\left( A_{orf} = \frac{d_{orf}^2 \pi}{4} \cdot n \right) )</td>
<td>7.96 mm²</td>
</tr>
<tr>
<td>Orifice area to volume ratio (\left( \frac{d_{orf}^2 \pi}{4} \cdot n \right) )</td>
<td>0.033 1/cm</td>
</tr>
<tr>
<td>Orifice diameter to length ratio (\frac{d_{orf}}{l_{orf}})</td>
<td>0.37</td>
</tr>
</tbody>
</table>

\(^{(1)}\) The volume ratio is for engine compression ratio CR = 12.8. In this case the engine clearance volume is \(V_{cl} = 60,689.9 \text{ mm}^3\). \(^{(2)}\) The length of the orifice is \(l_{orf} = 3.5 \text{ mm}\).

The volume ratio surpassed the suggested limit (4.2% compared to the 2–3% of the engines clearance volume), but the orifice area to PC volume ratio (0.03–0.04 L/cm) and the length to diameter ratio of the orifice (around 0.5) were met with the applied initial design. The initial PC ignition chamber was sized according to an engine compression
The design of the ignition chamber was greatly assisted by the CFD simulations, which were used for the assessment of the fuel mixing quality in the proximity of the spark plug [24]. The initial orifice cap was used in the initial measurements of the research engine. The measured in-cylinder and pre-chamber pressure, intake and exhaust manifold pressures, and air and fuel mass flows were used as reference data for the validation of 3D CFD and 0D/1D simulation models, as briefly described in the following sections.

2.2. Numerical Models

The presented experimental setup is not equipped with the measurement of in-cylinder flow data (e.g., in-cylinder velocity and turbulence) that are required for the correct calibration of simulation models. Since in-cylinder velocity and turbulence always have spatial features, a 3D CFD simulation model of the experimental engine was made with imposed measured boundary conditions at the intake and exhaust sides. Cold flow simulations for two different engine speeds were performed, and averaged results over the cylinder domain were used for the verification of the 0D turbulence model integrated into the cycle simulation model.

2.2.1. 3D CFD Simulation Model

The full-cycle 3D CFD simulation model of the experimental engine with the initial pre-chamber design, made in AVL Fire and shown in a previous study [24], was calibrated based on the newly obtained experimental results. A mesh sensitivity study was performed in order to achieve a good compromise between the model accuracy and the computational effort, and the final mesh obtained is shown in Figure 4.

![Figure 4. Computational mesh of the experimental engine with a pre-chamber, (a) during valve overlap at TDC, (b) and at FTDC. (c) Cross section of the pre-chamber.](image-url)
sizes for the characteristic regions of the entire computational domain are shown in Table 3, along with the maximum number of cells for the four distinctive moving mesh periods.

Table 3. Mesh refinement setup and the resulting mesh size.

<table>
<thead>
<tr>
<th>Selection</th>
<th>Cell Size [mm]</th>
<th>Maximum Number of Cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intake port</td>
<td>2.8</td>
<td>234,359</td>
</tr>
<tr>
<td>Intake seat—CA dependent</td>
<td>0.175–0.7</td>
<td></td>
</tr>
<tr>
<td>Exhaust port</td>
<td>2.8</td>
<td>264,547</td>
</tr>
<tr>
<td>Exhaust seat—CA dependent</td>
<td>0.175–0.7</td>
<td></td>
</tr>
<tr>
<td>Pre-chamber</td>
<td>0.7</td>
<td></td>
</tr>
<tr>
<td>Orifices</td>
<td>0.175</td>
<td>126,350</td>
</tr>
<tr>
<td>Spark plug (surface—1 mm depth)</td>
<td>0.175</td>
<td></td>
</tr>
<tr>
<td>Spark plug proximity (sphere—3 mm)</td>
<td>0.35</td>
<td></td>
</tr>
<tr>
<td>Main chamber</td>
<td>1.4</td>
<td>728,997</td>
</tr>
<tr>
<td>Jet penetration cone refinement</td>
<td>0.7</td>
<td></td>
</tr>
</tbody>
</table>

The imposed boundary conditions were obtained from the reduced 0D/1D simulation model, now calibrated according to the experimentally obtained results, and the procedure was the same as already explained in [24]. The entire solver setup was also explained in the previous study [24] and was kept unchanged. Only a single combustion model constant was recalibrated to achieve a good fit between the simulated and experimentally obtained pressure curves. Additionally, the heat transfer model was changed to the Han–Reitz model, as the previously used Standard Wall Function model underestimated the heat losses.

