



MARMARA UNIVERSITY
INSTITUTE FOR GRADUATE STUDIES
IN PURE AND APPLIED SCIENCES



**DEVELOPMENT OF A SINGLE CYLINDER
HIGH PERFORMANCE AND LOW
EMISSION COMPRESSION IGNITION
ENGINE WITH ADVANCED
EXPERIMENTAL AND NUMERICAL
SIMULATION METHODS**

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Ph.D. THESIS

Department of Mechanical Engineering

Thesis Supervisor

Prof. Dr. M. Zafer GÜL

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ÖZET

GELİŞMİŞ DENEYSEL VE SAYISAL SİMÜLASYON YÖNTEMLERİ İLE YÜKSEK PERFORMANSLI, DÜŞÜK EMİSYONLU TEK SİLİNDİRLİ DİZEL MOTOR GELİŞTİRİLMESİ

İçten yanmalı motorların en büyük dezavantajlarından biri fosil yakıtlardan kaynaklı olarak başta NO_x , CO_2 , HC ve CO gibi birçok zararlı gaz salınımı yapmasıdır. Küresel ısınma ve sera etkisinin artarak hissedildiği günümüzde, düşük yakıt tüketimi ve düşük emisyon değerlerine sahip içten yanmalı motor teknolojilerinin geliştirilmesi önem arz etmektedir. Bilindiği üzere motor içinde meydana gelen yanmanın sonucunda egzoz gazları açığa çıkmaktadır ve motorun emisyon değerleri, yanma işleminin verimine bağlıdır.

Deneysel teknikler, QD ve CFD modelleme yöntemleri kullanılarak mevcut dizel motor test edilmiştir ve modellenmiştir. Tez kapsamında mevcut motorun emisyon değerlerinin azaltılması hedeflenmiştir. Mevcut motorda, yanma verimine etki edecek, emisyon ve motor performansına etki eden değerler parametrik olarak incelenmiştir.

Piston çanak geometrisi, sıkıştırma oranı, enjeksiyon zamanı, enjeksiyon basıncı, sprey açısı, enjektör delik sayısı, EGR oranı gibi parametrelerin yanma verimi, motor performansı ve egzoz emisyonlarına etkisi incelenmiştir. Motorun çanak geometrisi, CFD simülasyon ve genetik algoritma kullanılarak emisyonları minimize edecek şekilde optimize edilmiştir. Ayrıca QD model ile genetik algoritma kullanılarak, enjeksiyon parametreleri ve supap zamanlamaları optimize edilmiştir.

Yapılan çalışmalar sonucunda motorun emisyonlarının en az olduğu ancak performansının azalmadığı optimum noktalar tespit edilmiştir. Nihai tasarımda, NO_x , CO ve is emisyonları önemli ölçüde azalmıştır. Motor performans değerinde ise bir miktar iyileşme gözlenmiştir. Optimize edilen yanma odası, iyileştirilen enjeksiyon parametreleri ve optimize edilen supap zamanlamaları ile motor günümüz emisyon standartlarını sağlayabilecektir.

Anahtar Kelimeler: Dizel motorlar, deneysel metotlar, optimizasyon, CFD, QD, emisyon

ABSTRACT

DEVELOPMENT OF A SINGLE CYLINDER HIGH PERFORMANCE AND LOW EMISSION COMPRESSION IGNITION ENGINE WITH ADVANCED EXPERIMENTAL AND NUMERICAL SIMULATION METHODS

The major disadvantage of internal combustion engines is the release of many hazardous gases, NO_x, CO₂, HC, and CO, from fossil fuels. Today, because of increasing global warming and the greenhouse effect, the development of internal combustion engine technologies with low fuel consumption and low emission values is very important. Exhaust gases are released as a result of combustion in the engine. The emission values of the engine depending on the efficiency of the combustion process.

The diesel engine was tested and modeled using experimental techniques, QD and CFD simulation methods. This thesis aims to reduce the emission values of the existing engine. In the engine, the values that affect the combustion efficiency, exhaust emission and engine performance have been examined parametrically.

The effects of the engine parameters such as piston bowl geometry, compression ratio, SOI, injection pressure, spray angle, number of injector holes, and EGR ratio on combustion efficiency, engine performance and exhaust emissions were investigated. The piston bowl geometry was optimized in order to minimize the emissions using CFD model and genetic algorithm. In addition, the injection parameters and valve timings were optimized using the QD model and the genetic algorithm.

As a result of the studies, the parameters that the engine emits the least emissions were determined. In the optimized engine, NO_x, CO, and soot emissions were significantly reduced and also the performance was improved slightly. The engine with the optimized combustion chamber, improved injection parameters and optimized valve timings will be able to meet today's emission standards.

Keywords: CI engine, experimental, optimization, CFD, QD, emissions

CLAIM FOR ORIGINALITY

DEVELOPMENT OF A SINGLE CYLINDER HIGH PERFORMANCE AND LOW EMISSION COMPRESSION IGNITION ENGINE WITH ADVANCED EXPERIMENTAL AND NUMERICAL SIMULATION METHODS

Single-cylinder diesel engines are widely used in marine, agricultural and construction sectors. However, emissions of combustion engines with adverse effects on health, environment, and climate are limited. Necessary improvements to diesel engines are required to meet the increasingly stringent emission legislation.

The diesel engine is considered one of the most effective types of internal combustion engines, although the disadvantage of the diesel engine is the high soot and NO_x emissions. Thus, the main current objective in diesel engine research is to come up with ways to reduce soot and NO_x while reducing fuel consumption. Significant progress has been made in the area of diesel exhaust post-processing in recent years; however, further reduction of exhaust emissions is still needed.

By using CFD and QD simulation tools, engine development with high engine performance and low emissions have been realized according to their equivalents. A new-type piston bowl design has been optimized using a genetic algorithm. This bowl design provides optimum combustion and mixture formation. NO_x emissions have been decreased by optimizing the valve timing. The injection strategy aims to provide the most appropriate injection. The thesis studies aim to improve combustion efficiency by re-designing different components without concentrating on a single parameter. Thus, the effects of the components on each other and the combustion and emissions have been evaluated together and their effectiveness has been evaluated mutually. Within this framework, a design methodology, experimental studies, and original design made to contribute to national knowledge.

SYMBOLS

a	: Thermal diffusivity (m^2/s)
A_s	: Droplet surface area (m^2)
C_d	: Discharge coefficient
c_f	: Friction coefficient
c_v	: Specific heat at constant volume (J/kgK)
c_p	: Specific heat at constant pressure (J/kgK)
c_μ	: Coefficient of k- ϵ model
C_s	: Swirl coefficient
C_t	: Tumble coefficient
D	: Mass diffusion coefficient (m^2/s)
$D_{d,\text{stable}}$	: Stable droplet diameter
D_d	: Instantaneous droplet diameter
ϵ	: Dissipation rate of turbulence (m^2/s^3)
E	: Internal energy (J)
k	: Turbulent kinetic energy (m^2/s^2)
F_m	: Mass transfer rate per unit surface area (kg/m^2)
F_{drag}	: Drag force (F)
H	: Total enthalpy (J)
h_g	: Heat transfer coefficient ($\text{W}/\text{m}^2\text{K}$)
L	: Characteristic length
N	: Engine speed (rpm)

Pr	: Prandtl number
R	: Gas constant (J/molK)
Re	: Reynolds number
T_{gas}	: Temperature of the gas (K)
T_{wall}	: Temperature of the wall (K)
U	: Radial velocity (m/s)
U_{eff}	: The outer boundary layer effective velocity
ρ	: Density (kg/m ³)
η	: Dynamic viscosity (Pa-s)
λ	: Heat conduction coefficient (W/m ² K)
ν	: Kinematic viscosity (m ² /s)
σ_d	: Surface tension coefficient (N/m)
S	: Source term
Sc	: Schmidt number
V	: Volume (m ³)

ABBREVIATIONS

3D	: Three-dimensional
aBDC	: After bottom dead center
AFR	: Air-fuel ratio
AHRR	: Apparent Heat Release Rate
AMR	: Adaptive mesh refinement
aTDC	: After top dead center
bBDC	: Before bottom dead center
bTDC	: Before top dead center
BDC	: Bottom dead center
BMEP	: Brake mean effective pressure (bar)
BB	: Base piston bowl
BSFC	: Brake specific fuel consumption (g/kWh)
CA	: Crank angle
CFD	: Computational Fluid Dynamics
CI	: Compression Ignition
CNG	: Compressed natural gas
CR	: Compression ratio
DI	: Direct Injection
DOE	: Design of Experiments
DSB	: Double-swirl piston bowl
DWEA	: Density-weighted and ensemble averaged

ECFM	: Extended coherent flame model
EGR	: Exhaust gas recirculation
EOI	: End of Injection
EPA	: Environmental protection agency
EVO	: Exhaust valve opening
HCCI	: Homogeneous charge compression ignition
HRR	: Heat release rate
ICE	: Internal Combustion Engine
ID	: Ignition delay
IMEP	: Indicated mean effective pressure
ISFC	: Indicated specific fuel consumption
IVC	: Intake valve closing
KH	: Kelvin-Helmholtz
LPG	: Liquefied petroleum gas
MOGA	: Multi-objectives genetic algorithm
MOSA	: Multi-objective simulated annealing
MSB	: Multi-swirl piston bowl
NG	: Natural gas
NTC	: No time counter
NTP	: Non-thermal plasma
NSGA	: Non-dominated sorting genetic algorithm
PISO	: Pressure implicit by splitting of operators

PM	: Particulate Matter
PPCI	: Partially Premixed Compression Ignition
RANS	: Reynold-Averaged Navier-Stokes
RB	: Reentrant piston bowl
RCCI	: Reactivity controlled compression ignition
RSM	: Response surface method
RT	: Rayleigh-Taylor
QD	: Quasi-dimensional
SAGE	: Detailed transient chemistry solver
SCR	: Selective catalytic reduction
SIMPLE	: Semi-implicit method for pressure-linked equations
SI	: Spark Ignition
SOC	: Start of Combustion
SOI	: Start of Injection
SRM	: Stochastic reactor model
TDC	: Top dead center
TKE	: Turbulence kinetic energy

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1. INTRODUCTION

Humankind needs the energy to provide essentials such as food (including water), shelter and clothing. Nowadays, while the population and needs are increasing, the energy requirements are increasing rapidly too. Although it is foreseen that a remarkable proportion of the energy requirement will be provided by renewable energy sources in the future, the dependence on fossil fuels will still constitute a significant amount in the coming decades.

Air pollution caused by the usage of fossil fuels also poses a great risk to human health (Salameh, 2014). The main causes of premature deaths are air pollution. The exposure of children and adults to short- and long-term air pollution leads to lung diseases and asthma. In addition to exposure to air pollution has negative effects on fertility (WHO, 2005, 2013). There is new information that exposure to air pollution is associated with diabetes in adults. It may also be associated with obesity, systemic inflammation, aging, Alzheimer's and dementia (Ornes, 2016).

The use of fossil fuels causes the emission of greenhouse gases, which is one of the most important reasons for climate change and global warming, one of the world's biggest problems (Nordell, 2003). Since global warming is a threat to the earth's ecosystem, it is of utmost importance to take necessary precaution (Lal, 2004; Ninawe, Indulkar, & Amin, 2017; Williams, 2002).

The necessary measures should be taken in this regard as a state policy, although individuals also have responsibilities. Therefore, measures are taken in many countries around the world to reduce harmful emissions to the environment. There are 160 countries have been signed the Kyoto Protocol to fight global warming and climate change. This protocol requires countries to decrease the carbon amount emitted into the atmosphere to 1990 levels (United Nation, 1998). European Union member countries are taking measures in this regard. In 2016, there was a 22% decrease compared to 1990 and a reduction in emissions of 80% to 95% is targeted in 2050 (EEA, 2017).

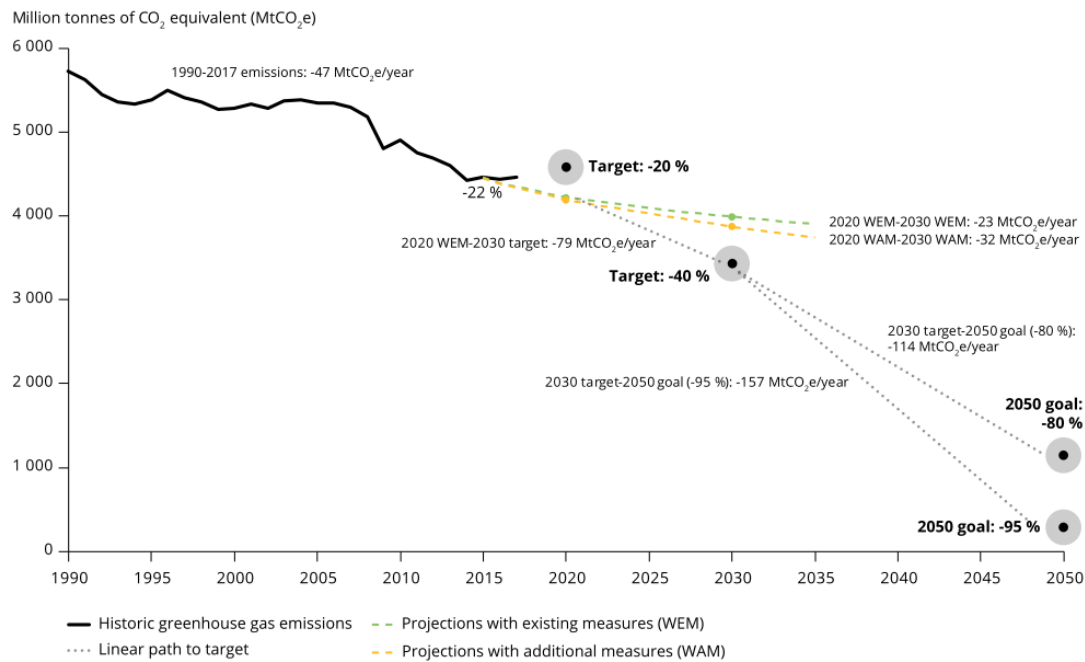


Figure 1.1. Trends of greenhouse gas emission, targets and projections in the EU, 1990-2050 (EEA, 2017)

As shown in Figure 1.1, it is aimed to reduce emissions continuously. On a sectoral basis, the share of transport and internal combustion engines in CO₂, and NO_x, CO and PM emissions is quite high (Figure 1.2). More than half of the NO_x emissions are emitted from vehicles. Since NO_x emissions increase the acidity of the rain, it has great harm to agricultural areas, forests and human health (Pawlowski, 1997). Both internal combustion engines of transportation vehicles and non-road internal combustion engines have a remarkable impact on air pollution and thus global warming. Therefore, it was introduced new regulations for minimization of emissions (Table 1.1 and Table 1.2). The production and use of engines that do not meet the emission requirements must be restricted. Engine manufacturers are required to work to minimize the exhaust emissions and they are making great efforts to meet emission standards. Vehicles with Euro 6 emissions standard should reduce NO_x emissions to levels of 0.46 g/kWh and below. Standards also limit HC, CO and PM emissions, which is very challenging for the engine manufacturers (Boccardo et al., 2019).

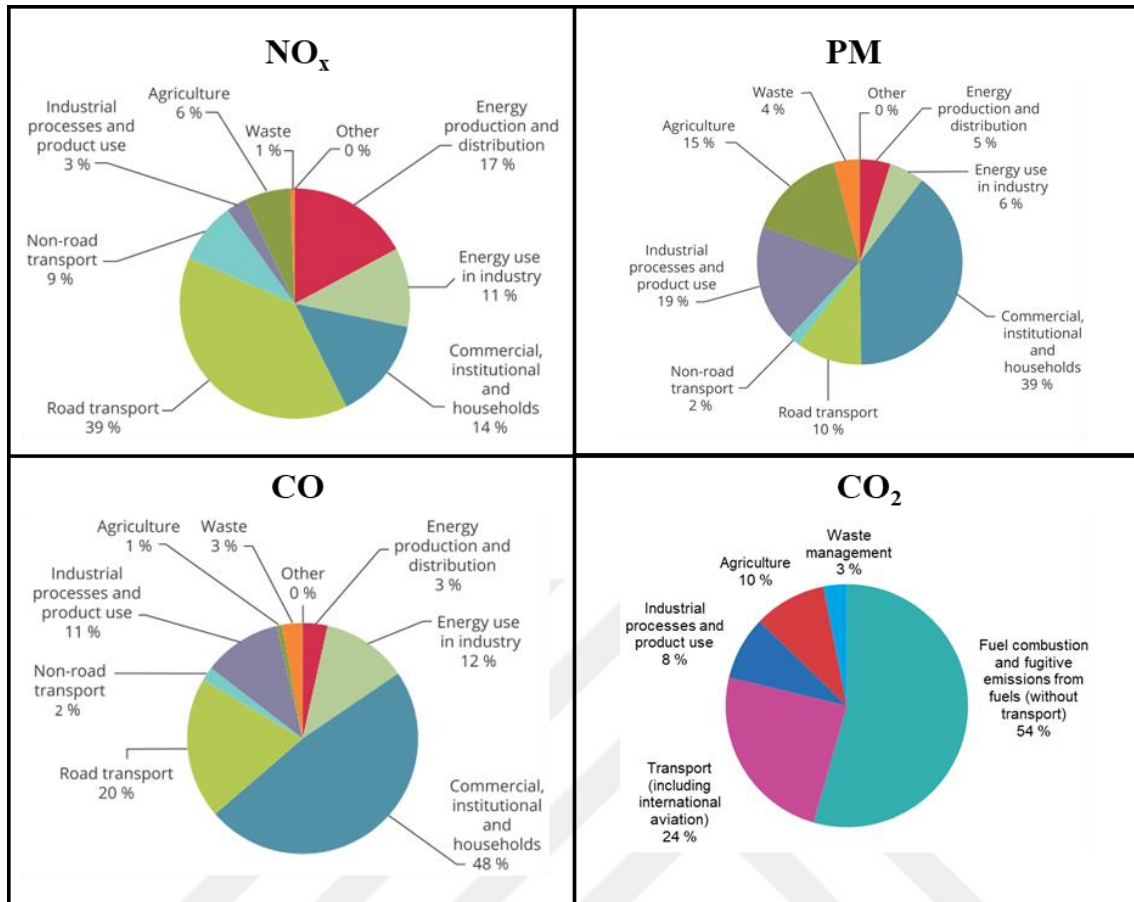


Figure 1.2. Sectoral trends in emissions in the EU (EEA, 2018)

Table 1.1. European emission standards for heavy-duty diesel engines

Stage	Date	CO	HC	NO _x	PM	PN
		g/kWh				1/kWh
Euro I	1993	4.5	1.1	8.0	0.612<85 kW 0.36>85 kW	
Euro II	1996	4.0	1.1	7.0	0.15	
Euro III	2000	5.5	0.78	5.0	0.16	
Euro IV	2005	4.0	0.55	3.5	0.03	
Euro V	2008	4.0	0.55	2.0	0.03	
Euro VI	2013	4.0	0.16	0.46	0.01	6.0x10 ¹¹

ICEs can be used for transportation purposes, as well as for non-road purposes, in agricultural areas and as generators. These non-road internal combustion engines are also regulated by emissions regulation and have to meet Stage V emission standards as of 2019 (Table 1.2) (The European Parliament and of The Council, 2016).