2.2.2. 0D/1D Simulation Model

The optimization process in this study was made by using a reduced 0D/1D simulation model that was made in AVL Boost v2013.2, as shown in Figure 5. The short intake pipe (1) has a length of 60 mm, and the measured intake pressure profile from the experimental setup was imposed on the intake system boundary (SB1) by means of the engine interface element (EI1). The intake temperature at SB1 was set to a constant value measured by the intake thermocouple element used on the experimental testbed. Since the port fuel injector on the experimental engine was located 320 mm upstream of the intake valve, the injector element was not used in the simulation model, and the mass fraction of fuel vapor was defined at SB1 to achieve the desired air excess ratio at the main chamber for each operating point.
The exhaust side is described by a pipe element with a length of 70 mm that corresponds to the location of the thermocouple on the experimental engine. Hence, constant exhaust pressure and temperature were set to SB2 for each operating point. The heat transfer was calculated at the intake and exhaust pipes using the Colburn model, while the pipe wall temperatures were set to 70 °C and 200 °C, respectively.

The zero-dimensional (0D) volumes were considered for both combustion chambers (pre-chamber and main chamber), which were connected via several equal orifices. The state in the pre-chamber volume was calculated with the original quasi-dimensional combustion model available in AVL Boost v2013.2, while the main chamber state was described with a new quasi-dimensional combustion model, including the integration of full K-\(k-\varepsilon\) turbulence and the multiple flame propagation model [25,26]. Since the new quasi-dimensional combustion model was already described in [24], it will not be given in this paper, while the governing differential equations and upgrade of the full K-\(k-\varepsilon\) turbulence model can be seen in Appendix A. This turbulence model is applied only for the main chamber, and it is extended to capture the additional production term (see Equation (A1)) caused by turbulent jets occurring with the development of the combustion process in the pre-chamber volume. The integration of the full K-\(k-\varepsilon\) turbulence model in a quasi-dimensional combustion model for PCSI combustion eliminates the necessity of case-by-case tuning of the turbulence model constant that was used in the previous study [24]. A single set of K-\(k-\varepsilon\) turbulence model constants was used for all analyzed operating points.

2.3. Optimization Methodology

The optimization of pre-chamber geometry was made using the 0D/1D simulation model in AVL Boost. Before the optimization process, the 0D/1D simulation model was calibrated with 3D CFD flow results and, after that, with initial experimental results at different engine operating conditions, as described in previous sections.

Figure 6 shows the operating points used in the optimization and calibration of the 0D/1D model. The calibration operating points are shown with yellow squared markers and represent the available experimental results obtained with the application of the initial pre-chamber design. It can be noted that the calibration position at OP5 contains several results with different spark timing, i.e., spark sweep.
The optimization operating points cover enhanced engine speed and load variation, as can be seen in Figure 6 (red circle markers). The maximum engine speed was set to 2000 rpm because of the limitations of the experimental engine. Additionally, high-efficiency engines usually operate at low engine speeds because there is an increase in losses with increased engine speed. At each engine speed, three engine loads were considered by the modification of the air excess ratio in the main chamber, resulting in 9 operating points in total. The stoichiometric mixture (\(\lambda_{MC} = 1\)) in the main chamber means that passive pre-chamber operation is achieved, and there is no added fuel in the pre-chamber.

The optimization was made using a genetic algorithm available in AVL Boost v2013.2. The optimization variables are the pre-chamber neck diameter, nozzle diameter, injected pre-chamber fuel mass and spark timing. In the first optimization approach (individual optimization), the objective function was set to minimize the indicated specific fuel consumption (ISFC) for each optimization operating point, while the occurrence of knock was considered a constraint and defined with the required octane number of fuel. This means that optimization was performed for each individual optimization operating point and resulted in a set of optimal geometrical and operating parameters, one for each operating point. In the second optimization approach (simultaneous optimization), the objective function was set to minimize the mean value of ISFC for all operating points while also considering the knock occurrence as a constraint. This means that optimization was performed on all operating points simultaneously, resulting in a single PC geometry for the defined operating range of the engine and optimal operating parameters for each operating point. To enable the simultaneous optimization that will result in a universal PC geometry along with the case-by-case optimized operating parameters, the definition of the optimization variables needs to be set up accordingly. The geometrical variables were defined once, and the single optimized solution was achieved for all operating points. On the other hand, the variables for spark timing and injected fuel mass were defined for each of the 9 considered operating points separately. Such an approach significantly increases the total variable count and, consequently, the required number of generations in the algorithm, but the optimization tool used in this study does not currently allow for a different approach.

Since the modification of pre-chamber volume on the experimental setup used in this study can be made by the change of neck diameter, the correlation between neck diameter and pre-chamber volume was derived. The dependency of pre-chamber volume on neck diameter, which has values from 5 to 9 mm, is plotted in Figure 7. Black circle markers show results of pre-chamber volumes defined in the CAD model, while the red dotted line represents the polynomial second-order fit curve defined by the expression given in

![Figure 6. Positions of calibration and optimization operating points in experimental engine map.](image-url)
Figure 7. The definition of the correlation function between neck diameter and pre-chamber volume reduces the optimization variables in terms of pre-chamber geometry. Hence, the pre-chamber neck diameter was optimized with imposed lower and upper limits set to 5 and 9 mm, respectively.

![Image](image-url)

**Figure 7.** Definition of total pre-chamber volume as a function of neck diameter.

3. Results and Discussion

In this section, first, the validation and calibration results of the 0D/1D simulation model are presented. The verification of the newly integrated turbulence model in the 0D/1D simulation model was made using 3D CFD results from the cold flow. The calibration of the combustion model with multiple flame propagations in the 0D/1D simulation was made using experimental results achieved with the initial pre-chamber geometry. After that, the optimization results of individual and simultaneous optimization of pre-chamber geometry are given. At the end of this section, the methodology for the definition of the final and most favorable pre-chamber design is described and discussed depending on the potential engine application.

3.1. Validation and Calibration of 0D/1D Simulation Model

The calibration of the 0D/1D simulation model with integrated new features (multiple flame propagation and K-\( k-\varepsilon \) turbulence model) was made by using 3D CFD and experimental results over several calibration points. Calibration points are partially described in the research methods section, and an overview of the calibration points is given in Table 4. Calibration points include variations of the engine speed, spark timing and air excess ratio.

| Table 4. Details of calibration operating points with initial pre-chamber design. |
|----------------------------------|---|---|---|---|---|
| **Name** | CP1 | CP2 | CP3 | CP4 | CP5 |
| \( n \) (rpm) | 1200 | 1600 | | | |
| \( \lambda \) (-) | 1.60 | 1.60 | 2.15 | | |
| ST (° BTDC) | 6 | 14 | 12 | 10 | 22 |

Since a newly integrated K-\( k-\varepsilon \) turbulence model is a single-zone model, and the experimental results do not contain results of flow and turbulence, the calibration of model constants was first performed by comparison with 3D CFD cold flow simulation results. The influence of combustion and subsequent high-velocity jet penetration on turbulence level in the main chamber was then calibrated simultaneously with other 0D combustion model constants to achieve a good agreement between simulated and experimentally obtained pressure curves. Since in the 0D/1D simulation model, only the specific turbulent kinetic energy is used in the calculation of the heat release rate, the comparisons of specific
turbulent kinetic energies for two engine speeds (1200 rpm and 1600 rpm) are given in Figure 8. Although the K-ke turbulence model is a single-zone model, if properly calibrated, it matches well with the reference results from the 3D CFD simulation. The most important period for good prediction of in-cylinder turbulence is around firing top dead center (FTDC) when combustion takes place and when calculated turbulence intensity is used for the calculation of turbulent flame speed in the 0D/1D simulation model.

**Figure 8.** Verification of turbulence model—comparisons of specific turbulent kinetic energies at 1200 rpm and 1600 rpm.

Experimental pressure traces for the pre-chamber and main chamber plotted with black dashed lines in Figure 9 are averaged results over 300 consecutive cycles. Simulation results of the 0D/1D model are shown with solid red lines. The top diagrams refer to the pre-chamber pressure, while the bottom diagrams of Figure 8 show pressure profiles in the main chamber.