Table 1.2. Stage V non-road engines emission standards

Category	Date	Ignition	Net Power	CO	HC	NO _x	PM	PN
			kW	g/kWh				1/kWh
NRE-v/c-1	2019	CI	$P < 8$	8.00	7.50		0.40 ^b	-
NRE-v/c-2	2019	CI	$8 \leq P < 19$	6.60	7.50		0.40	-
NRE-v/c-3	2019	CI	$19 \leq P < 37$	5.00	4.70		0.015	1×10^{12}
NRE-v/c-4	2019	CI	$37 \leq P < 56$	5.00	4.70		0.015	1×10^{12}
NRE-v/c-5	2020	All	$56 \leq P < 130$	5.00	0.19	0.015	0.015	1×10^{12}
NRE-v/c-6	2019	All	$130 \leq P \leq 560$	3.50	0.19	0.015	0.015	1×10^{12}
NRE-v/c-7	2019	All	$P > 560$	3.50	0.19	0.045	0.045	-

Compression-ignition (diesel) engines among the IC engines are widely used due to their high thermal efficiency compared to spark-ignition (gasoline) engines. Diesel engines emit less HC and CO. Even so, PM and NO_x emissions which have carcinogenic effects are higher (O'Driscoll, Stettler, Molden, Oxley, & ApSimon, 2018). Diesel engine technology is developing. Diesel engines with high efficiency, low fuel consumption, and low emission are being produced. These developments have led to an increase in the interest in diesel engines for agricultural and maritime sectors where fuel economy is a significant parameter and apparently the usage of diesel engines will continue to increase in these sectors.

Nowadays, there are different techniques for reducing diesel engine emissions. Alternative fuels, high-pressure injection systems, combustion chamber improvements, turbo and intercooler, EGR (exhaust gas recirculation), SCR (selective catalytic reduction) and particulate filter are used to limit exhaust emissions (Boccardo et al., 2019).

Alternative fuels with lower emissions to replace fossil fuels are studied to reduce fossil fuel usage that is a limited resource. Biodiesel, biogas, CNG, LPG, hydrogen, methanol, ethanol and butanol can be used in ICEs as fuel (Ashok & Nanthagopal, 2019; Yisong Chen et al., 2018; Köten, 2014; Shahir, Jawahar, & Suresh, 2015; I. T. Yilmaz & Gumus, 2017).

Optimization of piston bowl geometry and valve timing and improvement of injection parameters play an essential role in reducing emissions. The aim of improving the combustion chamber is to ensure combustion with maximum efficiency (Yue Chen & Lv, 2014; Hanson et al., 2012; Seokhwon Lee, Jeon, & Park, 2016; Seungpil Lee & Park, 2017). On the other hand, after-treatment systems are commonly used to control emissions including oxidation catalyst, particulate filters, NO_x absorber, SCR, lean NO_x catalyst and non-thermal plasma catalyst if previous methods are not enough to reduce emission to a desired level (Gül, Köten, Yilmaz, & Savci, 2018; Gupta, Chaturvedi, Dubey, & Rao, 2017; Praveena & Martin, 2018).

1.1.Literature Review

Hentschel and Schindler aimed to demonstrate in-cylinder flow and fuel injection. They analyzed with advanced techniques including the laser Doppler anemometer. Their study helps to understand the interaction of vortices in the flow, spray formation and self-ignition and combustion. So that engine development can be achieved with lower fuel consumption and lower emission values (Hentschel & Schindler, 1996).

Payri et al. designed different piston bowls for four-valve, direct injection diesel engine. Experimental verification is provided by performing 3D CFD simulation during expansion and compression stroke. CFD simulation results were compared with the laser doppler anemometry results for three different piston bowl designs. It was observed that the experimental data and numerical data were more compatible with the crank angles near the top dead center. Flow properties inside the cylinder were compared with different piston bowl configurations (Payri, Benajes, Margot, & Gil, 2004).

Shi and Reitz used the KIVA CFD code and NSGA-II method with an automated mesh generation method on heavy-duty CI engines to obtain low emission and high fuel economy. They investigated the combustion chamber design, swirl ratio and spray

targeting for CI engine at low and high loads. It was found that the optimal bowl geometry and spray targeting were used for minimum emission and maximum fuel efficiency. Optimization studies show that high load conditions are more sensitive to combustion chamber geometry than low load conditions. Thus, optimization may perform using high load conditions, and then this design can be applied to low load operating conditions (Y. Shi & Reitz, 2008).

Varol et al. analyzed the heat transfer and the fluid flow in a crescent type combustion chamber. They employed dynamic grid model to simulate intake stroke. The $k-\epsilon$ turbulence model was used to solve the in-cylinder flow of an incompressible fluid. They presented velocity profiles, temperature, and pressure. It was observed that the crescent type combustion chamber reduces the swirl effect. It could be used as a control parameter for fluid flow and heat (Varol, Oztop, Firat, & Koca, 2010).

Shi and Reitz investigated the injection strategy optimization for a CI engine fueled with diesel and gasoline-like fuels. They developed an efficient chemistry solver to calculate performance and emission with low CPU times. CFD code and NSGA-II method were coupled to find optimum injection parameters for efficient combustion. They found that heavy-duty CI engine fueled with gasoline-like fuels with an optimum injection parameters promises higher thermal efficiency, lower NO_x and soot emissions. Moreover, lower octane number gasoline-like fuels improve the controllability of the combustion and also decrease the noise of the engine. One challenge for high and low loads is the high pressure rise rate inside the cylinder (Yu Shi & Reitz, 2010).

Yilmaz et al. studied the effect of the compression ratio, injection timing, and cone angle on the HCCI performance and PM and NO_x emissions. They performed the CFD simulation with ECFM-3Z combustion model and analyzed the high-pressure fuel spray and the air motion inside the cylinder. They found that four times lower soot mass fraction and three times lower NO_x mass fraction in the PPCI case than the conventional case (M. Yilmaz, Köten, & Zafer Gul, 2012).

Jaichandar and Annamalai carried out experiments using a diesel engine with a plunger-type injection system and toroidal reentrant combustion chamber and hemispherical combustion chamber piston bowl designs. They were evaluated combustion chamber geometries and injection pressure on the combustion efficiency, engine performance and

exhaust emissions, using 20% PME (pongamia oil methyl ester) and diesel blend. Improvement in terms of thermal efficiency and specific fuel consumption for toroidal reentrant combustion chamber operated at high injection pressure found with the experiment. Toroidal reentrant combustion chamber with high injection pressure caused the reduction of the exhaust emission. However, NO_x increased owing to homogeneous air-fuel mixture inside the cylinder and high-pressure injection. When the injection pressure increased, ignition delay decreased, and also maximum pressure and gross heat release increased inside the cylinder (Jaichandar & Annamalai, 2013).

Taghavifar et al. performed simulation using the diesel engine applied the geometrical modification on the piston bowl movement and its size. It is demonstrated the air-fuel ratio by homogeneity factor and equivalence ratio. In addition, the indicated thermal efficiency, pressure curves, and rate of heat release were compared for different piston bowl geometries. They adopted the Extended Coherent Flame Model's sub-model (ECFM-3Z) to understand the combustion chemistry and reaction rate. They found that increasing the mixture homogeneity increase the pressure and rate of heat release rate. Moreover, it was shown that smaller bowl diameter induces better vortex formation and squish in the combustion chamber, and reduce ignition delay (Taghavifar, Khalilarya, & Jafarmadar, 2014).

Mohan et al. developed a new hybrid spray model and validated against the experimental results. They found that the new hybrid model grabs the detail of the process of spray and combustion (Mohan, Yang, & Chou, 2014).

Benajes et al. focused on describing a methodology for optimizing the combustion system of medium-duty direct injection CI engine, by combining CFD modeling, and DOE method and Response Surface Method (RSM). Their methodology is quite favorable to obtain the cause-effect correlations between the input and output parameters and to define the optimum input parameters value. They optimized the combustion system in order to maximize fuel efficiency and fulfill the exhaust emission limits. Optimization parameters of their studies were the injector nozzle configuration, the bowl geometry, and intake manifold design. The results confirmed that fuel consumption decreased by about 2% with the same NO_x emission value when optimizing only the engine hardware. Moreover, the optimization including injection settings and air management besides engine hardware

improvement resulted in the fuel consumption of about 5% decrease with keeping the emission value (Jesus Benajes et al., 2016).

Benajes et al. studied the influence of the combustion chamber on heat transfer, combustion losses, and efficiency using the RCCI engine. The engine has three different piston bowl designs with a constant compression ratio of 14.4:1. They performed the experiments at 1200 rpm and low, medium, and high loads. The engine with the shallow bowl geometry which has a 16% smaller surface area than baseline bowl geometry improves the gross work (Jesús Benajes, García, Pastor, & Monsalve-Serrano, 2016).

Kakaee et al. used three piston bowl designs that were base, bathtub and cylindrical with constant compression ratio (CR) on RCCI engine fueled with NG and diesel. They examined the double injection strategy, the influence of the bowl depth, engine speed, and chamfered ring-land. They found that the piston bowl profile did not remarkable affect the combustion characteristics at low engine speed, although it was noticeable important at high speed and it was highly important for NO_x emissions. The other result of the study was increasing engine speed results in increase UHC and CO emissions (Kakaee, Nasiri-Toosi, Partovi, & Paykani, 2016).

Nazemi et al. analyzed fuel injection parameters on an RCCI engine. They coupled Converge CFD modeling tool and GT-Power QD modeling tool. They found that the dominant parameter affecting the RCCI engine is spray angle and least affecting parameter is the injection pressure. So, decreasing the spray angle from 55 to 74 results CO and HC emissions decreased by 27% and 15% respectively. They obtained that NO_x decreases by increasing P_{inj} and premixed ratio (PR) and HC, CO emissions increases for narrow spray angles (i.e. 25° and 35°) by increasing P_{inj} and PR. They suggested that the optimum fuel injection parameters and spray angle [55°], SOI [55° aTDC], P_{inj} [580 bar] and PR [0.76] for RCCI engine. These parameters are decreasing HC and CO emissions by 23% and 39%, respectively and enhancing combustion efficiency (Nazemi & Shahbakhti, 2016).

Chemical and physical processes, which are responsible for engine performance and exhaust emissions of compression-ignition engine, can be described by CFD. The CFD is useful for predicting ignition and combustion of CI engine. CFD simulations put the sophistication and fidelity of spray, turbulence, and chemistry models at investigators'

disposal. The treatment of oxidation chemistry is important in CI CFD calculations. There are 1000s–10,000s of elementary reactions and 100s–1000s of species in modern chemical kinetic mechanisms of fuel. Such a large number of reactions and species are handicap for engine simulations. The number of species and reactions must be decreased due to computational cost. Huang et al. tried to predict the ignition behavior of a light-duty CI engine in their paper. RANS approach was used for turbulence, the KH–RT model, and a reduced reaction mechanism. Predictions were similar to experimental data as ignition delays, energy release, cylinder and post-combustion pressures (M. Huang, Gowdagiri, Cesari, & Oehlschlaeger, 2016).

Ela et al. used a single-cylinder CI engine with a CR of 17, displacement volume of 825 cm³, and run at speed of 1500 rpm for the CFD simulation analysis. They validated their model with the experimental results. Replacing nitrogen with helium increased in cylinder pressures via the numerical results. Besides this, a percentage of 0.5–10% of the helium on a mass basis failed to satisfy the recovery needed to get over the drop in-cylinder pressure (Abo El Ela, Eldrainy, Elkasaby, & Nour, 2016).

Kim and Park described the optimum operating conditions of diesel and dimethyl-ether fuel blend in a CI engine using the GA method. They studied parameters as the injection pressure, start of injection, spray angle, and equivalence ratio. They performed numerous CFD simulation at different operating condition using the KIVA-3V code in order to find optimum condition for minimum fuel consumption and exhaust emission. They found that the lower equivalence ratio and late injection strategy were optimal cases of diesel and DME fuels for lower NO_x emissions than baseline cases. The late injection strategy increases soot emission, however, the DME-fueled engine emits extremely small soot emission (Kim & Park, 2016).

Soni and Gupta used CFD software AVL-FIRE for optimization to obtain minimum possible emissions from single cylinder CI engine by means of optimum diesel- methanol blends and different variations of initial swirl, EGR percentage and water emulsion methods. CFD simulations show that the most effective method is water addition among the three methods for the reduction of exhaust emission (Soni & Gupta, 2016).

Benajes et al. focused on optimizing the combustion of a medium-duty and 4-stroke diesel engine with using CFD modelling and the statistical Design of Experiments (DOE)

technique and RSM in their study. Their optimization parameters were the piston bowl geometry, injector nozzle configuration, and mean swirl number for the first optimization study; air management and injection settings for the second optimization study. They said that a 40% NO_x reduction could be achieved using S2 Opt2 combustion system while indicated specific fuel consumption and soot emissions are constant (Jesus Benajes et al., 2016).

Huang et al. used CFD simulation tool (Converge CFD) to predict the ignition timing for the diesel engine. They compared the CFD simulation and experimental results. They found that CFD simulations showed good agreement with experimental results. CFD simulations emphasize the importance of turbulence, spray breakup, and chemistry, to predict ignition delay (M. Huang et al., 2016).

Lee et al. employed the experimental methods and CFD model to increase the fuel economy of CI engine running with a diesel-gasoline fuel blend. The combustion chamber design and operating conditions were optimized using a micro genetic algorithm. The result shows that the optimized combustion chamber improves fuel efficiency. When the gasoline fraction increase, ignition delay, and pressure raise rate increase and combustion duration and IMEP reduce. Soot emissions were decreased by about 90% using gasoline-diesel fuel blends (Seokhwon Lee et al., 2016).

By the means of computational modelling, combustion and emissions can be predicted accurately under favor of properly calibrated and validated models. Besides of this, the current measurement techniques are not adequate to perform an experimentally in-depth analysis. Computational modeling can be used for examining the effects of the bore-to-stroke ratio in CI engines. One-dimensional models are proper for such study because they are rapid and straight on predicting the whole engine behavior. On the other hand, these models are simplifying the combustion processes considerably and appealing to correlations while simulating combustion behavior. Benajes at al. performed a CFD study of the effect of different bore and stroke dimension on the efficiency and pollutants of the diesel engine. They found that efficiency and NO_x emissions increased due to lower heat losses and quicker mixing and combustion with lower bore-stroke ratio. On the other hand, lower bore-stroke ratio decreased fuel-rich zones in squish zone and soot emission formation (J. Benajes, Novella, Pastor, Hernández-López, & Duverger, 2017).

Li et al. proposed a new multi-swirl bowl design and analyzed emission and combustion characteristic using experimental and computational simulation tools. Results show that new design multi-swirl bowl has lower BSFC by 4-5 g/kWh and lower soot emission by about 60% according to double-swirl bowl because a multi-swirl bowl enlarges the fuel diffusion volume and improves the fuel/air mixture ratio (X. Li, Qiao, Su, Li, & Liu, 2017).

Li et al. studied the wall impinging jet in the omega (ω) and the lateral swirl (LS) combustion chamber to obtain the combustion and spray characteristic using a constant volume vessel. They investigated the ω and LS combustion system through the high-speed photography and image processing. They found that LS combustion system improves the mixing of the air and fuel, and accelerate the combustion and also decrease soot emissions by the guiding effect of convex edge on the wall jet (X. R. Li, Yang, Su, & Liu, 2017).

Poorghasemi et al. investigate the influence of DI strategies of a modified RCCI engine on the combustion efficiency and exhaust emission characteristics. They used dual fuel, which are NG, port-injection and diesel, direct-injection. They analyzed premixed ratio of NG, start of injection, diesel mass fraction, injection pressure and spray angle. They found that these parameters affect exhaust emission and engine performance, significantly. Also, decreasing injection pressure from 450 to 300 bar, the gross indicated efficiency increases by 5% and reducing spray angle from 144 to 100 degree, the gross indicated efficiency decreases by 4% and higher premixed ratio increases HC and CO emission and decreases NO_x emission (Poorghasemi et al., 2017).

Sideri et al. used CFD simulations to predict the wall heat fluxes through the combustion chamber walls of a diesel engine in their paper. The heat transfer models of Angelberger, and GruMo–UniMORE was used. GruMo–UniMORE's model was found much the same with the experimental results. The heat lost through the walls of the cylinder is directly responsible for determining the thermal efficiency of ICEs. If the wall heat fluxes are high then lower indicated work is gained. Heat transfer affects cylinder temperatures. Temperatures play an important role in pollutant emissions. By the way, higher cylinder temperatures cause excessive thermal loads and thermo-mechanical failures (Sideri, Berton, & D'Orrico, 2017).

Mattarelli et al. analyzed the influence of a combustion system optimization on the performance of an opposed-piston engine. This two-stroke diesel engine produces 270 kW of power at 3200 rpm. This opposed-piston engine was compared to a traditional four-stroke, turbocharged diesel engine. The numerical study eventually shown that opposed-piston engine had lower in-cylinder pressures, turbine inlet temperatures and improved the efficiency 10% in comparison to traditional engine at full load conditions (Mattarelli, Cantore, Rinaldini, & Savioli, 2017).

Zhao et al. developed a skeletal diesel and natural gas reaction mechanism including 61 species and 199 reactions for CI engines. They combined a reduced reaction mechanism for diesel and GRI-Mech 3.0 reaction mechanism for natural gas fuel. This dual-fuel mechanism presented effective results of ignition, combustion and emission characteristics. They reported that using a calculation method based on the round-robin algorithm of KIVA4-Chemkin code, CFD simulation time for the combustion in CI engines reduced considerably (Zhao, Yang, Fan, Zhou, & Ma, 2017).

Chuahy and Kokjohn worked with CFD using KIVA-3V code. They found that effects of different boiling curves of test fuels on the combustion phases at early and late injection timings were unimportant. Instead of cetane number, chemical characteristic of test fuels had an important role in differences of combustion phases (D.F. Chuahy & Kokjohn, 2017).

Jafari et al. investigated spray angle, start and duration of injection on the entropy generation. Different optimization methods were utilized for comparison like a multi-objective Genetic algorithm (MOGA), a multi-objective simulated annealing (MOSA), a multi-objective particle swarm optimization (MOPSO) and a non-sorted genetic algorithm (NSGA). While the first law efficiency and emissions were strongly effected by start of injection, the effect of spray angle was insignificant. On the other hand, they found that injection duration were highly influenced the second law efficiency (Jafari, Parhizkar, Amani, & Naderan, 2016).

Torelli et al. performed the simulations to model the nozzle flow in a five-hole mini-sac diesel injector. Homogeneous Relaxation Model (HRM) and a multiphase flow representation depend on the assumption of the mixture model with the Volume of Fluid technique were used for simulations. They used full-range naphtha and light naphtha and

also n-Dodecane as CI engine fuel. More cavitation was observed in the use of naphtha fuels than n-Dodecane. Because of the lower mass flow rate of naphtha fuels, the injected energy was lower than n-Dodecane (Torelli, Som, Pei, Zhang, & Traver, 2017).

Petranovic et al. presented a numerical model for pollutant prediction of bio-fueled ICE using FIRE software in their study. Fuel disintegration, spray particles, and evaporation, combustion and the chemical models were included in their numerical model. According to their study, biodiesel blends were more successful decreasing nitrogen oxide emissions than the regular diesel. While comparing different fuels in experiments, the operating parameters like the same start and the end of injection are often difficult to ensure them constant. In these situations, numerical simulations succor to investigators for analyzing and comprising different fuels in the same test conditions (Petranović, Bešenić, Vujanović, & Duić, 2017).

Varun et al. studied the effects of varied combustion chamber designs on performance, emission and combustion parameters using a CI engine. The experimental and numerical results were discussed. According to results, biodiesel can be used more successful in CI engines with small modifications in combustion chamber (Varun, Singh, Tiwari, Singh, & Kumar, 2017).

Maurya and Mishra investigated the performance, and emission characteristics of a six cylinder, turbocharged dual fuel engine. They used 0D-SRM and 3D-CFD models for numeric analyses. NG premixing ratio, engine speed and EGR percentage were changed during parametrical analysis. They found that not only engine performance was improved but also carbon monoxide and unburned hydrocarbon emissions were reduced at higher engine loads (Maurya & Mishra, 2017).

Mauro et al. compare the single-zone thermodynamic model and 3D CFD model for Gross Heat Release characterization of the internal combustion engine. Single Zone model, derived from the First Law of Thermodynamics, has an accuracy of the physic of the phenomenon and its very low computational time, although 3D CFD model provides a high spatial resolution within the combustion chamber and describes turbulent flow inside the cylinder. They found that the CFD model is more accurate but time-consuming but SZ model is can be used for the first approaches with low computational time (Mauro et al., 2018).