**Figure 9.** Experimental and 0D/1D simulation results of pressure traces in pre-chamber and main chamber for several calibration points.
A single set of turbulence and combustion model parameters was defined within the 0D/1D model calibration, while the lower heating value of fuel was reduced as the air excess ratio was increased. If the lower heating values are not changed, the pressure profiles in the pre-chamber and main chamber for CP5 are overpredicted. In real engine operations with such a lean mixture ($\lambda > 2$), incomplete combustion will be significant due to the lowering of the laminar flame speed and flame quenching. Since the flame quenching effect cannot be captured by the applied simulation model, the reduction of the lower heating value of the fuel is the applied method that compensates for the lack of the simulation model in terms of flame quenching. The reduction factor for lower heating value is equal to combustion efficiency, and it was calculated from measured raw emissions. It is equal to 98.3%, 96.4% and 85.3% for $\lambda = 1$, $\lambda = 1.6$ and $\lambda = 2.2$, respectively. The calibrated simulation model matched well with the experimental pressure profiles, especially in the main chamber, which is responsible for the indicated work. The same approach was used in the optimization by defining the fixed value of combustion efficiency for each of the 9 optimization points since the excess air ratio in the main chamber was predefined rather than used as the optimization variable.

Since the objective function in the optimization algorithm was set to minimize the indicated specific fuel consumptions (ISFC) over 9 operating points, the ISFC result obtained from the calibrated simulation model was compared to the experimentally obtained result, as shown in Figure 10. It can be seen that a very good match is achieved with a single set of model constants, and, more importantly, the influence of spark timing and mixture dilution changes are captured correctly. The average accuracy of the simulated results for ISFC is 98.5%.

![Figure 10](image_url)  
*Figure 10.* Experimental and 0D/1D simulation results for indicated specific fuel consumption (ISFC) over calibration points.

In Figure 11, the calibration of knock prediction is shown by comparing the simulated octane number requirement and the experimentally obtained maximum amplitude of pressure oscillations (MAPO). The calibration point CP2 was identified during the post-processing of the experimental results as the operating point in which knocking is evident, while the calibration point CP3 was at the knock-limited spark timing. The simulation model correctly captured the knock-limited spark timing, as the required octane number simulated for the CP3 was equal to 95, which is the actual octane number rating of the fuel used in this study.
Figure 11. Comparisons of maximum amplitude of pressure oscillations (MAPO) and calculated fuel octane number (ON) from 0D/1D simulation.

The calibration results plotted in Figures 8–11 confirmed that the 0D/1D simulation model captures well the changes in engine operating parameters, such as engine speed, air excess ratio and spark timing. Hence, the applied simulation model can be used for the optimization of pre-chamber volume, nozzle diameter, injected pre-chamber fuel mass and spark timing while considering the limit of knock occurrence.

3.2. Optimization Results

In the commercial version of AVL Boost v2013.2, the optimization algorithm is integrated, which enables definitions of objective functions (responses), optimization variables and the selection of an optimization algorithm with specific settings. The optimization was made using the genetic algorithm with the default settings, except for the simultaneous optimization, where the number of generations was increased because of the simultaneous optimization of all 9 optimization points. The optimization settings, objective functions, and variables with their limits and constraints are shown in Table 5.

Table 5. Overview of optimization settings, objective functions, variables and constraints for individual and simultaneous optimization.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Distribution for crossover probability</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>Distribution for mutation probability</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>Crossover probability</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td>Mutation probability</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td>Population size</td>
<td>50</td>
<td></td>
</tr>
<tr>
<td>Number of generations</td>
<td>10</td>
<td>40</td>
</tr>
<tr>
<td>Objective function</td>
<td>min ISFC</td>
<td>min ISFC&lt;sub&gt;mean&lt;/sub&gt;</td>
</tr>
<tr>
<td>Neck diameter, d&lt;sub&gt;PC&lt;/sub&gt; (mm)</td>
<td>5 ≤ d&lt;sub&gt;PC&lt;/sub&gt; ≤ 9</td>
<td></td>
</tr>
<tr>
<td>Orifice diameter, d&lt;sub&gt;orf&lt;/sub&gt; (mm)</td>
<td>1 ≤ d&lt;sub&gt;orf&lt;/sub&gt; ≤ 3</td>
<td></td>
</tr>
<tr>
<td>Spark timing, ST (° CA BTDC)</td>
<td>42 ≤ ST ≤ −3</td>
<td></td>
</tr>
<tr>
<td>PC fuel mass, m&lt;sub&gt;LPC&lt;/sub&gt; (mg)</td>
<td>0 ≤ m&lt;sub&gt;LPC&lt;/sub&gt; ≤ 1.5</td>
<td></td>
</tr>
</tbody>
</table>

The overview of optimization results for individual and simultaneous optimization performed in this study is given in Table 6.
Table 6. Overview of optimization results for individual (A) and simultaneous (B) optimization of pre-chamber geometry and operating parameters.