Boccardo et al. evaluated the performance of non-road diesel engine with low-pressure EGR system, turbocharger and high-pressure fuel injection system. The fuel injection pressure is very high that reaches 3000 bar. They are trying to ensure Stage V emissions regulation without selective catalytic reduction (SCR) system. They found that high injection pressures ensured about 50% smoke reduction and up to 3% BSFC improvement (Boccardo et al., 2019).

Jaliliamtabar et al. developed the EGR system for light-duty CI engine. Besides, they made a mathematical model to predict CO, HC, NO_x, smoke emissions, power and BSFC with less than 10% error value. This mathematical model coupled with the NSGA-II method to optimize factors such as EGR percent, engine load, speed, and biodiesel percent. They found that NO_x emission decreases 63.76% using EGR and fueled with a B10 fuel blend (Jaliliantabar, Ghobadian, Najafi, Mamat, & Carlucci, 2019).

Pei et al. aim to optimize a diesel engine fueled with RON80 gasoline. The piston bowl design, in-cylinder swirl ratio, and injection strategies were studied in order to improve fuel efficiency. The generation of 256 combustion chamber designs at different operation conditions was produced to find the best results. After simulated over 3000 cases, they obtained optimum bowl geometry with up to 6.3% improvement in ISFC and maintaining the baseline NO_x emission value (Pei et al., 2019).

As seen in the studies described, the combustion chamber geometry, compression ratio, SOI, injection pressure, EGR, spray angle have a major effect on engine performance and exhaust emissions. The combustion chamber geometry is critical as guiding air-fuel mixture. SOI has an impact on emissions and performance as it affects the crank angle where the start and end the combustion. The higher the injection pressure, the better the pulverizes the fuel and reduces soot emissions. But since in-cylinder pressures can rise excessively, they should be controlled. As the EGR rate increases, NO_x emissions decrease, but combustion efficiency and volumetric efficiency decrease. EGR application in a controlled manner will reduce NO_x emissions. Spray angle should be determined according to the bowl geometry and affect combustion efficiency. In these studies, Experimental, CFD, and QD simulation studies were performed to examine the combustion and exhaust emission of a diesel engine. The optimum injection parameters were found by selecting the appropriate injector with parametric preliminary studies. In

order to define the optimum piston bowl design, the genetic algorithm optimization method was used. In addition, the valve timings were optimized to obtain minimum NO_x emission. High-efficiency and low emission diesel engine design has been made with these studies and the literature guidance.

1.2.Objectives

There are certain standards (Tier, NRE-v/c standards etc.) that limit the emission values of non-road diesel engines in our country and in the world. The diesel engines must not emit more than the limits specified in these standards. The most successful method of reducing emissions is to optimize the combustion chamber and the fluid motion inside the engine.

The main objective of this thesis is to develop a single-cylinder diesel engine with low emissions according to NRE-v/c standards. For this purpose, experimental and numerical methods have been used to analyze the engine fluid motion, combustion process, and exhaust emission. According to baseline experimental and numerical results, optimization studies have been carried out on the four-stroke single-cylinder diesel engine.

Another aim of the thesis is to systematize the R&D studies and to expand the diesel engine development methodology. This will contribute to the national knowledge on this subject.

1.3. Hypothesis

It is aimed to reduce emissions in non-road light-duty diesel engines, while the engine power and torque are desired to remain the same value. The combustion chamber of the engine is one of the most important components affecting the combustion efficiency and emissions. Therefore, improvements to the combustion chamber will reduce emissions. Thus, exhaust emissions will be decreased with modification of the combustion chamber geometry, valve timing, and injection parameters.

1.4. Methodology

In this thesis, the methodology is designed to achieve the objectives.

Literature review: Books and journal papers is important to understand the engine development, exhaust emission control and optimization of the engines.

Experimental study: The engine is tested on the experimental setup.

Modeling the engine: A base simulation carried out using CFD and QD software. These results were validated with experimental data.

Optimization study: Optimization studies were performed on the baseline model using QD, CFD and optimization software. Some modification applied to the test engine.

Analysis of the results: Validated results of the baseline engine were comprised with results of the modified engine using post-processing tools.

Conclusion: The results were analyzed and interpreted.

1.5. Structure of Thesis

Chapter 1 presents a review of relevant literature about experimental, and simulation studies of the engines. Experimental setup and test procedure are explained in chapter 2. The governing differential equations of QD and CFD simulation, simulation setup, the engine geometry, boundary conditions and optimization methods are described in chapter 3. This chapter gives the basic information about the simulation and optimization studies. Chapter 4 shows the results of the experimental, QD, and CFD simulations, and optimization. Chapter 5 deals with conclusions and recommendations.

2. EXPERIMENTAL METHODS AND PROCEDURE

In this section, the devices and equipment used in the experiments are introduced and the methods used in the analysis of the experimental data and the experimental process are explained.

2.1. Experimental Equipment

Experiments were carried out in the Internal Combustion Engine Laboratories of Marmara University, Faculty of Engineering, Mechanical Engineering Department. The test setup consists of the dynamometer, test engine, in-cylinder pressure measurement system and exhaust gas analysis system. The cooling tower was used to cool the test engine during operation. The photographic view of the test setup is given in Figure 2.1 and the schematic diagram of the test setup is given in Figure 2.2. Standard diesel fuel was used in the experiments (Table 2.1).

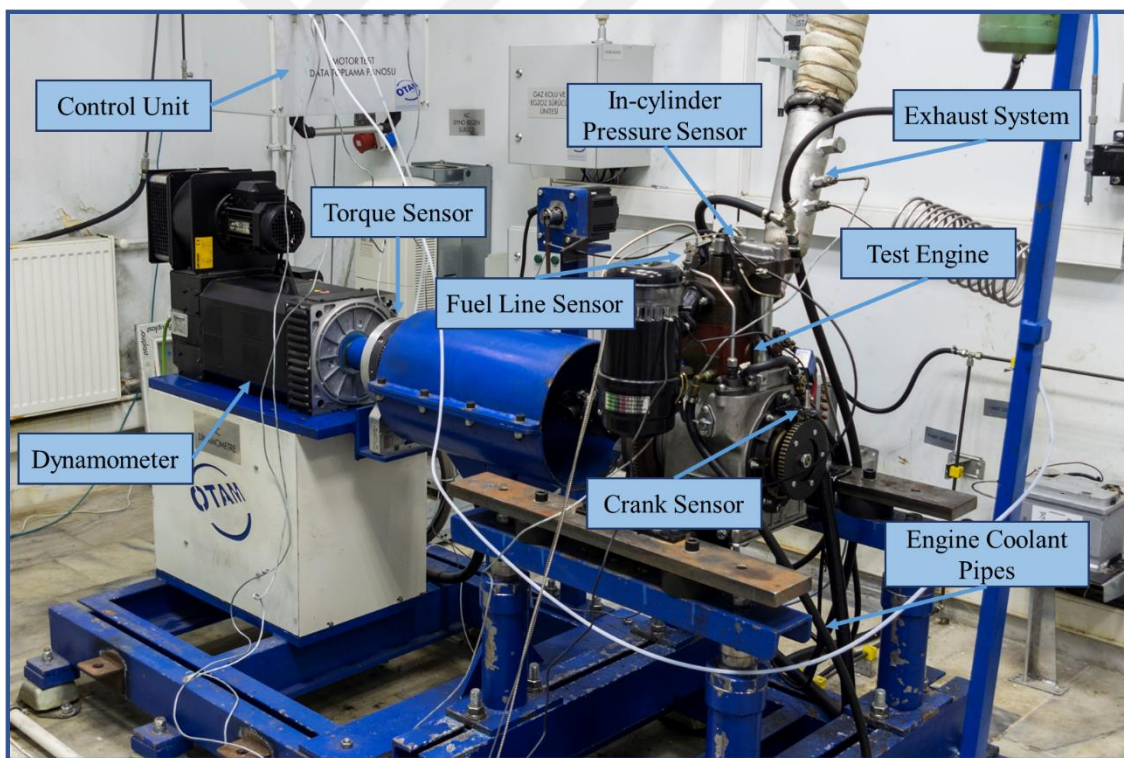


Figure 2.1. Photographic view of the test setup

Table 2.1. Properties of diesel fuel

Properties	Value
Chemical formula	$C_{12}H_{26}$
Density	786 kg/m ³
Boiling point	214 - 218°C
Cetane number	52 - 53
Self-ignition temperature	205 - 210°C
Lower heating value	45.6 MJ/kg
F/A ratio	0.0714
Vapor pressure	< 38 kPa at 20°C

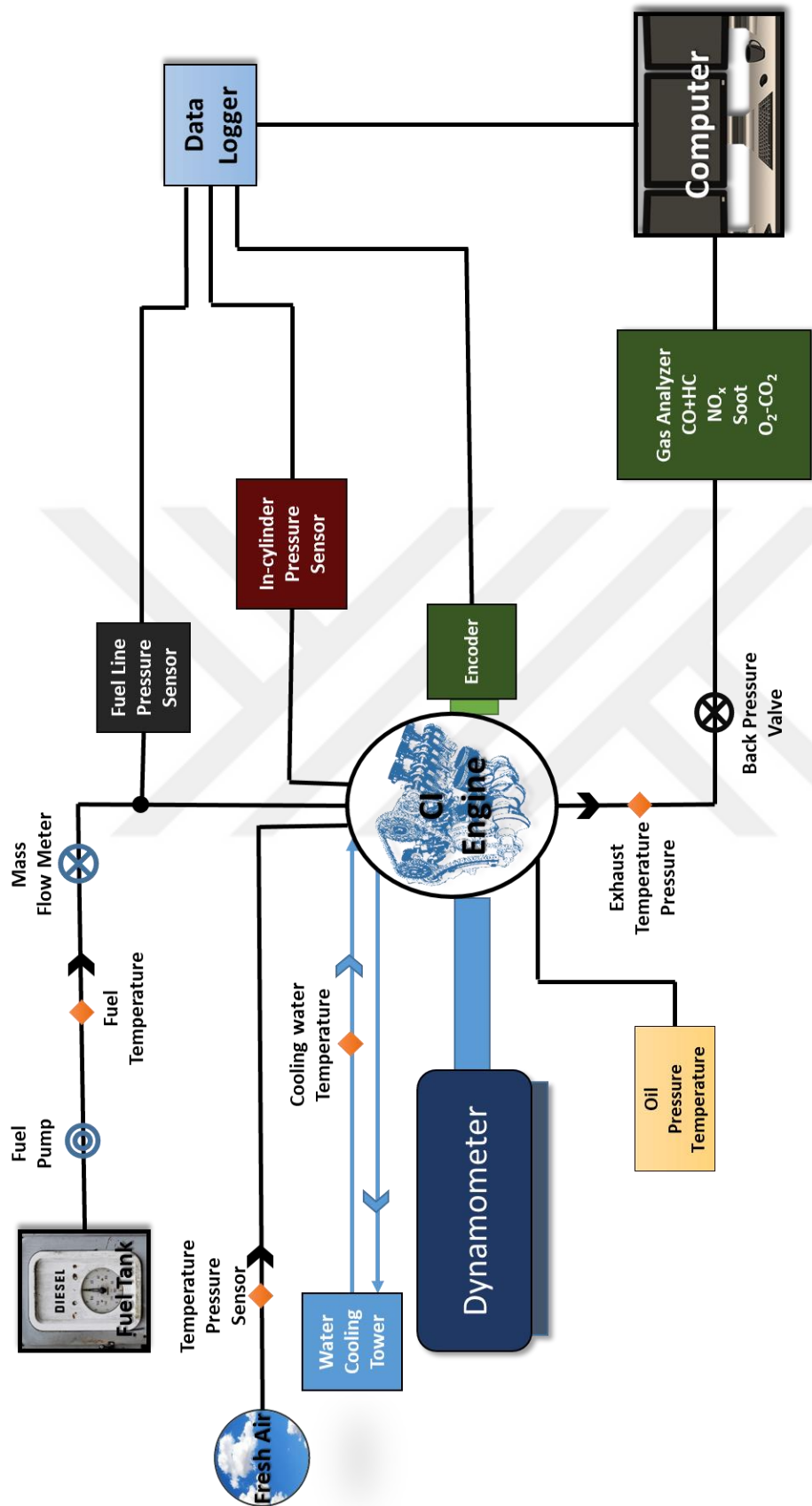


Figure 2.2. The schematic diagram of the experimental setup

2.1.1. Test engine

The experiments were performed using a single-cylinder, four-stroke, direct injection diesel engine. The test engine is shown in Figure 2.3. Table 2.2 shows some characteristics of the test engine.

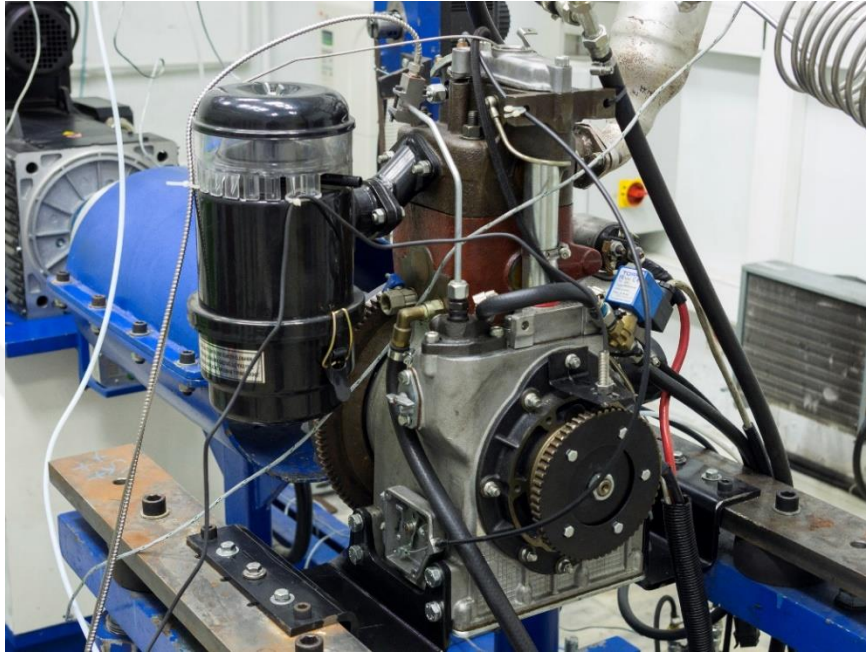


Figure 2.3. The test engine

Table 2.2. Characteristics of test engine

Engine Model And Type	Single Cylinder, Compression Ignition and naturally aspirated, four-stroke engine
Total Displacement	510 cm ³
Bore	85 mm
Stroke	90 mm
Maximum power	11.2 HP
Maximum torque	33.1 Nm
Compression ratio	17.5
Connecting rod length	144.5 mm
Bore/Stroke	0.944
Injection type	Mechanical, 200 bar
Cooling	Water

2.1.2. Engine dynamometer

The test engine is loaded with ABB IP23 AC dynamometer with a maximum power of 53 kW, a maximum torque of 338 Nm and a maximum speed of 8000 rpm. Figure 2.4 shows the engine dynamometer. The AC dynamometer is capable of applying power to the test engine as well as braking by the connected driveshaft. This allows the dynamometer to apply external forces on the engine. The system with an AC dynamometer does not require an engine-mounted starter. In addition, it uses air-cooling to dissipate energy. ABB ACS800 single drive unit is used for controlling the AC dynamometer.

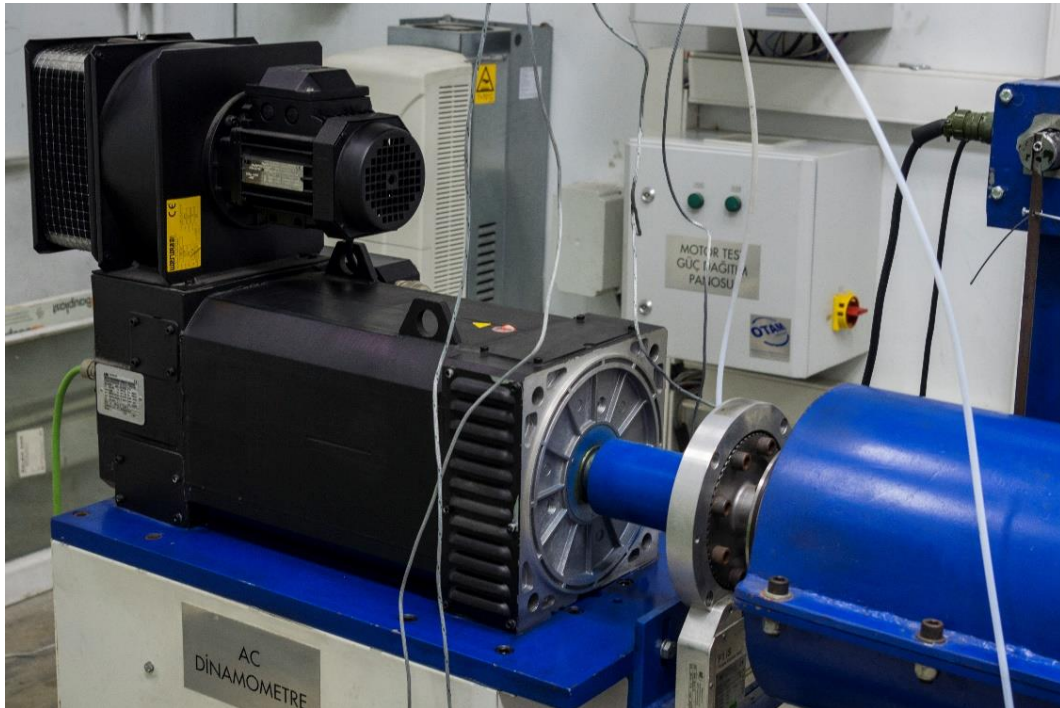


Figure 2.4. The engine dynamometer

The engine is controlled using the dynamometer control software (MpiCON). The engine data are recorded using the software. Engine tests could be performed at different speeds and loads. By entering the engine speed and the load to the dynamometer control software, the engine test data are collected. In addition, the engine coolant inlet and outlet temperature, fuel flow mass, fuel temperature, intake air temperature, exhaust gas temperature, exhaust emissions can be measured and recorded. The interface of the engine dynamometer control software is illustrated in Figure 2.5.



2.1.4. Fuel mass flowmeter

Rheonik RHM 03 coriolis fuel mass flow meter is used to measure the fuel mass flow (Figure 2.7 and Table 2.3).



Figure 2.7. Rheonik RHM 03 fuel mass flow meter

Table 2.3. Rheonik RHM 03 Coriolis mass flow meter

Typical Application Range	0.0038 – 5 kg/min
Max. Pressure	122.4 MPa
Temperature	-196 – 350°C
Accuracy	0.1% of rate
Process Connections	1/8" – 1"

2.1.5. Emission measurement system

ICE takes air from the atmosphere and mixed with fuel, and combustion occurs and creates the desired effect of heat and pressure inside the cylinder by the combustion process. Engine power and torque are produced with the release of chemical energy of the fuel. The hydrocarbon reacts with the oxygen and produces CO₂ and H₂O during the

complete combustion process. Due to some reason besides complete combustion products, ICE produces CO, HC, NO_x and soot emissions, which are harmful to human health. CO₂, however, is a complete combustion product, but it has a negative impact on the environment because it causes global warming. Diesel engines generally produce NO_x and soot emissions, while spark ignition engines produce HC and CO emissions. The technical specification of the exhaust emission measurement device used in the experiments are shown in Table 2.4. LumaSense Andros 6500 emission system was used for HC, CO and CO₂ and ITG-A-22 sensor was used for NO, and ITG-A-01 sensor was used for O₂ in the experiments (Figure 2.8).

Table 2.4. Emission measurement system specification

	Measurement Range	Resolution	Accuracy
CO	0-15 % vol.	0.001 % vol.	± 3-5 % rel.
NO _x	0-5000 ppm	1 ppm	± 4-5 % rel.
CO ₂	0-20 % vol.	0.01 % vol.	± 3-5 % rel.
HC	0-30000 ppm	1 ppm	± 3-8 % rel.
O ₂	0-25 % vol.	0.01 % vol.	± 3 % rel.
Lambda	0.5-9.99	0.1	± 3 % rel.
Opacity	0-100 %	0.1 %	± 3 % rel.

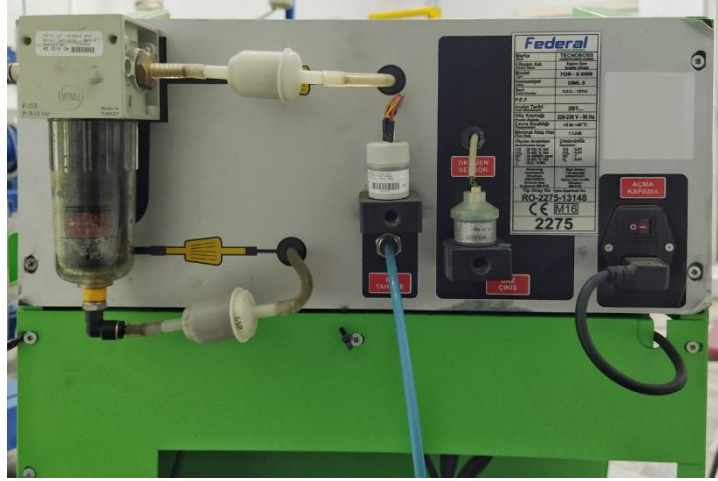


Figure 2.8. Exhaust emission measurement system

Exhaust emissions of the engine are typically measured in parts per million (ppm) or volume percent (vol%) using a gas analyzer. Measured emission values must be converted to g/kWh to be compared with European emission standards. The measured values are converted according to the standards with the use of the following equations (Chintala, Benaerjee, Ghodke, & Porpatham, 2019; Pilusa, Mollagee, & Muzenda, 2012):

$$ME_{species} = MF_{species} \times \frac{MW_{species}}{MW_{Exh}} \times \frac{\dot{m}_{Exh}}{P_{brake}} \quad (2.1)$$

where, $ME_{species}$ is mass emission of species as g/kWh, $MF_{species}$ is mole fraction of species as ppm, $MW_{species}$ is molecular weight of species, MW_{Exh} is molecular mass of exhaust gas, $\dot{m}_{Exh}$ is exhaust mass flow rate as kg/h, and P_{brake} is brake power as kW. The ratio of exhaust mas flow and power was obtained using the empirical constants:

$$\frac{\dot{m}_{Exh}}{P_{brake}} = 3.873 \quad g / kWh \quad (2.2)$$

The conversion from the exhaust emissions concentration (ppm) to specific fuel consumption (g/kWh) is summarized as follows:

$$CO \quad (g / kWh) = 35.897 \times CO \quad (vol\%) \quad (2.3)$$

$$NO_x \quad (g / kWh) = 5.896 \times 10^{-3} \times NO_x \quad (ppm) \quad (2.4)$$

$$Soot \quad (g / kWh) = 1.538 \times 10^{-3} \times Soot \quad (ppm) \quad (2.5)$$

$$CO_2 \text{ (g / kWh)} = 56.409 \times CO_2 \text{ (vol\%)} \quad (2.6)$$

2.1.6. In-cylinder pressure analyzer

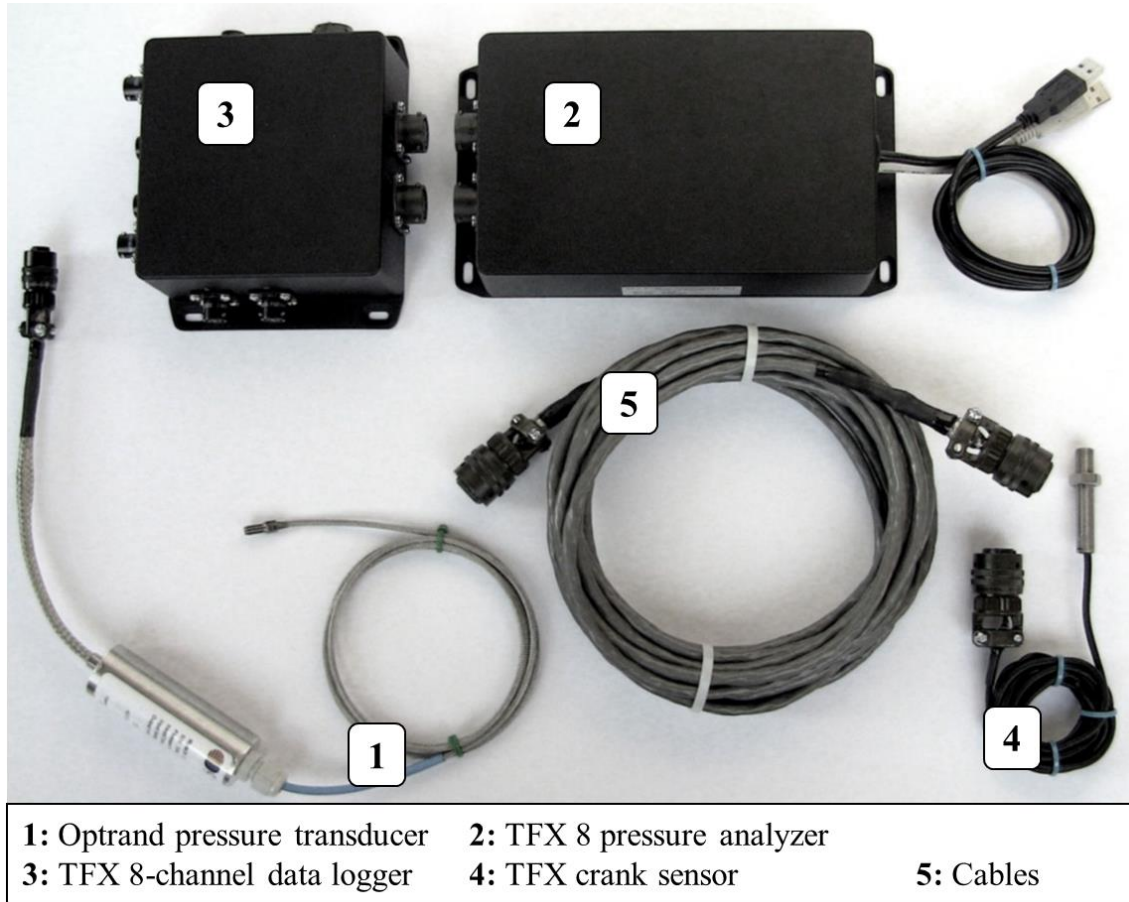


Figure 2.9. In-cylinder pressure measurement system

In-cylinder pressure measurement system consists of the TFX crank encoder, Optrand pressure transducer, TFX 8-channel data logger, TFX combustion analysis software and computer. The in-cylinder pressure transducer specifications are given in Table 2.5. In-cylinder pressure sensor has been installed using an adapter with minimum alteration in the combustion chamber. High-temperature red RTV silicone gasket is applied to the adapter and the sensor connection and insulated. Figure 2.9 shows the in-cylinder pressure measurement system. In-cylinder pressure sensor has no contact with the engine coolant, and it is air-cooled.

Table 2.5. In-cylinder pressure sensor specifications

Model	Optrand AutoPSI
Pressure Range	0-200 bar
Over pressure	2 x 200 bar
Non-Linearity & Hysteresis	±1% FSO (combustion), ±0.5% FSO (non-combustion)
Frequency Range	0.1 Hz to 15 kHz (typical)
Diaphragm Resonant Frequency	>120kHz
Sensor Housing Temperature Range	-40° to 350°C
Fiber Optic Cable Operating Temperature	-40° to 200°C
Vibration	100G
Sensor Input Signal	9-18V DC
Sensor Output Signal	Analog, 0.5 to 5V
Lifetime	200 Million Pressure Cycles or 2 Years

Figure 2.10 shows TFX combustion analyzer software user-interface. Using the software, fuel line pressure and in-cylinder pressure sensor can be measured relative to the crank angles. The software generates P-V and P-CA graphs, combustion and compression pressure. Burn rate, and IMEP can be calculated.

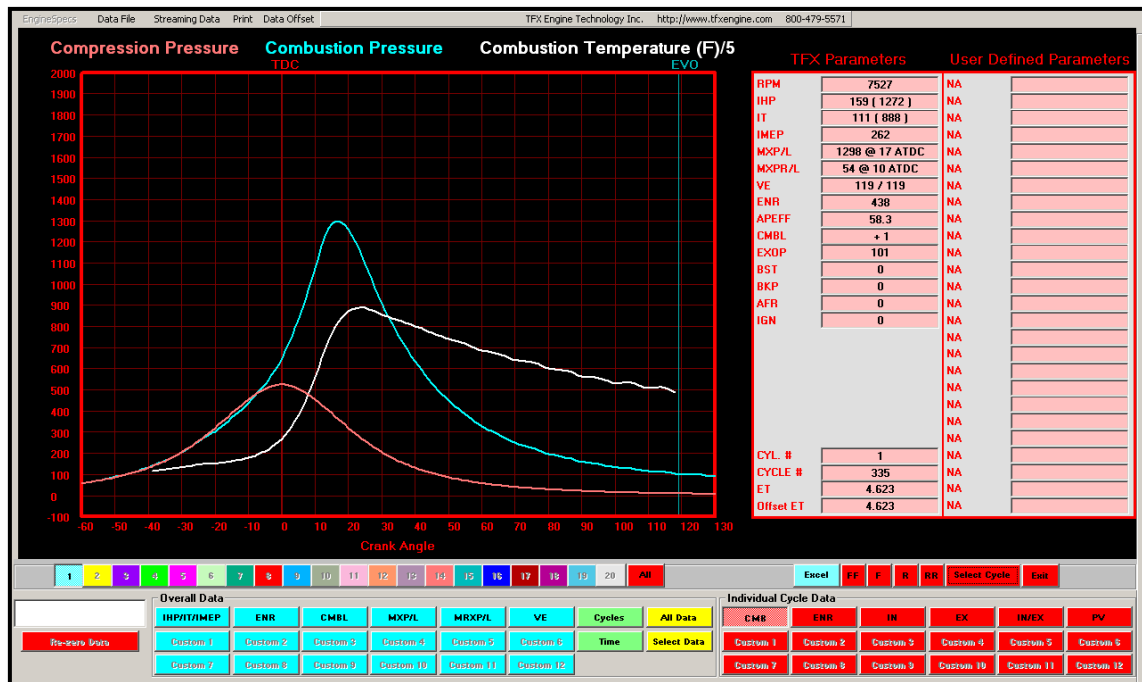


Figure 2.10. User-interface of the combustion analyzer software

2.1.7. Fuel line pressure sensor

Optrand AutoPSI-S2000 fuel line pressure sensor shown in Figure 2.11 is connected to the TFX data logger. The data from the sensor is collected in the TFX combustion analysis software. The fuel line pressure sensor is mounted on the high-pressure fuel line using an adapter. The fuel line sensor, adapter and fuel line are insulated using high-temperature silicone gasket. The specifications of the fuel line sensor are shown in Table 2.6.



Figure 2.11. Fuel line pressure sensor

Table 2.6. Optrand AutoPSI-S2000 fuel line sensor specifications

Pressure Range	0 - 2000 bar
Over Pressure	0 - 3000 bar
Accuracy	0.3333 mV/MPa
Frequency Range	0.1 Hz to 15 kHz
Natural Frequency	> 150 kHz
Operating Temperature	-40 - +300°C
Non-Linearity and Hysteresis	± 1.0% FSO
Interface Power Supply	9 - 18 DC, 85 mA
Output Signal	0.5 - 5 V Analog

2.1.8. Crank encoder

The crank encoder used in the experiments generates 1440 signals at each revolution (4 signals per crank angle). The characteristics of the crank encoder are listed in Table 2.7. The crank encoder is connected to crankshaft using adapter. Figure 2.12 shows the crank encoder and adapter.

Table 2.7. Crank encoder specifications

Type	TFX crank encoder
Pulse speed	1440 pulse/revolution
Operating Temperature	-40 - +80°C
Power Supply	5 - 30V DC
Pulse Frequency	300 kHz
Shock resistance	2500 m/s ²
Vibration resistant	100 m/s ²

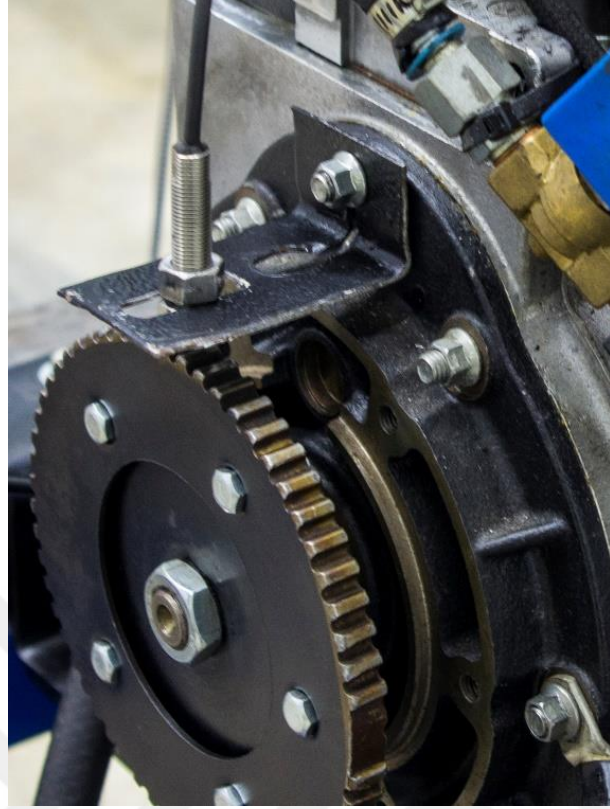


Figure 2.12. Crank encoder

2.2. Uncertainty Analysis

The uncertainty analysis of the experimental data was carried out using Kline and McClintock method (Kline & McClintock, 1953). In this method, the total error was calculated using the sensitivities of the sensors (Genceli, 1995; Yılmaz, 2015). The calculated percentage error are given in Table 2.8.

$$w_t = \sqrt{a^2 + b^2 + c^2} \quad (2.7)$$

where w_t is the total percentage error [%], a , b and c are percentage error [%].

Table 2.8. Measurement accuracies

Parameter	Apparatus	Accuracy	Total Error
Engine torque	Load cell	$\pm 0.25 \%$	$\pm 0.25 \%$
Engine speed	Crank encoder	$\pm 0.10 \%$	$\pm 0.1 \%$
Engine power	Torque	$\pm 0.25 \%$	$\pm 0.27 \%$
	Crank encoder	$\pm 0.1 \%$	
BSFC	Fuel mass flow meter	$\pm 0.1 \%$	$\pm 0.29 \%$
	Torque	$\pm 0.25 \%$	
	Crank encoder	$\pm 0.1 \%$	
In-cylinder pressure	In-cylinder pressure sensor	$\pm 0.05 \%$	$\pm 0.11 \%$
	Crank encoder	$\pm 0.1 \%$	
Fuel line pressure	Fuel line pressure sensor	$\pm 0.05 \%$	$\pm 0.11 \%$
	Crank encoder	$\pm 0.1 \%$	
CO	LumaSense Andros 6500	$\pm 5 \%$	$\pm 5 \%$
NO _x	LumaSense Andros 6500	$\pm 5 \%$	$\pm 5 \%$
CO ₂	LumaSense Andros 6500	$\pm 5 \%$	$\pm 5 \%$
HC	LumaSense Andros 6500	$\pm 8 \%$	$\pm 8 \%$
O ₂	LumaSense Andros 6500	$\pm 3 \%$	$\pm 3 \%$
Lambda	LumaSense Andros 6500	$\pm 3 \%$	$\pm 3 \%$
Opacity	LumaSense Andros 6500	$\pm 3 \%$	$\pm 3 \%$

2.3. Experimental Procedure

The study was started by installation the test engine on the dynamometer. Adapters were manufactured to install the test engine to the dynamometer. The fuel system of the diesel engine was made to be fed from the fuel tank on the dynamometer. The cooling system of the diesel engine was connected to the cooling tower in test laboratory. Utilizing the cooling tower, the engine coolant can be maintained at a constant temperature. The exhaust manifold of the test engine was connected to the gas analyzer.

Experimental data were collected when the engine coolant temperature reached 80°C to ensure stable operation. The experiments were carried out at an increase of 200 rpm between 1200 and 3000 rpm. Load values were increased of 10% between 10 and 100%. Therefore, 100 operation points were taken at different speeds and loads. In this way, the performance curve of the engine was derived. To minimize the percentage error during the combustion analysis, 100 cycles of data were obtained in each operation point.

3. NUMERICAL METHODS AND MODELING

The modeling a process in engineering means developing and using appropriate assumptions and equations to analyze the critical properties of the process. Modeling of an internal combustion engine will develop as our understanding and knowledge of the physics and chemistry mechanism of the phenomena and as computers continue to increase their ability to solve complex equations. The models describe the thermodynamics, fluid flow, heat transfer, combustion and emission formation events that calculate the performance parameters of the engines. Two basic models have been developed to solve engine performance and emissions. These can be classified as Thermodynamic and CFD models, depending on whether the model is used solely for the conservation of energy and mass or for examining the entire fluid flow inside the domain.

The thermodynamic models are ground solely on the conservation of energy and mass. The terminology of single-zone and multi-zone models is often used in thermodynamic models. The single-zone model is derived from the first law of thermodynamics and the conservation of mass and energy and it is dimensionless, and single-volume considered. Since all thermodynamic properties are evaluated as a uniform. In the multi zone thermodynamic model, however, the combustion chamber is disunited to sundry zones with the same thermodynamic features. Mathematical equations of these models consist of a group of differential equations with independent variables of time (or crank angle). Quasi-dimensional (QD) model is a particular type of such models. The QD model is obtained by adding diesel fuel injection patterns and specific geometric features to the basic thermodynamic approach in CI engines (Lakshminarayanan & Aghav, 2010; Mauro et al., 2018; Medina et al., 2014).

Computational Fluid Dynamics (CFD) model is multi-dimensional model derived from the conservation of energy, mass, momentum and chemical reaction mechanism inside the combustion chamber. Mathematically, the primary equations of these models are depend on the system of partial differential equations namely the Navier-Stoke equations. The coordinates of time and spatial variables are assessed as independent. Therefore, the properties of the liquid in the combustion chamber can be obtained in 3D and full spatial resolution (Lakshminarayanan & Aghav, 2010; Mauro et al., 2018; Medina et al., 2014).

Due to the complexity and lack of understanding of engine operation and combustion, most engine models have some deficiencies. Empirical relationships and ad hoc approximations are often needed to close gaps in the analysis of critical events. Hence, the models will continue to be developed for greater completeness and generality (Heywood, 1988).

3.1. Quasi-Dimensional Models

3.1.1. Combustion model

3.1.1.1. Single-Zone model

The single-zone model is based on the thermodynamic analysis of the processes inside the combustion chamber. The conservation equations are applied to the cylinder for air, fuel, and residuals during each stroke in this model. In the compression and expansion stroke, the system is considered as closed while it is considered as open during intake and exhaust stroke and the mass passing through the ports must be calculated. The composition inside the cylinder is different during all phases, since before combustion phase contains an air-fuel and residual mixture, but after combustion phase merely contains residuals. Thermodynamic properties (pressure, temperature, mixing, etc.) and transport properties (viscosity, conduction, etc.) of the mixture are evaluated as spatially uniform and it solved as time-dependent (Mauro et al., 2018).

3.1.1.2. Multi-Zone model

Multi-zone model divides the domain into several regions such that each zone has identical thermodynamic properties. Sensitivity analysis determines the optimum number of zones. Conservation equations are applied to each region and it is assumed that there is mass, heat, and mass exchange between regions. Any other thermodynamic properties of each region are evaluated as uniformly. The properties may be however different from other regions. This model allows analyzing the temperature effects and species stratification. This approach provides a better estimate of the precise combustion duration, pressure increment, and exhaust emissions (Medina et al., 2014).