<table>
<thead>
<tr>
<th></th>
<th>n (rpm)</th>
<th>A</th>
<th>Neck Diameter</th>
<th>Orifice Diameter</th>
<th>m_{\text{I,PC}} (mg)</th>
<th>ST (° CA BTDC)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>d_{\text{rc}} (mm)</td>
<td>d_{\text{orf}} (mm)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OP1</td>
<td>1200</td>
<td>2.2</td>
<td>8.50</td>
<td>1.01</td>
<td>1.049</td>
<td>17.3</td>
</tr>
<tr>
<td>OP2</td>
<td>1200</td>
<td>1.6</td>
<td>8.97</td>
<td>1.66</td>
<td>0.292</td>
<td>7.7</td>
</tr>
<tr>
<td>OP3</td>
<td>1200</td>
<td>1.0</td>
<td>8.76</td>
<td>2.34</td>
<td>-</td>
<td>1.6</td>
</tr>
<tr>
<td>OP4</td>
<td>1600</td>
<td>2.2</td>
<td>6.88</td>
<td>1.19</td>
<td>0.704</td>
<td>24</td>
</tr>
<tr>
<td>OP5</td>
<td>1600</td>
<td>1.6</td>
<td>8.76</td>
<td>2.65</td>
<td>0.333</td>
<td>11.25</td>
</tr>
<tr>
<td>OP6</td>
<td>1600</td>
<td>1.0</td>
<td>8.08</td>
<td>2.50</td>
<td>-</td>
<td>4.2</td>
</tr>
<tr>
<td>OP7</td>
<td>2000</td>
<td>2.2</td>
<td>8.92</td>
<td>1.31</td>
<td>0.832</td>
<td>31.7</td>
</tr>
<tr>
<td>OP8</td>
<td>2000</td>
<td>1.6</td>
<td>7.00</td>
<td>2.86</td>
<td>0.337</td>
<td>12</td>
</tr>
<tr>
<td>OP9</td>
<td>2000</td>
<td>1.0</td>
<td>8.02</td>
<td>2.60</td>
<td>-</td>
<td>7.3</td>
</tr>
</tbody>
</table>

Figure 12 shows the change in pre-chamber volume ratio for individually optimized operating points and for simultaneous optimization. The optimized pre-chamber volume ratio for lower engine speeds is higher (near the upper limit) than the volume ratio for higher engine speeds, while at the same time, the volume ratio is higher for lean mixtures except for a small drop in volume ratio for an engine speed of 1200 rpm, which is already near the upper limit for all three mixtures. For the simultaneous optimization, the optimized pre-chamber volume ratio is also near the upper limit.

Figure 12. Optimized pre-chamber volume ratio for individual and simultaneous optimization.

In Figure 13, the orifice diameters for each optimization point are plotted against the air excess ratio, and the orifice diameters for lean mixtures ($\lambda = 2.2$) are close to the lower limit, while the orifice diameters for the stoichiometric case have higher values. This is because small orifice diameters create stronger turbulent jets, which result in higher turbulence levels and combustion speed, while the bigger orifice diameters result in lower turbulence levels but also in lower residual gas concentration in the pre-chamber for the stoichiometric cases and $\lambda = 1.6$. The bigger orifice diameters also result in slightly lower heat losses because of lower combustion speeds. The contribution of engine performance at lean mixtures is the dominant one when performing simultaneous optimization, so the orifice diameter is at the lower limit for this approach of optimization.
When comparing the individual optimization results to the initial results, the combustion duration for $\lambda = 2.2$ is decreased by 39.0%, 35.1% and 16.3% for engine speeds of 1200 rpm, 1600 rpm and 2000 rpm, respectively. For $\lambda = 1.6$ and $\lambda = 1.0$, the combustion duration is increased between 16.7% and 34.2%, depending on the operating point, because of the bigger orifices, but the scavenging of the pre-chamber is improved, and the residual gas concentration at spark timing is decreased between 7.8% and 45.3%. The decrease in combustion speed is also responsible for the reduction in heat losses, ranging between 0.2% and 13.1%.