Two-Zone model divides the combustion chamber into burned and unburned zones in order to model combustion. The following energy equations are solved for the two regions.

Unburned Zone:

$$\frac{d(m_u e_u)}{dt} = -p \frac{dV_u}{dt} - \frac{dQ_u}{dt} + \left(\frac{dm_f}{dt} h_f + \frac{dm_a}{dt} h_a \right) + \frac{dm_{f,i}}{dt} h_{f,i} \quad (3.1)$$

Burned Zone:

$$\frac{d(m_b e_b)}{dt} = -p \frac{dV_b}{dt} - \frac{dQ_b}{dt} + \left(\frac{dm_f}{dt} h_f + \frac{dm_a}{dt} h_a \right) \quad (3.2)$$

In the above equations, p is in-cylinder pressure, e energy, m mass, m_a air mass, m_f fuel mass, $m_{f,i}$ injected fuel mass, V volume, Q heat transfer rate, h_f enthalpy of fuel mass, h_a enthalpy of air mass, $h_{f,i}$ enthalpy of injected fuel mass. Subscript “b” means burned and subscript “u” means unburned zone.

Wiebe function is used to carry out combustion model. The Wiebe function is shown as follows:

$$x_b = 1 - \exp \left(-a \left(\frac{\theta - \theta_0}{\Delta \theta} \right)^{m+1} \right) \quad (3.3)$$

where x_b is the mass fraction burned, θ is the crank angle, θ_0 is the crank angle at the start of the combustion, $\Delta \theta$ and a determine the combustion duration and m fixes the shape of the combustion curve. $\Delta \theta$, a , and m are adjustable constants.

The Apparent Heat Release Rate (AHRR) can be calculated by solving the single zone energy equation (Gamma Technologies, 2016a). The following equation is calculated for each time step according to the pressure inside the cylinder (Yoon & Park, 2019).

$$AHRR = \left(-p \frac{dV}{dt} - \frac{dQ}{dt} - \frac{d(me)}{dt} \right) \quad (3.4)$$

3.1.2. In-cylinder flow model

The in-cylinder flow model splits the combustion chamber into several zones: the central core zone, the squish zone, the head recess zone, and the piston bowl zone. At each time-step in each zone, the average radial velocity, axial velocity and vortex velocity are calculated taking into account cylinder geometry, piston movement and the flow rates of

incoming and outgoing gases through the valves. These velocities are used in the "flow" heat transfer model. The flow model also includes single-zone turbulence and tumble models.

Swirl and tumble values can be predicted or imposed. When these values are predicted, the most significant factors in the simulations are the tumble and swirl produced by the fluids entering the cylinder from the valves. The tumble and swirl coefficients specified in the valves are used to calculate the tumble and swirl torque applied to the in-cylinder fluid. Generally, increasing the magnitude of the tumble and swirl coefficients will increase the swirl and tumble formation along with the valve flow. When using the impose option, the swirl and tumble profiles are defined as a function of the angle. Swirl and tumble coefficients are determined by the user according to Lift / Diameter. Swirl and tumble coefficients are described as the ratio of angular momentum flux to linear momentum flux, and tumble and swirl torque measurements from a flow bench can be calculated as follows (Uzkan, Borgnakke, & Morel, 1983).

$$C_s = \frac{2T}{\dot{m}U_{is}B} \quad (3.5)$$

$$C_t = \frac{2T}{\dot{m}U_{is}B} \quad (3.6)$$

$$U_{is} = \sqrt{RT_0} \left\{ \frac{2\gamma}{\gamma-1} \left[1 - P_R^{\frac{\gamma-1}{\gamma}} \right] \right\}^{\frac{1}{2}} \quad (3.7)$$

$$|C_s| + |C_t| \leq 1 \quad (3.8)$$

where C_s is swirl coefficient, C_t tumble coefficient, T torque, $\dot{m}$ mass flow rate, U_{is} isentropic valve velocity, B bore, P_R absolute pressure ratio, T_0 upstream stagnation temperature and γ specific heat ratio.

3.1.3. In-cylinder heat transfer model

WoschniGT, Flow, WoschniClassic, WoschniSwirl, WoschniHuber and Hohenberg models are used for the calculation of engine heat transfer. In this thesis, Woschni model was used because of its widespread use in the literature (Chang et al., 2004; Sanli, Sayin,

Gumus, Kilicaslan, & Canakci, 2009). Convective heat transfer coefficient defined in Woschni model is (Nabi, Rasul, & Brown, 2019):

$$h_{c, \text{ Woschni}} = \frac{K_1 p^{0.8} w^{0.8}}{B^{0.2} T^{K_2}} \quad (3.9)$$

where B is the bore diameter (m), K_1 and K_2 are constants 3.01426 and 0.5, respectively for WoschniGT model, p in-cylinder pressure (kPa), T in-cylinder temperature (K), and w average cylinder gas velocity (m/s) as given below:

$$w = C_1 \bar{S}_p + C_2 \frac{V_d T_r}{P_r V_r} (p - p_m) \quad (3.10)$$

where C_1 and C_2 are constant defined below for WoschniGT model, $\bar{S}_p$ the mean piston speed (m/s), T_r working fluid temperature prior to combustion (K), p instantaneous fluid pressure (kPa). V_d is displacement volume (m^3), V_r working fluid volume prior to combustion (m^3), p_m motoring fluid pressure at same angle as p (kPa) and p_r working fluid pressure prior to combustion (kPa).

$$C_1 = 2.28 + 3.9 \times \left(\frac{\text{Net mass flow into cylinder from valves}}{\text{Trapped mass} \times \text{Engine frequency}} \right) \quad (3.11)$$

$$C_2 = 0 \quad (\text{during cylinder gas exchange and compression}) \quad (3.12)$$

$$C_2 = 3.24e^{-3} \quad (\text{during combustion and expansion}) \quad (3.13)$$

3.1.4. Flow within the manifolds

Fluid flow inside the ports and manifolds are solved by one-dimensional Navier-stoke and heat transfer equations. Conservation equations solve the flow direction in the model. Conservation of mass is described by the change rate in the sub-system:

$$\dot{m}_{sub} = \sum_i \dot{m}_i - \sum_e \dot{m}_e \quad (3.14)$$

The rate of mass flow is defined as follows:

$$\dot{m} = \rho AU \quad (3.15)$$

where, U is the fluid velocity, A the cross sectional area of a flow and ρ the density. Energy conservation is equal to the change rate in subsystems and the total energy transfer of the system. Related equation:

$$\frac{dE}{dt} = \frac{\partial Q}{\partial t} - \frac{\partial W}{\partial t} \quad (3.16)$$

$$\frac{d(me)}{dt} = p \frac{dv}{dt} + \sum_i \dot{m}_i H - \sum_e \dot{m}_e H - h_g A (T_{gas} - T_{wall}) \quad (3.17)$$

where H is total enthalpy, e internal energy, h_g heat transfer coefficient, T_{gas} gas temperature and T_{wall} wall temperatures. The heat transfer from the fluids to the walls depends on the heat transfer coefficient, the wall and fluid temperatures. At each step, the heat transfer coefficient determined as function of wall surface roughness, fluid velocity, and thermo-physical properties. The wall temperatures set as input (M. Yilmaz, 2009).

$$h_g = \frac{1}{2} C_f \rho U_{eff} C_p Pr^{\frac{2}{3}} \quad (3.18)$$

where C_f is the friction coefficient, U_{eff} the outer boundary layer effective velocity, and Pr the Prandtl number. The friction coefficient is connected with Reynolds number:

$$Re = \frac{\rho U_c L_c}{\eta} \quad (3.19)$$

where ρ is the density, L_c the characteristic length, U_c the characteristic speed, and η the dynamic viscosity. Friction coefficient on smooth surfaces:

$$C_f = \frac{16}{Re_D} \quad (3.20)$$

$$C_f = \frac{0.08}{Re_D^{0.25}} \quad (3.21)$$

Equation 3.20 is used for laminar region ($Re_D < 2000$) and equation 3.21 is used for linear transitional region ($Re_D < 2000$). The Prandtl number is:

$$Pr = \frac{\eta C_p}{\lambda} = \frac{\nu}{a} \quad (3.22)$$

where η is the dynamic viscosity, λ the heat conduction coefficient, α the thermal diffusivity and ν the kinematic viscosity.

Providing that the flow is not laminar and the wall surface is rough, the value of the above friction coefficient is given by the formula of Nikuradse (M. Yilmaz, 2009):

$$C_{f(rough)} = \frac{0.25}{\left(2 \log_{10} \left(\frac{1}{2} \frac{D}{h} \right) + 1.74 \right)^2} \quad (3.23)$$

where D is the pipe diameter and h the roughness height. The friction characteristics in ducts and flow division can be used to scale the determined friction if necessary.

Momentum conservation, pressure forces acting on a subsystem and wall shear forces are equal to the rate of change of momentum in the system.

$$\frac{d\dot{M}}{dt} = \frac{dpA + \sum_i \dot{m}_i u + \sum_e \dot{m}_e u - 4C_f \frac{\rho u^2}{2} \frac{dx A}{D} - C_p \frac{1}{2} \rho u^2 A}{dx} \quad (3.24)$$

where dx is the element length, C_p the pressure loss coefficient, C_f the friction loss coefficient, D the equivalent diameter and u is fluid velocity. In order to achieve the correct coefficient of pressure and friction loss, the model uses empirical correlations to define the surface roughness and the pipe curvature.

The pressure loss coefficient is:

$$C_{pressure} = \frac{p_1 - p_2}{\frac{1}{2} \rho V_1^2} \quad (3.25)$$

where p_1 is the inlet pressure, p_2 the outlet pressure, and V_1 the inlet velocity.

All subsystem is evaluated in small-scale volumes where a single volume represents a flow split. The manifold flow is divided into sundry small volumes. Scalar properties like pressure, temperature, density, etc. are estimated homogeneous for each volume. Improvements to accuracy can be considered by selecting an appropriate period of discretization. However, the discretization length is restricted by the time step size. The explicit method is used for time integration of governing equations. This method solves the system status at the next time step from the current system state. If we put $Y(t)$ in the

existent state of the system and $Y(t + \Delta t)$ in a later state (small time step Δt), the explicit method is:

$$Y(t + \Delta t) = F(Y(t)) \quad (3.26)$$

The Courant–Friedrichs–Lewy condition limits the time step with given resolution of the element volume:

$$\frac{\Delta t}{\Delta x}(u + c) \leq 0.8 \quad (3.27)$$

where Δt the time step, Δx is the discretized length, c the speed of sound and u the fluid velocity. Discretization length and time step are interrelated. In the system, a duct is divided into small volumes according to the discretization length. However, flow split is single volume. They are linked to other volumes by boundaries. Mass, momentum and energy equation are solved as one-dimensional. Therefore, averaged numerical quantities are used throughout the flow direction area. The scalar quantities are calculated at the center of the sub-system. The vector quantities are determined at the faces of the subsystem. The flow is achieved with explicit time integration of equations for mass, energy, and momentum using a small time step (M. Yilmaz, 2009).

GT-Suite commercial code was used to model test engine in this thesis (Gamma Technologies, 2016a, 2016b). This commercial code has the capability for combustion analysis, turbocharger matching including waste gates, variable geometry turbines, and control strategies, manifold design, valve lift profile and timing optimization, EGR system performance, thermal analysis of engine components, design of active and passive control systems, noise analysis, and after-treatment systems.

An engine can be modeled according to speed and load. The valve lift can be simulated depending on the crank angle as mass input and output in the model.

3.2. Multi-Dimensional Models

A multi-dimensional or Computational Fluid Dynamics model allows solving the valve movement, fuel injection, in-cylinder flow with a higher spatial resolution inside the cylinder. Computational Fluid Dynamics (CFD) model describes the effects of turbulence in detail.

The aviation industry has integrated CFD modeling techniques into the design since the 1960s. Nowadays, with the increase in the computing capability of CPU, it is used for the design of ICEs and gas turbines. CFD model solves partial differential equations for the conservation of momentum, energy, mass, and species concentrations for the combustion chamber and the intake and exhaust ports. Basic steps in the solution are defining the geometry, meshing, defining the liquid-gas properties and the boundary conditions (Medina et al., 2014).

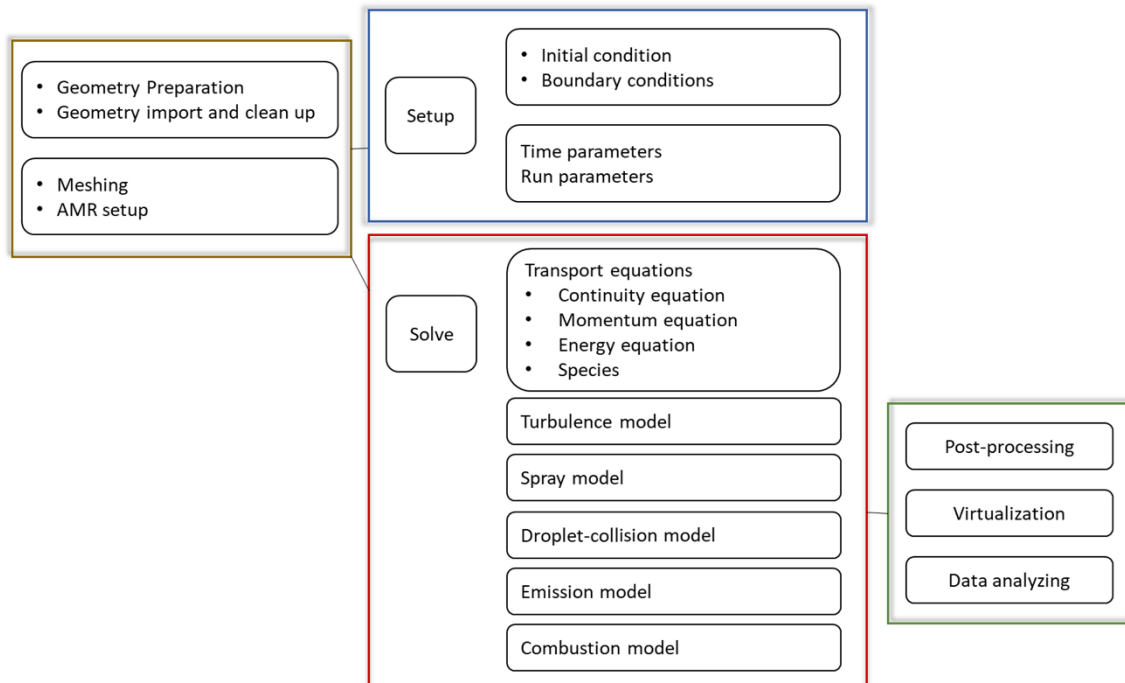


Figure 3.1. Simulation process flow chart for multi-dimensional case

Commercial CFD code, Converge CFD[®], used to simulate in-cylinder flow, spray and combustion for a test engine (Richards, Senecal, & Pomraning, 2019). The CFD commercial code solves full Reynolds-averaged Navier-Stokes (RANS) equations including turbulence models. For meshing, modified cut-cell Cartesian grid method has been used. For moving boundaries, the domain is re-meshed at each time-step. Adaptive

mesh refinement (AMR) is used to refine the mesh based on moving and fluctuating conditions such as velocity or temperature. Simulation flow process chart illustrated in Figure 3.1.

3.2.1. Solution procedure

The solution algorithm of the transport equations is very important to configure the simulation parameters. Figure 3.2 illustrates the algorithm for solving transport equations used by commercial code. The PISO algorithm (Issa, 1986) begins with a prediction step in which the momentum and pressure equation is solved following the prediction. The momentum equation is corrected and solved again. This procedure is repeated enough to achieve the necessary convergence. Other transport equations are solved in order when the momentum prediction and correction steps have been completed.

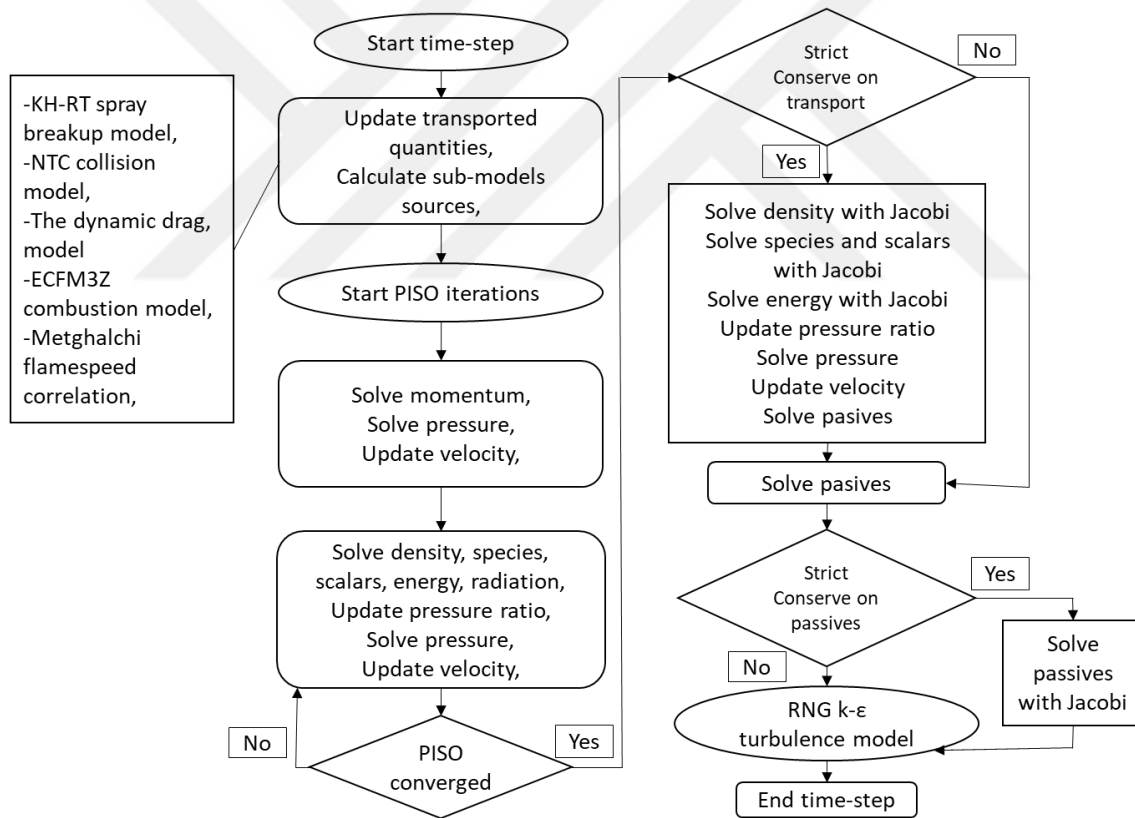


Figure 3.2. Solution algorithm of CFD simulation

Toward the beginning of each time-step, the previous values are collected for all transported amounts. Next, explicit sources are determined for each sub model that is actuated and radiation is solved if energy and radiation are decoupled. Toward the start of the PISO loop, it is solved for momentum and pressure, which sets the velocity for the

other transport equations. After each PISO iteration, it is important to check for PISO loop convergence. For compressible cases, it is considered the PISO loop to be converged.

3.2.2. Governing equations

The dynamics of fluid flow are governed by equations defining the conservation of momentum, energy, and mass. Additional equations describe turbulence and passive, scalar and transport of species.

3.2.2.1. Mass and momentum transport

It is necessary to solve the gradient of mass and momentum equations. Equations for mass and momentum transport of compressible fluids are as follows respectively (Gül, 1994):

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = S \quad (3.28)$$

and

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + S_i \quad (3.29)$$

Here viscous stress tensor (Maia et al., 2020) is given as:

$$\sigma_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \left(\frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \quad (3.30)$$

where P is pressure, S the source term, δ_{ij} the Kronecker delta, and μ viscosity.

Equations 3.28 and 3.29 both allow source terms. While for the momentum equation, source terms may arise, for example, from gravitational acceleration, spray convection, or mass sources, the source term for the mass conservation equation may arise from evaporation or other sub-models.

Momentum equation is solved by using finite volume method. When solving the momentum equation, the conserved values on the solid surfaces should be expressed in terms of the primitive values at the cell center.

3.2.2.2. Energy transport

The energy equation can be solved independently or together with the momentum and mass equations. If the energy equation is solved without momentum and mass, the transport will not be included in the energy transport equation, which contains only diffusion terms (Richards et al., 2019). The energy equation for compressible flows is given below:

$$\frac{\partial \rho e}{\partial t} + \frac{\partial u_j \rho e}{\partial x_j} = -P \frac{\partial u_j}{\partial x_j} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left(K \frac{\partial T}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\rho D \sum_m h_m \frac{\partial Y_m}{\partial x_j} \right) + S \quad (3.31)$$

where Y_m the mass fraction of species m , e the specific internal energy, D the mass diffusion coefficient, K the conductivity, h_m the enthalpy of species, T temperature, σ_{ij} the stress tensor and S the source term. If the turbulence model is included, the conduction term is replaced by turbulence conduction:

$$K_t = K + C_p \frac{\mu_t}{Pr_t} \quad (3.32)$$

where μ_t is the turbulent viscosity, and Pr_t the turbulent Prandtl number. The turbulent Prandtl number is:

$$Pr_t = \frac{c_p \mu_t}{k_t} \quad (3.33)$$

where μ_t is the turbulent viscosity, and k_t the turbulent conductivity.

3.2.2.3. Species transport

The equations of species transport solve the mass fractions of species in the region. Mass fraction of species:

$$Y_m = \frac{M_m}{M_t} = \frac{\rho_m}{\rho_t} \quad (3.34)$$

where M is the mass of species, ρ is the density of the cell, sub script m means mass of species m and sub script t means total mass of the cell.

Equations of the species can be solved alone or together with other equations of transport. If the momentum equation is not solved, the species transport equation will not be taken into account in the transport equation. Therefore, the conservation equation of the species will include only diffusion terms.

Conservation equation of species for compressible flow:

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial \rho_m u_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial Y_m}{\partial x_j} \right) + S_m \quad (3.35)$$

where ρ_m is the density equals to $Y_m \rho$, Y_m mass fraction of species m , Sc is Schmidt number, D is the mass diffusion coefficient, equals to $\frac{\nu}{Sc}$, and S_m is the source term. This source term in the species equation regards to combustion, evaporation and other sub-models.

3.2.2.4. Turbulent modeling

Turbulence is a highly complicated fluid motion. Turbulent flow is three-dimensional, time-dependent, intermittent, rotational, diffusive, dissipative and disordered. Turbulence transport the energy to smaller spatial scales across a continuous wave-number spectrum. The primary mechanisms of turbulence are eddy that is a typical turbulence pattern, covering a range of wavelengths. Many sized eddies can exist in the same volume of fluid and high-vorticity regions. Turbulence, which is a characteristic of the liquid, is defined by the eddy viscosity as a local property of the liquid (Launder & Spalding, 1974; Markatos, 1984).

Turbulent mixing is a convective process resulting from the existence of turbulent vortices in the flow. These turbulent effects occur on lots of length scales. If a CFD solver does not contain a discrete area (grid) that can solve the smallest vortex length scale, the solver cannot fully take into account the improved mixing effects of the turbulence in the simulations. Currently, it is impractical to solve all length scales in a typical CFD simulation, and therefore turbulence models are used to take into account additional mixtures.

It is generally accepted that turbulence can be defined by Navier-Stokes momentum-transport equations (O. Reynolds, 1895). Reynold-Averaged Navier-Stokes (RANS) statistical approach is quite wide spread in CFD simulations in general (A. J. Reynolds, 1974). However, for the ICE simulations density-weighted ensemble averaging (DWEA) was used in these studies. Nevertheless, both equations are written in Reynolds averaging, and DWEA averaging yields the same form of partial differential equations. RANS approach in which flow variables are decomposed into a mean term and a fluctuating term (Gül, 1994):

$$\rho = \bar{\rho} + \rho' \quad (3.36)$$

$$U_i = \bar{U}_i + u_i \quad (3.37)$$

Moreover, averaging the equations for compressible flow produces the following:

Conservation of mass:

$$\frac{\partial}{\partial t}(\bar{\rho}) + \frac{\partial}{\partial x_j}(\bar{\rho}\bar{U}_j + \bar{\rho}\bar{u}_j) = 0 \quad (3.38)$$

Conservation of momentum:

$$\frac{\partial}{\partial t}(\bar{\rho}\bar{U}_i + \bar{\rho}'u_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\bar{U}_j\bar{U}_i + \bar{\rho}\bar{u}_j\bar{U}_i + \bar{U}_j\bar{\rho}'u_i + \bar{U}_i\bar{\rho}'u_j) = -\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial}{\partial x_j}\bar{\sigma}_{ij} \quad (3.39)$$

Transport of scalar, ϕ :

$$\frac{\partial}{\partial t}(\bar{\rho}\bar{\phi} + \bar{\rho}'\phi') + \frac{\partial}{\partial x_j}(\bar{\rho}\bar{U}_j\bar{\phi} + \bar{\rho}\bar{u}_j\bar{\phi}' + \bar{U}_j\bar{\rho}'\phi' + \bar{\phi}\bar{\rho}'u_j + \bar{\rho}\bar{u}_j\phi') = \frac{\partial}{\partial x_j}\left(\Gamma_\phi \frac{\partial \bar{\phi}}{\partial x_j}\right) + \bar{S}_\phi \quad (3.40)$$

Reynold stress:

$$\tau_{ij} = -\overline{\rho u_i' u_j'} \quad (3.41)$$

1) The k- ϵ turbulence model

Two equation model was first developed from interpolates Boussinesq's eddy viscosity concept by (Jones & Launder, 1972). The standard k- ϵ turbulence model (Launder &

Spalding, 1972) widely used in engine simulation (Yu Shi, Ge, & Reitz, 2011). It was later derived by the Renormalization Group (RNG) k-ε model (Yakhot & Orszag, 1986) using Renormalization Group theory. The RNG k- ε model was extended to compressible and two phase flows by (Han & Reitz, 1995). Gul has also developed a three-equation turbulence model for in-cylinder engine flow simulations (Gül, 1994). The RNG k- ε model has been preferred in this thesis for solution accuracy, simplicity and effectiveness. The model is widely used in the literature (H. Huang et al., 2018; Z. Li et al., 2019; Richards et al., 2019; Shu, Fu, Liu, et al., 2019; Shu, Fu, Zhao, et al., 2019). The turbulence length scale is given for all two-equation k- ε models:

$$l_e = C_\mu^{3/4} \frac{k^{3/2}}{\varepsilon} \quad (3.42)$$

k term for the turbulence kinetic energy (Launder & Spalding, 1974):

$$k = \frac{1}{2} \overline{u_i u_i} \quad (3.43)$$

Turbulence kinetic energy is half of the traces of the Reynolds stress tensor. Turbulence viscosity is given by:

$$\mu_t = C_\mu \frac{k^2}{\varepsilon} \quad (3.44)$$

where C_μ is the constant and can be tune according to species flow. Mean strain rate tensor is given as:

$$S_{ij} = \frac{1}{2} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \quad (3.45)$$

The model uses the terms of turbulent conductivity and turbulent diffusion in order to clarify the existence of turbulence in the transport of energy and mass. The terms of conductivity and turbulent diffusion is given as:

$$D_t = \frac{\mu_t}{\rho Sc_t} \quad (3.46)$$

and

$$K_t = \frac{\mu_t}{\rho Pr_t} C_p \quad (3.47)$$

where D_t is the turbulent diffusion, Sc_t the turbulent Schmidt number, K_t the turbulent conductivity, and Pr_t the turbulent Prandtl number.

The k- ϵ models require additional equations to obtain turbulence viscosity. One equation is the turbulent kinetic energy for turbulent kinetic energy, k and the other equation is the turbulent kinetic energy dissipation for the turbulent kinetic energy dispersion, ϵ . Turbulent kinetic energy transport equation for the RNG k- ϵ model is given as:

$$\frac{\partial \rho k}{\partial t} = \frac{\partial \rho u_i k}{\partial x_i} = \tau_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \frac{\mu + \mu_t}{Pr_k} \frac{\partial k}{\partial x_j} - \rho \epsilon + \frac{C_s}{1.5} S_s \quad (3.48)$$

In the above equation 1.5 value is empirical constant in the RNG k- ϵ model. Transport equation for the dissipation of turbulent kinetic energy is:

$$\begin{aligned} \frac{\partial \rho \epsilon}{\partial t} + \frac{\partial (\rho u_i \epsilon)}{\partial x_i} = & \frac{\partial}{\partial x_j} \left(\frac{\mu + \mu_t}{Pr_\epsilon} \frac{\partial \epsilon}{\partial x_j} \right) + C_{\epsilon 3} \rho \epsilon \frac{\partial u_i}{\partial x_i} + \\ & \left(C_{\epsilon 1} \frac{\partial u_i}{\partial x_j} \tau_{ij} - C_{\epsilon 2} \rho \epsilon + C_s S_s \right) \frac{\epsilon}{k} + S - \rho R \end{aligned} \quad (3.49)$$

where S is the user-defined source term and S_s is the spray source term. The $C_{\epsilon i}$ terms are model constant that account for expansion and compression. R equals to zero for standard k- ϵ model but R equation for RNG k- ϵ model is:

$$R = \frac{C_\mu \eta^3 \left(1 - \frac{\eta}{\eta_0} \right)}{(1 + \beta \eta^3)} \frac{\epsilon^2}{k} \quad (3.50)$$

where η is:

$$\eta = \frac{k}{\epsilon} |S_{ij}| = \frac{k}{\epsilon} \sqrt{2 S_{ij} S_{ij}} \quad (3.51)$$

3.2.2.5. Discrete phase modeling

The droplet parcels are defined to the region at the injector location at a specified size and number in order to calculate the spray in a simulation. The parcels represent the same set

of droplets (such as the same radius, speed, temperature, etc.) and they are used to represent the entire spray volume statistically. Using the droplet parcel concept significantly reduces the calculation time of a spray-containing simulation (Richards et al., 2019).

The identification of the spray is a process and the solution is achieved using specific models at each stage. In this thesis, solid cone injection is defined for fuel injection. KH-RT spray breakup model, dynamic drag model, NTC collision model, post collision results model, O'Rourke droplet turbulent dispersion model, drop/wall interaction rebound/slide model and multi-component vaporization evaporation model were used.

1) Spray breakup model

Fuel particles may become unstable because of interface forces acting on their surfaces during notional movement relative to the steady phase. Spray Breakup is used to solve this problem. For the spray breakup mechanism, although there are many different models, the Kelvin Helmholtz - Rayleigh-Taylor (KH-RT) model has been preferred due to widespread use in the literature for similar cases (Frassoldati et al., 2015; Reitz, 1987). The comparison of the photograph and modeled spray is shown in the Figure 3.3 (Kong, Senecal, & Reitz, 1999).

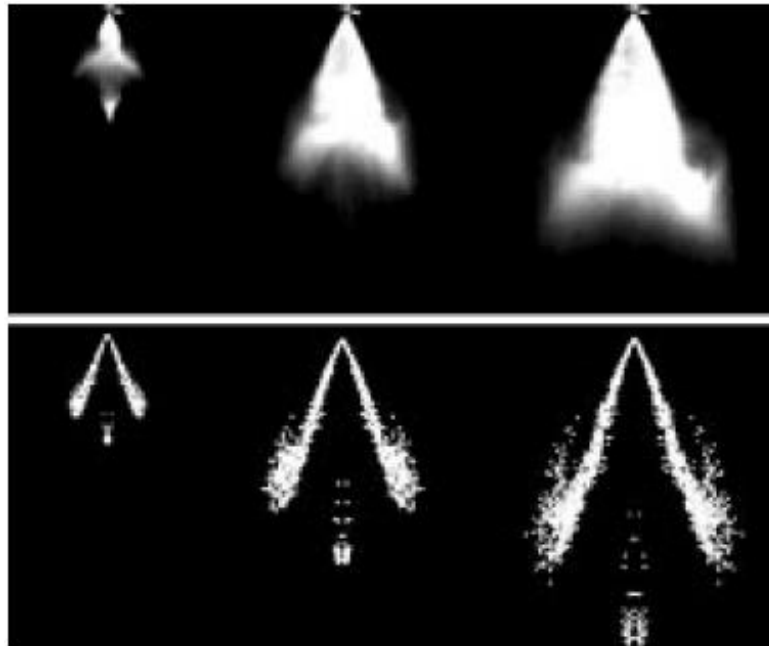


Figure 3.3. Photographs (top) and model predictions (bottom) for 0.7, 1.7 and 2.7 ms after the SOI (from left to right)

a) Kelvin-Helmholtz breakup model

It considers the stability of a cylindrical, liquid jet, viscous as a stationary, incompressible, inviscid gas stability at a rate of U which issuing from a circular orifice. The liquid has a radius r_0 , a density ρ_l and a viscosity μ_l . The polar coordinate system that moves with the jet is used.

Mechanical relationships for the definition of liquid and gas motion are combined with linearized hydrodynamic equations. The result is obtained by converting the equation of motion into flow and potential function (Reitz, 1987).

$$\begin{aligned} \omega_{KH}^2 + 2\nu_l k_{KH}^2 \omega_{KH} \left[\frac{l_1'(k_{KH} r_p)}{l_0(k_{KH} r_p)} - \frac{2k_{KH} L}{k_{KH}^2 + L^2} \frac{l_1(k_{KH} r_p)}{l_0(k_{KH} r_p)} \frac{l_1'(L r_p)}{l_0(L r_p)} \right] = \\ \frac{\sigma k_{KH}}{\rho_l r_p^2} (1 - k_{KH}^2 r_p^2) \left(\frac{L^2 - r_p^2}{L^2 + r_p^2} \right) \frac{l_1(k_{KH} r_p)}{l_0(k_{KH} r_p)} + \\ \frac{\rho_g}{\rho_l} \left(U - i \frac{\omega_{KH}}{k_{KH}} \right)^2 \left(\frac{L^2 - r_p^2}{L^2 + r_p^2} \right) \frac{I_1(k_{KH} r_p)}{I_0(k_{KH} r_p)} \frac{K_0(k_{KH} r_p)}{K_1(k_{KH} r_p)} \end{aligned} \quad (3.52)$$

where I and K are Bessel function, ω wave growth rate, k wave number and ν_l liquid viscosity. the maximum rate of growth, Ω_{KH} , and the corresponding wave length, Λ_{KH} , and are given by (Reitz, 1987):

$$\frac{\Lambda_{KH}}{r_p} = 9.02 \frac{(1 + 0.45 Z_l^{0.5})(1 + 0.4 T^{0.7})}{(1 + 0.87 We_g^{1.67})^{0.6}} \quad (3.53)$$

and

$$\Omega_{KH} \left[\frac{\rho_l r_p^3}{\sigma} \right]^{0.5} = \frac{(0.34 + 0.38 We_g^{1.5})}{(1 + Z_l)(1 + 1.4 T^{0.6})} \quad (3.54)$$

$$Z_l = \frac{\sqrt{We_l}}{Re_l} \quad (3.55)$$

$$T = Z_l \sqrt{We_g} \quad (3.56)$$

$$We_l = \frac{\rho_l U^2 r_p}{\sigma} \quad (3.57)$$

$$We_g = \frac{\rho_g U^2 r_p}{\sigma} \quad (3.58)$$

$$Re_l = \frac{U r_p}{\nu_l} \quad (3.59)$$

$$U = |u_i - v_i| \quad (3.60)$$

where Z_l is the Ohnesorge number, T is the Taylor number, We_l is the liquid Weber number, We_g is the gas Weber number, Re_l is the Reynold number, u_i is the fluid-phase velocity and v_i is the droplet velocity.

KH model, the first parcel size, nozzle orifice diameter d_0 is set equal and relatively large blobs injected into the atomization process is modeled using the liquid jet stability analysis as described above. The breakup of the parcels and the resulting droplets are calculated assuming that the droplet radius r_c , the quicker growing unstable surface wave given by Equation 3.61, is proportional to the wavelength.

This equation is:

$$r_c = B_0 \Lambda_{KH} \quad (3.61)$$

where B_0 is a model constant, 0.61 (Reitz, 1987). The change rate of droplet radius in a main parcel is given by:

$$\frac{dr_p}{dt} = -\frac{|r_p - r_c|}{\tau_{KH}} \quad (3.62)$$

The time of breakup, τ_{KH} is:

$$\tau_{KH} = \frac{3.726 B_l r_p}{\Lambda_{KH} \Omega_{KH}} \quad (3.63)$$

Stripping regime breakup criterion:

$$\frac{We_g}{Re_g^{0.5}} > 0.5 \quad (3.64)$$

The breakup size:

$$r_c = \frac{\sigma^2}{2\rho_g^2 U^3 v_g} \quad (3.65)$$

b) Rayleigh-Taylor breakup model

The unstable Rayleigh-Taylor (RT) waves occur on account of the quick retardation of the droplets from the drag force magnitude, which is given as (Ricart, Xin, Bower, & Reitz, 1997):

$$|F_{D,i}| = M_d |a_i| = M_d \frac{3}{8} C_D \frac{\rho_g |U_i|^2}{\rho_l r_o} \quad (3.66)$$

where $|a_i|$ is the droplet deceleration, C_D the drag coefficient, and M_d the drop mass. RT breakup model ignore the viscosity of fluids. Therefore, the quickest growing wavelength for the Rayleigh-Taylor instabilities is given by (Xin, Ricart, & Reitz, 1998):

$$\Lambda_{RT} = 2\pi \sqrt{\frac{3\sigma}{a(\rho_l - \rho_g)}} \quad (3.67)$$

In addition, growth rate used in model is:

$$\omega_{RT} = -k_{RT}^2 \left(\frac{\mu_l + \mu_g}{\rho_l + \rho_g} \right) + \sqrt{k_{RT}^2 \left(\frac{\rho_l - \rho_g}{\rho_l + \rho_g} \right) a - \frac{k_{RT}^3 \sigma}{\rho_l + \rho_g} + k_{RT}^4 \left(\frac{\mu_l + \mu_g}{\rho_l + \rho_g} \right)^2} \quad (3.68)$$

k_{RT} is the wave number.

c) KH-RT breakup length model

In the simulation, running KH and RT model together is to use the so-called KH-RT breakup length model. Breakup length L_b is specified:

$$L_b = C_{bl} \sqrt{\frac{\rho_l}{\rho_g}} d_0 \quad (3.69)$$

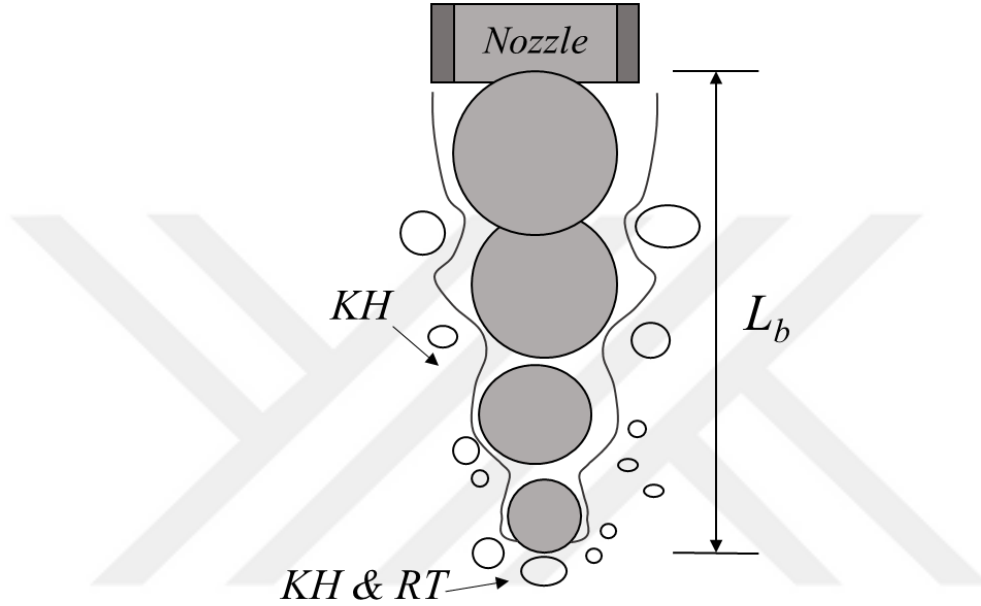


Figure 3.4. Schematic of the KH-RT spray breakup model.