When comparing the simultaneous optimization results to the initial results, the combustion duration for $\lambda = 2.2$ is also decreased by 41.5%, 34.8% and 9.9% for engine speeds of 1200 rpm, 1600 rpm and 2000 rpm, respectively. In this approach, for $\lambda = 1.6$ and $\lambda = 1.0$, the orifice diameters are smaller, so the combustion duration for OP3 and OP6 are decreased by 2.3% and 1.7%, but for the other operating points, there is an increase in combustion duration. Because of the single geometry parameters (smaller orifices), the residual gas concentration in the pre-chamber is increased for all operating points between 2.3% and 34.7%, but the heat losses for $\lambda = 1.6$ and $\lambda = 1.0$ are reduced between 0.5% and 19.5%, except for OP6, where an increase by 1.0% can be observed. Because of an increase in residual gas concentration and heat losses, OP6 is the only operating point where no improvement in ISFC was achieved.

When changing the pre-chamber volume and the air excess ratio in the main chamber, it is important to adjust the injected fuel mass into the pre-chamber to achieve a favorable mixture for better ignition. When increasing the air excess ratio in the main chamber, the pre-chamber injected fuel mass also needs to be increased (Figure 14), except for the stoichiometric case, where passive pre-chamber operation is achieved. The injected fuel mass needs to be simultaneously optimized with the spark timing to achieve a favorable air excess ratio in the pre-chamber because the air excess ratio in the pre-chamber changes with the crank angle.
The most favorable air excess ratio in the PC at spark timing, for both optimization approaches, ranges between $\lambda = 0.9$ and $\lambda = 0.7$ at a global excess air ratio value of $\lambda = 2.2$, where $\lambda$ decreases with an increase in engine speed. At $\lambda = 1.6$, the most favorable air excess ratio in the PC at spark timing, for the individual optimization, ranges between $\lambda = 1.3$ and $\lambda = 1.2$, and for the simultaneous optimization, the values are between $\lambda = 1.46$ and $\lambda = 1.42$, where $\lambda$ decreases with an increase in engine speed. The difference in the optimal values between the two optimization approaches is due to the different orifice diameters, where the results of the simultaneous optimization have smaller orifice diameters. The difference in the optimal air excess ratio in the PC at $\lambda = 1.6$ is the reason why there is less injected fuel in the PC for the simultaneous optimization when compared to the individual optimization.

The optimized orifice cross-section area to pre-chamber volume ratio is plotted against the air excess ratio and shown in Figure 15. For the stoichiometric case, the optimized orifice area to pre-chamber volume is higher than the initial design because of the higher values of orifice diameters, which result in lower residual gas concentration. For lean mixtures, the ratio is at the lower limit because of the small orifice diameters, which result in higher turbulence levels. For the simultaneous optimization, the ratio is also at the lower limit because the contribution of engine performance at lean mixtures is dominant.
Figure 15. Optimized orifice area to PC volume ratio over individual and simultaneous optimization.

The results of the indicated specific fuel consumptions (ISFC) after the optimization are compared to the results of the initial pre-chamber design and are shown in Figure 16. For each operating point, an improvement in ISFC is achieved, ranging from 0.1% to 5.4%, with greater improvements in ISFC for leaner mixtures, except for OP6, where an 0.1% increase in ISFC can be seen for simultaneous optimization. This is not an issue because for the simultaneous optimization of geometrical and operating parameters for all operating points, it is less likely to achieve an improvement in ISFC for all points individually, but there is an improvement in the mean value of ISFC of all operating points.

In Figure 16, the comparisons of the octane numbers (ON) of the initial and the optimized results are shown because the knock occurrence was considered a constraint. Excessive knock combustion is not reached because the calculated ON is below 95.
The optimization results plotted in Figure 16 confirmed that the applied optimization methods can be used for the optimization of geometrical and operating parameters of a turbulent jet ignition engine by minimizing ISFC while considering the limit of knock occurrence.