KH-RT spray breakup model schematic is shown in Figure 3.4. Liquid blobs are injected with a radius equal to that of the injector nozzle. Besides that, the KH mechanism is utilized to a drop along with its existence, while the RT model is only begun when the droplet attains a characteristic length, L_b , from the injector.

3.2.2.6. Collision model

The collision model of No Time Counter (NTC) method was used in the simulation (Schmidt & Rutland, 2000). The NTC technique is depend on the gas dynamics for Direct Simulation Monte Carlo (DSMC) calculations. The NTC method is derived from the basic probability model for stochastic collision without assumptions. In the basic probability model, the cell size should be so small that spatial changes in spray quantities can be negligible.

The equation of NTC method for application to parcels representing varying number of drops:

$$M_{coll} = \sum_{i=1}^{\sqrt{M_{cand}}} q_i \sum_{j=1}^{\sqrt{M_{cand}}} \frac{q_j V_{i,j} \sigma_{i,j}}{(qV\sigma)_{max}} \quad (3.70)$$

3.2.2.7. Evaporating model

Evaporating model is used to clarify the effect of the alteration on the discrete phase whenever the droplet reaches the critical or boiling temperature. The boiling temperature is described as the temperature at which the saturation pressure compensating the gas pressure. If the temperature of the droplet reaches or exceeds the critical temperature, the droplet evaporates suddenly. The rate of mass transfer can be defined as below (M. Yilmaz, 2009):

$$\frac{dm_d}{dt} = \frac{-2\pi k D_d}{c_p} (1 + 0.23 Re^{0.5}) \ln \left[1 + \frac{c_p (T - T_d)}{h_{fg}} \right] \quad (3.71)$$

Throughout boiling, the temperature of the droplet is constant. Therefore, heat transfer rate from droplet to steady phase can be given as below:

$$\dot{q}_g = -h_{fg} \frac{dm_d}{dt} \quad (3.72)$$

3.2.2.8. Combustion Model

1) Extended Coherent Flame Model - 3 Zones (ECFM-3Z)

For partially- or non-premixed combustion, Extended Coherent Flame Model - 3 Zones (ECFM-3Z) is coupled with a mixing model and the ECFM model. ECFM-3Z build by a mixed zone between air (or air and EGR) and fuel zones (Colin & Benkenida, 2004; Richards et al., 2019). The mixing of air and fuel forms the mixed zone (Figure 3.5).

The ECFM-3Z model calculates the auto-ignition pre-reactions of the premixed charge of air and fuel, with the ignition delay governed by the pressure, temperature, equivalence ratio, and residual gas. Premixed combustion in the fuel, air and residual is modeled as stated by a flame propagation process after SOI, and auto-ignition. Diffusion combustion

occurs in a thin zone separating the fuel and oxidizer. Most of the fuel is consumed during premixed combustion (Mobasheri, 2015).

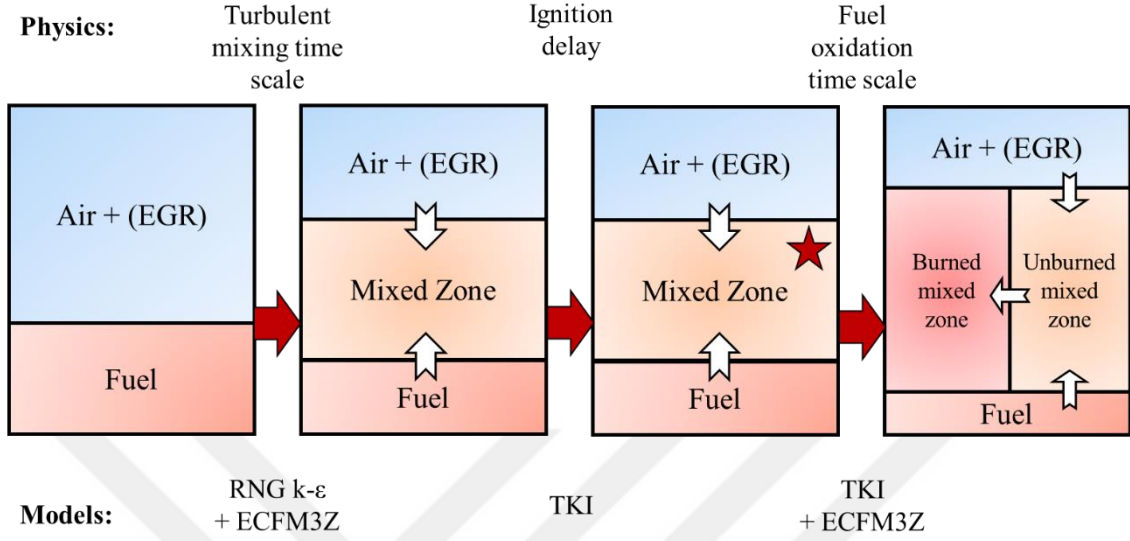


Figure 3.5. Mixing model.

Unmixed fuel and O₂ are solved as:

$$\frac{\partial \bar{\rho} \tilde{Y}_{Fu}^F}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{Y}_{Fu}^F}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\mu}{Sc} \frac{\partial \tilde{Y}_{Fu}^F}{\partial x_i} \right) + \bar{\rho} \dot{S}_{Fu} + \bar{\rho} \tilde{E}_{Fu}^{F \rightarrow M} \quad (3.73)$$

and

$$\frac{\partial \bar{\rho} \tilde{Y}_{O_2}^A}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{Y}_{O_2}^A}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\mu}{Sc} \frac{\partial \tilde{Y}_{O_2}^A}{\partial x_i} \right) + \bar{\rho} \tilde{E}_{O_2}^{A \rightarrow M} \quad (3.74)$$

where $\dot{S}_{Fu}$ is evaporation source term and mixing terms $\tilde{E}_{Fu}^{F \rightarrow M}$ and $\tilde{E}_{O_2}^{A \rightarrow M}$ are a turbulence time scale function, which is given by:

$$\frac{1}{\tau_m} = \beta_m \frac{\varepsilon}{k} \quad (3.75)$$

where β_m is the constant of the mixing rate.

2) Detailed Transient Chemistry Solver (SAGE)

The SAGE (detailed transient chemistry solver) combustion model calculates the rates of reaction and species concentrations within each cell and each time step using CHEMKIN-

formatted input files. The model uses a reduced reaction mechanism for n-heptane (C_7H_{16}) to represent the diesel fuel. This mechanism has 42 species and 168 reversible reactions performing hydrocarbon combustion and NO formation (Senecal et al., 2003). Multi-step reaction mechanism can be expressed:

$$\sum_{j=1}^J \nu_{ji}' X_j \leftrightarrow \sum_{j=1}^J \nu_{ji}'' X_j \quad \text{for } i = 1, 2, \dots, I \quad (3.76)$$

where ν_{ji}' is the stoichiometric coefficient for the reactants and ν_{ji}'' is the stoichiometric coefficient for the products for species j and reaction i, and X_j is the chemical symbol of species j. The generation amount of species j is:

$$\dot{\omega}_j = \sum_{i=1}^I \nu_{ji} q_i \quad j = 1, 2, \dots, J \quad (3.77)$$

and

$$\nu_{ji} = \nu_{ji}'' - \nu_{ji}' \quad (3.78)$$

The progress variable rate is:

$$q_i = k_{fi} \prod_{j=1}^J [X_j]^{\nu_{ji}'} - k_{ri} \prod_{j=1}^J [X_j]^{\nu_{ji}''} \quad (3.79)$$

where X_j is the molar concentration of species j, and k_{fi} is the forward rate coefficient and k_{ri} is the reverse rate coefficients of reaction i, respectively. The forward-rate coefficient is expressed in the form of Arrhenius:

$$k_{fi} = A_i T^{b_i} \exp(-E_i / R_u T) \quad (3.80)$$

where b_i is the exponent for temperature, A_i is the pre-exponential factor, R_u is the gas constant and E_i is the activation energy.

The governing conservation equations can be solved for a specific cell in the domain. These equations are:

$$\frac{d[X_j]}{dt} = \dot{\omega}_j \quad (3.81)$$

$$\frac{dT}{dt} = \frac{V \frac{dP}{dt} - \sum_j (\bar{h}_j \dot{\omega}_j)}{\sum_j ([X_j] \bar{c}_{p,j})} \quad (3.82)$$

where $\bar{h}_j$ is the molar specific enthalpy and $\bar{c}_{p,j}$ is the specific heat of species j. Equations 3.81 and 3.82 are resolved at each time step, then the species are properly updated (Senecal et al., 2003).

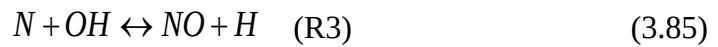
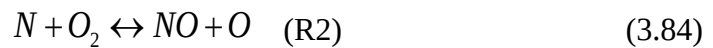
3.2.2.9. Emission model

Species of CO, CO₂ and unburned HC are calculated or interpolated in the commercial code (Converge CFD). They are solved with reaction mechanism inside the combustion model.

1) NO_x modeling

a) Thermal NO_x model

The formation of NO_x is dependent on the reaction temperature. If the temperature increase to a specific value, the NO_x emission occurs. The expanded Zeldovich mechanism is used to calculate NO formation. This mechanism forms of the below reactions (Heywood, 1988):



The reactions rate constants (cm³/mol):

$$k_{R1,f} = 7.6 \cdot 10^{13} e^{\left(\frac{-38000}{T}\right)} \quad (3.86)$$

$$k_{R1,r} = 1.6 \cdot 10^{13} \quad (3.87)$$

$$k_{R2,f} = 6.4 \cdot 10^9 T e^{\left(\frac{-3150}{T}\right)} \quad (3.88)$$

$$k_{R2,r} = 1.5 \cdot 10^9 T e^{\left(\frac{-19500}{T}\right)} \quad (3.89)$$

$$k_{R3,f} = 4.1 \cdot 10^{13} \quad (3.90)$$

$$k_{R3,r} = 2.0 \cdot 10^{14} e^{\left(\frac{-23650}{T}\right)} \quad (3.91)$$

where the subscript f denotes a forward reaction and the subscript r denotes a reverse reaction.

b) Prompt NO_x model

Prompt NO_x mechanism is completely related to the chemistry of hydrocarbon combustion. NO_x occurs in fuel-rich and low-temperature zones where the concentration of oxygen is high. Source term because of the prompt NO_x formation is given as (De Soete, 1975; Fenimore, 1971; Richards et al., 2019):

$$S_{prompt,NO} = M_{w,NO} \frac{dNO}{dt} \quad (3.92)$$

2) Soot modeling

The onset of soot is the formation of the small solid particles from the gas-phase hydrocarbon molecules, and soot surface growth is required to achieve the two-way connection with the gas phase. Soot coagulation is a physical process of collisions between small soot particles that lead to the formation of larger soot particles. Soot condensation indicates that the gas-phase species come together and form large soot particles. Figure 3.6 illustrates the soot formation in combustion (Bockhorn, 1994).

Hiroyasu-NSC empirical soot model used to simulate soot oxidation. Soot oxidation rate (Hiroyasu & Kadota, 1976; Richards et al., 2019):

$$\dot{M}_{so} = A_{so} \frac{6M_s}{\rho_s D_s} R_{total} MW_c \quad (3.93)$$

A_{so} is a scaling factor, M_s is the total soot particle mass (g), MW_c is the molecular weight of carbon (g/mol), D_s is the nominal soot particle diameter (cm), R_{total} is total reaction rate and ρ_s is the soot density (g/cm³).

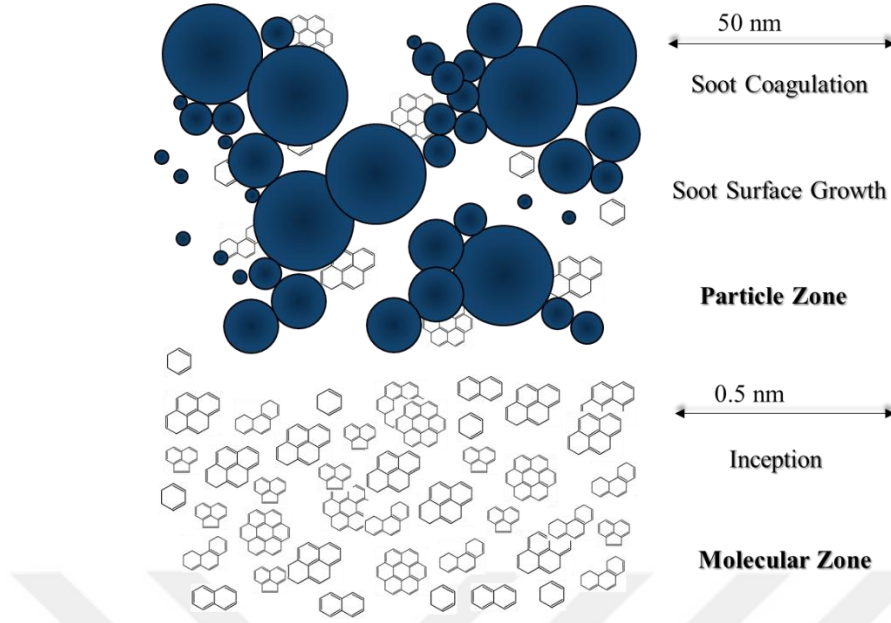


Figure 3.6. Soot formation in combustion.

The difference in soot density at the start and end of the computational time-step:

$$\rho_s^{n+1} - \rho_s^n = \left(\frac{SF \rho_{form}}{SO} - \rho_s^n \right) \cdot \left[1 - e^{(-SO \Delta t)} \right] \quad (3.94)$$

3.3. Optimization

Optimization is the study of achieving the best results under certain conditions. When making decisions in any design or process, decisions are made with the least effort and maximum gain. Since the necessary effort or desired gain can be defined as a function of specific decision variables, optimization is the process of finding conditions that give the minimum or maximum value of this function (Rao, 2009).

It is expected from engineers to find terms that give a minimum or maximum value with certain constraints in the design or process. However, sometimes it can be unsatisfactory in small projects by increasing engineering time and cost. Optimizing a complex design or process is often difficult. In these cases, it may be possible to optimize the subsystems and select the optimum combinations. But, there is no guarantee that this procedure will result in an optimum system or design (Stoecker, 1989).

There are many ways to solve optimization problems in the most efficient way. Various optimization methods have been developed for different types of optimization problems.

The Optimum search method is often part of operations research, which is a branch of mathematics related to the creation of the best solutions. Modern optimization methods are emerging as powerful methods for solving complex engineering problems. These methods are Genetic algorithms, Simulated annealing, Ant colony optimization, Particle swarm optimization, Neural networks, Fuzzy optimization (Rao, 2009). Genetic algorithms (GAs) are based on natural genetics and natural selection mechanics. Genetic algorithms were first proposed by John Holland (Holland, 1975). Although all methods have advantages, disadvantages and application areas, one of the most efficient optimization methods for bowl optimization and valve optimization is genetic algorithm methods. Thus, the genetic algorithm used in this thesis will be described in this chapter.

3.3.1. Genetic algorithm

Many classical optimum design problems are portrayed by mixed continuous-discrete variables and discontinuous and non-convex design spaces. When traditional non-linear programming techniques are used for this problem type, they will be ineffective, computationally expensive, and reach a relative optimum nearest to the starting point for most cases. GA is well suited for solving these problems and are likely to find the optimum global solution. GA is based on the concepts of natural genetics and natural selection. The genetic research procedure uses reproduction, crossover, and mutation, which are the basic elements of natural genetics. If the number of design variables is n , the population size is taken as $2n$ to $4n$. In GAs, the design variables are represented as binary variable strings corresponding to chromosomes in natural genetics. The design vector's objective function value plays the role of fitness in natural genetics. A new set of strings is generated in each new generation by using a randomized crossover from the old set of strings. The algorithm explores the new combinations with a better objective function value. The flow chart and main process of the genetic algorithm are shown in Figures 3.7 and 3.8 (Gökkuş, Yildirim, & Aydin, 2017).

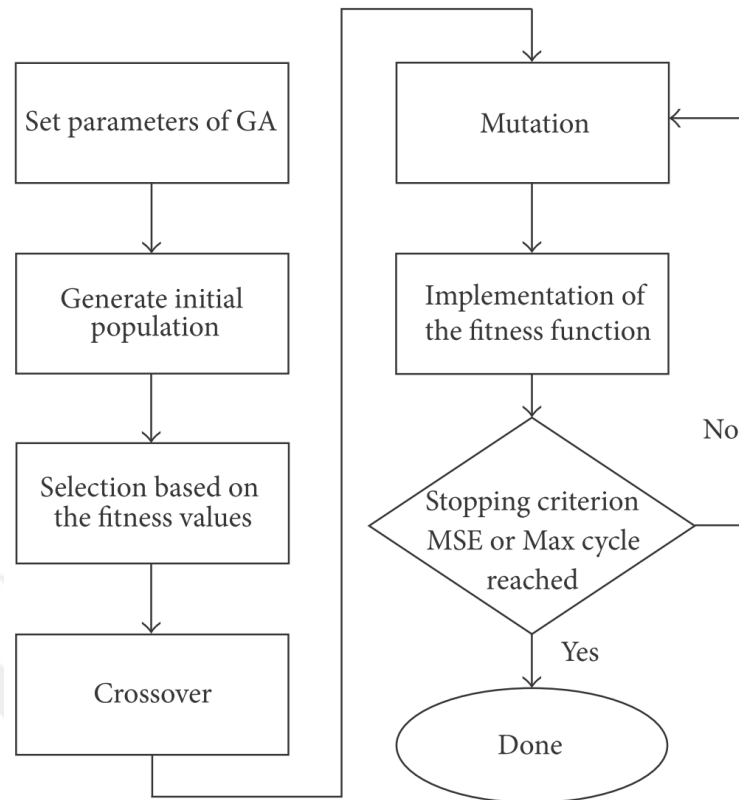


Figure 3.7. Basic process of the genetic algorithm.

The basic genetic algorithm steps are as follow (Yaktubay, 2018):

- 1- Set the parameters of GA for the problem
- 2- Generate the initial population
- 3- Evaluate the fitness values of each chromosome in the population.
- 4- Generate a new population. The genetic operators changes the chromosome structure until new population is completed.
- 5- Select the parent chromosomes for the reproduction from the population. The selection criteria related to the fitness values.
- 6- The chromosomes are recombined with a crossover probability to generate the offspring.
- 7- Alter each offspring with a mutation probability.
- 8- Replace the parent chromosomes with a new population after evaluating the fitness value of each offspring.
- 9- Stop and take optimum solution in the current population, if the stopping criterion or max cycle is reached.

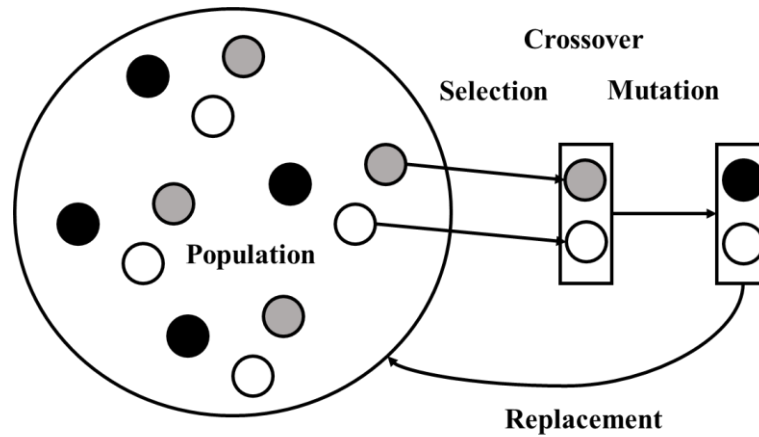


Figure 3.8. Main process of the genetic algorithm.