3.3. Strategy for PC Geometry Selection from Optimization Results

By looking at the results of individual optimization of each optimization operating point, it is not clear which pre-chamber geometry would be optimal to cover the operating range of the engine. It is evident from the results that greater pre-chamber volume ratios \( (V_{pc}/V_k) \) are more favorable for all optimization operating points, especially for lower engine speeds. There is also a clear trend for picking the orifice diameters, where smaller diameters result in better fuel economy for leaner mixtures and bigger diameters for richer mixtures. However, this methodology could be used for the definition of the most favorable pre-chamber geometry for engines that have naturally restricted operating ranges, which operate in quasi-stationary conditions, i.e., the drive of an electric generator that requires a constant engine speed or a marine engine that operates at low engine speeds.

The second optimization approach (simultaneous optimization) of pre-chamber geometry and operating parameters of a turbulent jet engine can be used to find optimal and single geometry parameters applicable in a wider range of engine speeds and loads, i.e., for vehicle powertrains. Although the simultaneous optimization in this study gives good results, a simple mean value of ISFC in multi-point optimization might not be the best solution for the objective function because the probability of operation of a passenger car engine in each operating point of the engine map is not the same, and some operating points will be operated with higher frequency than some others. Therefore, the pondered optimization approach could be implemented that evaluates operating points differently by using weighting factors for each operating point. Since the intended application of the engine defines the frequency of expected operation for each operating point, the weighting factors should depend on that.

Another possible approach for simultaneous optimization could be carried out by combining two different optimization algorithms in a nested loop optimization setup. For example, the genetic algorithm can be used for the optimization of the PC geometry, and for each member of such generated population, the optimization of the operating parameters would be performed by the Nelder–Mead algorithm. This would result in optimal operating parameters for each PC geometry variation generated by the genetic algorithm, which eliminates the potential problem of disregarding possibly good geometry solutions because of non-optimal operating parameters, especially in the initial populations.

4. Conclusions

Combustion results of an experimental turbulent jet ignition engine and 3D CFD results of cold flow were used for the calibration of an 0D/1D simulation model with an integrated new \( K-k-e \) turbulence model and multiple flame propagations. The calibration results covered different engine speeds, loads and spark timings where a single set of 0D/1D model parameters was determined, which provided a very good agreement between simulation and experimental data. The average accuracy of 98.5% was achieved in the simulation result of indicated specific fuel consumption, while the trend of calculated octane number matched well with the experimental indicator of knock combustion. Once the 0D/1D simulation model was calibrated, it was used for the optimization of pre-chamber geometry (volume and orifice diameter) and operating parameters (fuel mass injected in pre-chamber and spark timing) over 9 operating points to minimize indicated specific fuel consumption while avoiding excessive knock combustion. The genetic algorithm was used for the optimization, which was performed separately in two different manners. The
first method represented individual optimization of the geometrical and operating parameters for each operating point, while the second method entailed simultaneous optimization, which resulted in a single solution of optimal pre-chamber geometry for the considered engine operating map and optimal operating parameters for each operating point. From the performed analysis and optimization in this study, the following conclusions can be drawn:

- The upgraded 0D/1D simulation model is detailed enough to match well with experimental data with a single set of model constants;
- The pre-chamber volume is independent of engine operating conditions. A greater pre-chamber volume ($V_{pc}/V_k \approx 5\%$) is more favorable at most of the operating points;
- Results from individual and simultaneous optimization of injected fuel mass in PC clearly indicate the necessity for increasing the injected fuel mass in the PC as the main chamber mixture becomes leaner;
- Results from individual optimization of the orifice diameter show that at lean mixtures in MC ($\lambda = 2.2$), smaller orifice diameters are more favorable. A decrease in orifice flow area increases cross-flow velocities, which elevate the turbulence level in the MC. This, in turn, increases combustion speed under lean conditions. At stoichiometric conditions and for $\lambda = 1.6$ in MC, the most favorable orifice diameters are around 2.5 mm, where a compromise between MC turbulence level and residual gas concentration in the PC is achieved.
- Simultaneous optimization of the pre-chamber geometry and the operating parameters of the turbulent jet engine can be used to find optimal and single geometry parameters applicable in a wider range of engine speeds and loads;
- Simultaneous optimization of pre-chamber geometry for all considered operating conditions resulted in a single solution of pre-chamber volume that was equal to 5.14% of clearance volume with an orifice diameter of 1.1 mm. The contribution of engine performance at lean mixtures is the dominant contribution to total objective function when simultaneous optimization is performed.

Further research activities could include the experimental verification of optimal geometrical and operating parameters that were found in the presented study. Moreover, the 0D/1D simulation model could be additionally upgraded to directly optimize the number of orifices and to include additional objective functions, e.g., the minimization of engine raw emissions.

**Author Contributions:** Conceptualization, M.S. and V.D.; methodology and investigation, D.K., M.S., R.T., J.K., V.D. and S.U.; software and validation, M.S., J.K. and V.D.; writing—original draft preparation, M.S., R.T., J.K., V.D. and S.U.; writing—review and editing, D.K., M.S.; supervision and project administration, D.K., R.T. and M.S.; funding acquisition, D.K. All authors have read and agreed to the published version of the manuscript.

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**Conflicts of Interest:** The authors declare no conflict of interest.

**Appendix A**

The $K$-$\varepsilon$ turbulence model used in this study is already validated for swirl flow and published in [27]. It belongs to a group of $K$-$k$ turbulence models that is extended for swirl (or tumble) angular momentum equations. The change of mean flow kinetic energy $K$, turbulent kinetic energy $k$, dissipation rate $\varepsilon$, and swirl angular momentum $S$ are calculated using the following set of differential equations:
\[
\frac{d(mK)}{dt} = (\dot{m}K)_m - (\dot{m}K)_{out} - f_d \frac{mK}{t_S} + mK \frac{\dot{P}}{\rho} - P + \frac{1}{2} \dot{m}_{pre} \left(C_{\text{PM}} v_{in} \right)^2,
\]
(A1)

\[
\frac{d(mk)}{dt} = (\dot{m}k)_m - (\dot{m}k)_{out} + \frac{2}{3} \frac{\dot{P}}{\rho} \left( -mv \dot{\rho} + mk \right) + P - me,
\]
(A2)

\[
\frac{d(me)}{dt} = (\dot{m}e)_m - (\dot{m}e)_{out} + C_{st} \frac{e}{k} \left( P - \frac{2}{3} mv \dot{\rho} \left( \frac{\dot{\rho}}{\rho} \right)^2 + \frac{2}{3} mk \dot{\rho} \right) - C_{e2} \frac{me^2}{k} - C_s \frac{me^3}{\rho} - \frac{C_{\mu} \eta \left( 1 - \frac{\eta}{\eta_0} \right)}{1 + \beta \eta^3} \frac{me^2}{k},
\]
(A3)

\[
\frac{d(mS)}{dt} = (\dot{m}S)_m - (\dot{m}S)_{out} - f_d \frac{mS}{t_s}.
\]
(A4)

The first terms in these governing equations describe the inflow convective effect over the intake valves, while the second terms are related to the outflow over the exhaust valves. The turbulent production term \( P \) subtracts mean flow kinetic energy in Equation (A1) and adds it to the turbulent level in Equation (A2), describing the energy cascade mechanism. It is calculated as:

\[
P = C_{PKS} \frac{m}{t_s} \left( \frac{K - K_s}{t_s} \right),
\]
(A5)

where the swirl characteristic time scale \( t_s \) can be calculated if the swirl radius is divided by the turbulent intensity \( u' \). The kinetic energy of swirl flow \( K_s \) is equal to half of the squared swirl velocity \( U_s \):

\[
K_s = \frac{1}{2} U_s^2 = \frac{1}{2} \left( \frac{S}{r_s} \right)^2,
\]
(A6)

where \( r_s \) is the average radius of swirl vortex that is correlated to the cylinder bore. Compared to the original equations of the \( K-k-\varepsilon \) turbulence model already published in [27], the last term in Equation (A1) is a new source term considering an increase in mean flow kinetic energy governed by mass flow \( \dot{m}_{pre} \) from the pre-chamber to main chamber volume and calculated orifice velocity \( v_{in} \). The tuning constant \( C_{PM} \) was calibrated to capture the increase in mean flow and turbulent kinetic energies during pre-chamber combustion close to reference 3D CFD results. Since the same experimental engine was used in this study and in previous research [27], turbulent model constants (denoted as \( C \) with different subscripts) were not specified in this paper.

References