This theory begins with generating random individuals to form a population. The population of individuals that occur in each iteration. It is called a generation and a process that continues in iteration. The fitness of each individual generated in the population is assessed. The value of the objective function in the optimization study is considered the fitness value. Each individual genome is haphazardly mutated to a new generation. The algorithm uses next generation genomes in its next iteration. The algorithm stops when it has been produced a maximum number of generations or when the population has been reached satisfactory fitness. Multiplying the number of generations by the size of the population gives the total number of iterations.

The population size depends on the important problem. It should be considered along with the number of generations. Table 3.1 gives the initial recommendation about population size according to independent variables.

Table 3.1. Recommended population size of the genetic algorithm

n	Population size
3	10
4	16
5	20
6	26
7	30
8	40
9+	50

The mutation rate for the genetic algorithm is determined from the number of independent variables. The mutation rate is calculated by multiplying the number of independent variables by the number of active cases and adding the number of sweep variables.

3.3.2. Non-dominated sorting genetic algorithm

Engineering problems often require simultaneous optimization of multiple conflicting objectives. It may not always be possible to find one solution that provides all the objectives. In these cases, it needs to choose from alternative solutions for each of the objectives. A better solution is chosen for any of the objectives. Each of these solutions is called a Pareto-Optimal solution.

The Non-dominated Sorting Genetic Algorithm (NSGA) design engine implements a multipurpose evolutionary algorithm. The input parameters are determined for a number of generations, population size, mutation probability, and crossover probability. This algorithm is a good option (not only one objective) for optimization problems where several - often conflicting - targets that need to be minimized or maximized and also include some constraints. In addition to many optimization algorithms, it has been observed in the literature that NSGA is the algorithm that gives the best results (Tütüncü, 2009; Zitzler et al., 2000). Therefore, NSGA Algorithm was used in this thesis.

The NSGA determines the cost of each individual depend on dominance. First, all individuals are copied to a temporary population, T which includes all non-dominated individuals. These individuals, referred to as set B, are assigned the lowest cost value. B is subtracted from T and all non-dominated individuals in the reduced set T are found. They are assigned the second lowest cost value. This process is repeated and a cost depend on its level of non-domination for each individual is obtained. Figure 3.9 summarizes NSGA (Dan, 2013; Srinivas & Deb, 1994).

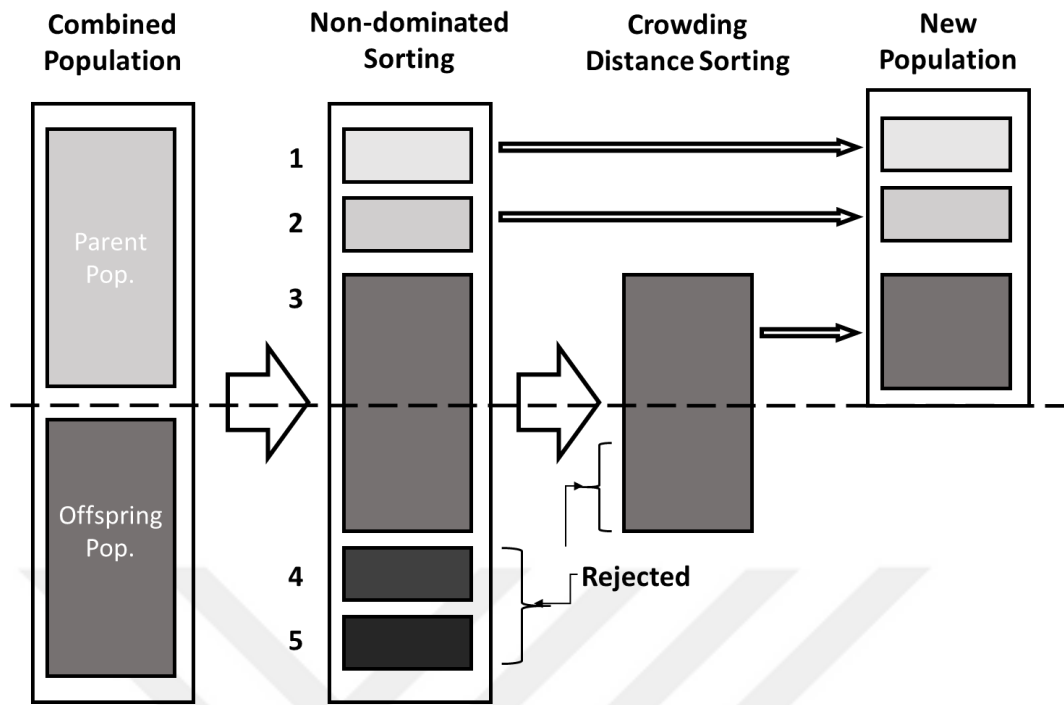


Figure 3.9. Schematic of NSGA-II algorithm.

NSGA-II is a modification of NSGA (Deb, Pratap, Agarwal, & Meyarivan, 2002). NSGA-II calculates the cost of an individual x by taking into account both the individuals that dominate it and the individuals that are dominated. In addition, a crowding distance for each individual is computed using the distance to the nearest individuals along each objective function dimension. The crowding distance is used to modify the fitness of individuals. This method apply an evolution strategy approach in order to fulfill elitism (Dan, 2013).

NSGA-II procedure begins with forming both the parent population and the offspring population. Then, the non-dominant sorting procedure is applied to all generations. This procedure ensures global non-domination control between offspring and parent solutions. This control causes NSGA-II to converge faster. The crowding distance is used in the selection of the parent for a new individual and the selection of the new population based on the comparison of the congestion in a solution. A larger crowd distance should be preferred to maintain the diversity of the solution (Ibrahim, Shamsuddin, Ahmad, & Qasem, 2013).

3.3.3. Multi objective genetic algorithm

Multi Objective Genetic Algorithm (MOGA) is a modified version of the genetic algorithm to find a set of multiple non-dominant solutions in a single run (Deb & Jain, 2014; Hu, Zhou, & Yang, 2017).

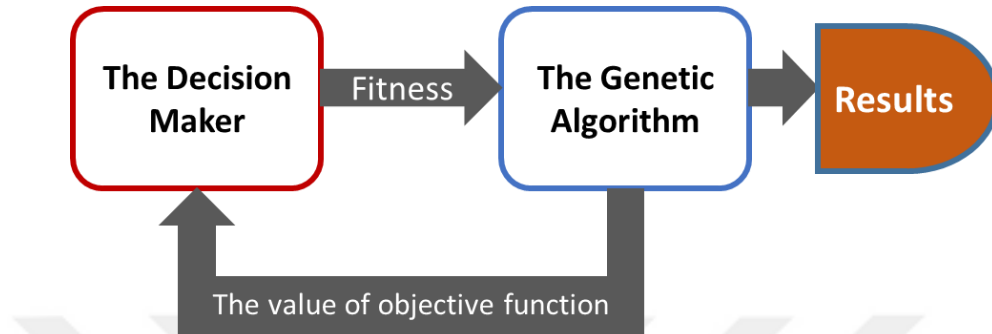


Figure 3.10. Schematic of the MOGA

Because the designer is usually looking for a single solution to the multi-objective problem, it should be used to influence the selection if some high-level information affecting the outcome can be explained by objectives. In this case, the fitness of a candidate solution does not have to be constant throughout the whole generation. It is a value that depends on the decision maker and is usually subjective. The interaction between the decision maker and the genetic algorithm is shown in Figure 3.10 (Konak, Coit, & Smith, 2006).

It is very important to use optimization tools because there are many variables, input and outputs at the engine development stage. The main purpose in the engine design is to maximize performance and minimize emissions. In this thesis study, the valve timing, injection strategy and bowl shape have been optimized using the GT-Suite direct optimizer tool, CAESES and Dakota software with Genetic Algorithm method (Adams et al., 2018; CAESES, n.d.; Gamma Technologies, 2016b).

4. RESULTS AND DISCUSSION

In this section, the results of experimental, QD, and CFD studies are presented. The effects of various parameters on performance and emissions are discussed. Optimization studies using QD and CFD models are presented in figures and interpreted. As a result of optimization studies; parameters, and geometry of the optimized engine were determined.

4.1. Experimental Results for the Baseline Engine

The experiments were performed with different engine speeds and loads. The engine power, torque and BSFC were measured at full load conditions to find maximum performance characteristics of the engine (Table 4.1, Figures 4.1 and 4.2).

Table 4.1. The experimental performance parameters of the test engine

Speed	Torque	Power		BSFC
<i>rpm</i>	<i>Nm</i>	<i>kW</i>	<i>HP</i>	<i>g/kwh</i>
3000	17.65	5.65	7.69	351.54
2800	27.46	8.21	11.17	342.26
2600	28.93	8.03	10.92	334.91
2400	30.65	7.85	10.68	324.68
2200	31.38	7.37	10.03	333.68
2000	32.12	6.86	9.33	330.95
1800	33.10	6.36	8.65	348.96
1500	32.61	5.22	7.10	384.84

A diesel engine is able to deliver maximum torque across a wide speed range. The volumetric efficiency decreases due to the shorter time allocated to exhaust and intake processes above 2200 rpm for this engine. Nevertheless, the engine torque decreases as the time allocated for the combustion process decreases. Despite the reduction of torque, the engine power continues to increase up to 2800 rpm. While the engine produces its

highest torque at 1800 rpm as 33.10 Nm, it delivers the highest power value at 2800 rpm as 8.21 kW (Figure 4.1).

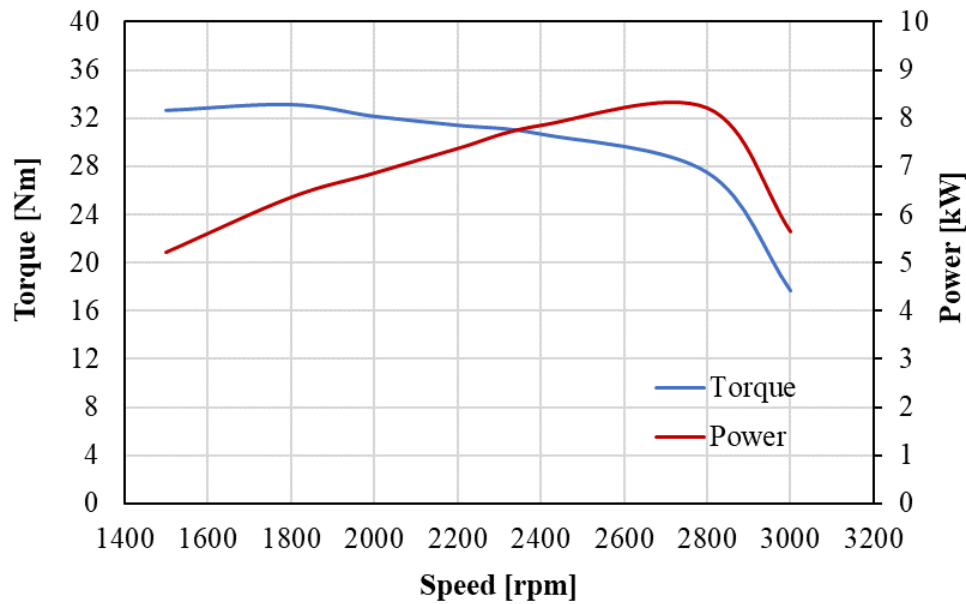


Figure 4.1. Power and Torque curve for a range of engine speed and full-load

The pattern of the BSFC curve shows that the BSFC diminishes with the increase in speed, which reaches a minimum at 2400 rpm. It is seen that the speed range in which the engine runs most economically at full load is between 2000 and 2400 rpm. Afterward, BSFC increases with the increase in speed until 3000 rpm (Figure 4.2).

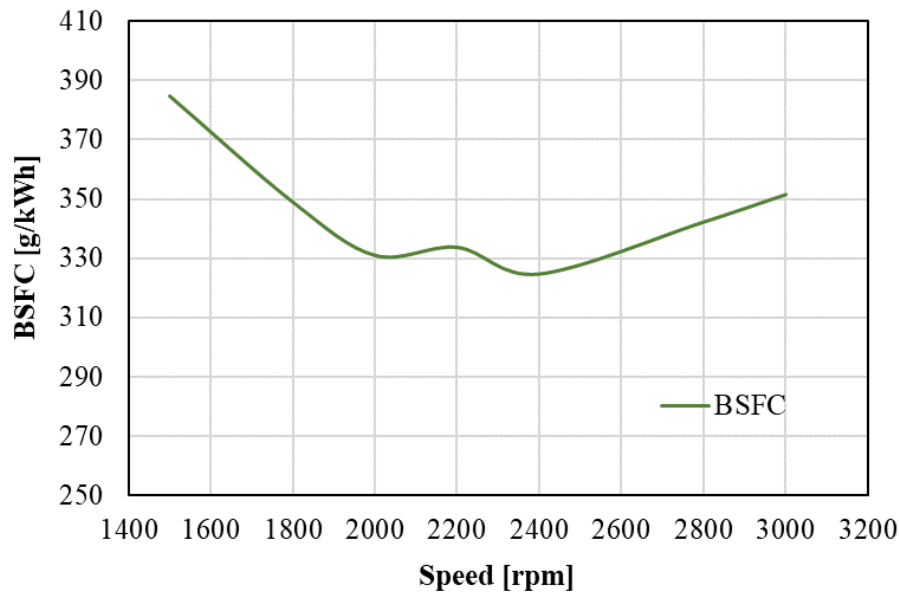


Figure 4.2. BSFC curve for a range of engine speed and full-load

The engine performance map was plotted for BSFC versus Load and Engine Speed (Figure 4.3). The lowest BSFC value for this engine is achieved as 276.56 g/kWh at 1800 rpm and 75% load. The most inefficient point of the engine is 3000 rpm and 15% load. At this point, the consumption occurs as 592.06 g/kWh. The most economical zone of the engine is 1800-2400 rpm and 50-75% load range.

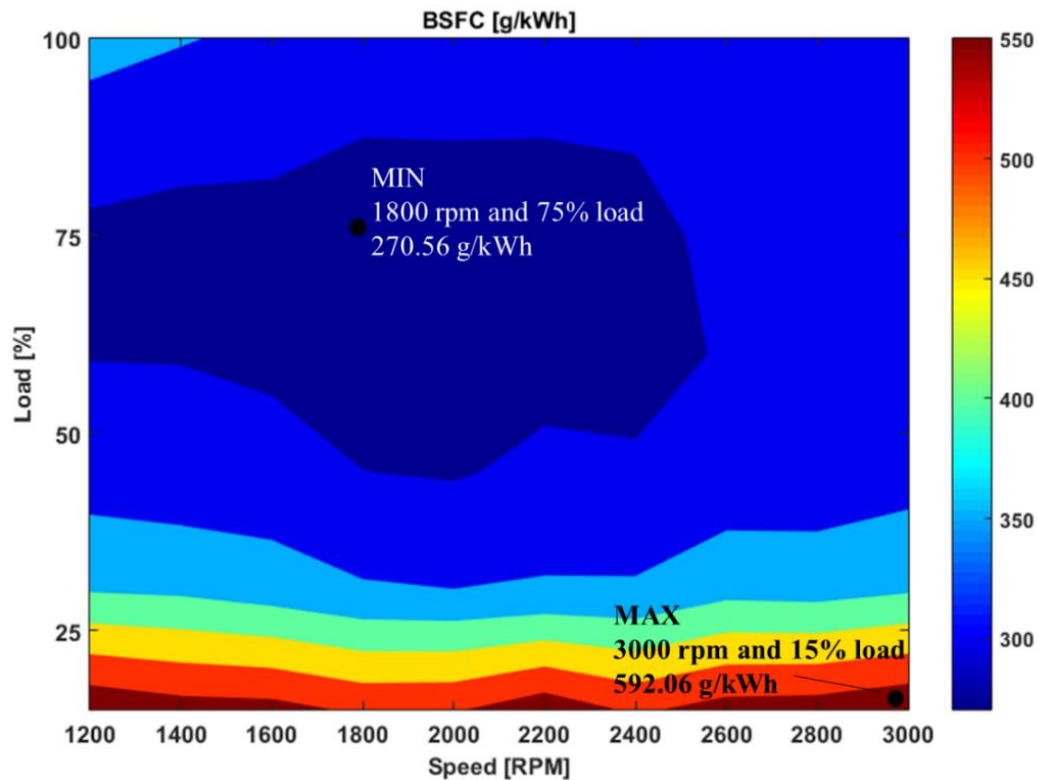


Figure 4.3. Engine performance map: BSFC versus Load and Engine Speed

The in-cylinder pressure of the test engine was measured from 1500 to 3000 rpm. The maximum pressure inside the cylinder rises to 100 bar. Fluctuations are observed in the region where the intake and exhaust valves are opened zone (Figure 4.4).

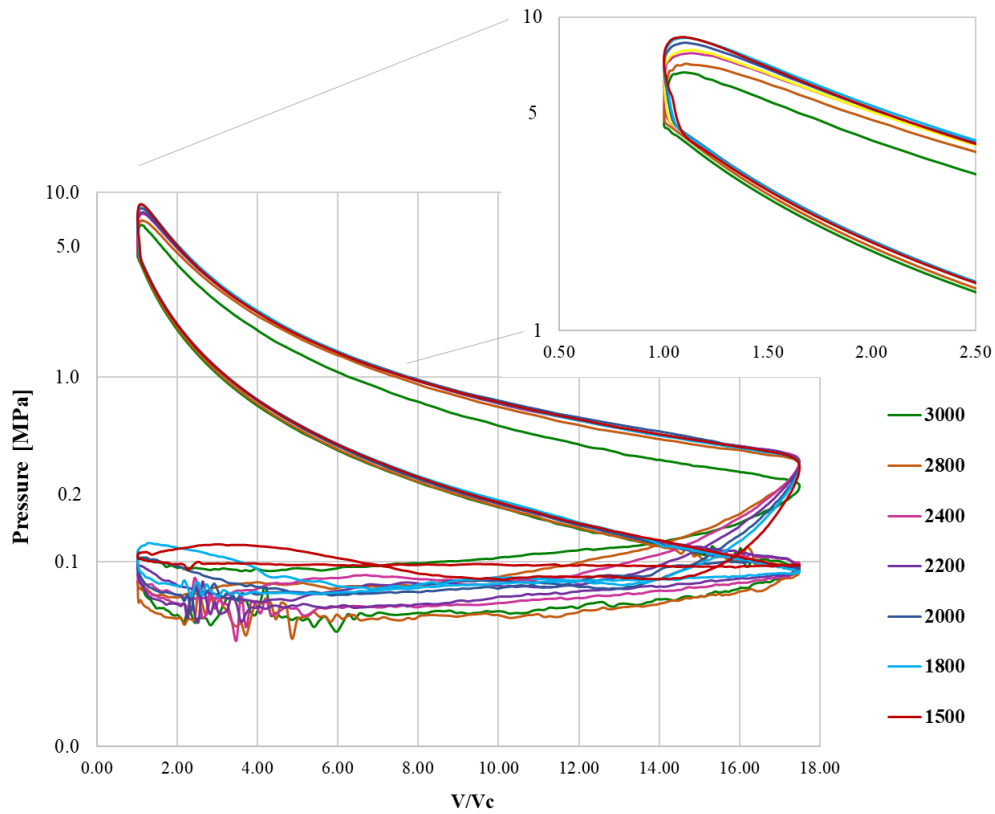


Figure 4.4. In-cylinder pressure-Volume/Clearance volume diagram for different engine speeds

Fuel line pressure value was also measured. It increases to an average of 200 bar pressure during fuel injection (Figure 4.5). After the injector is closed, fluctuations occur in the fuel line.

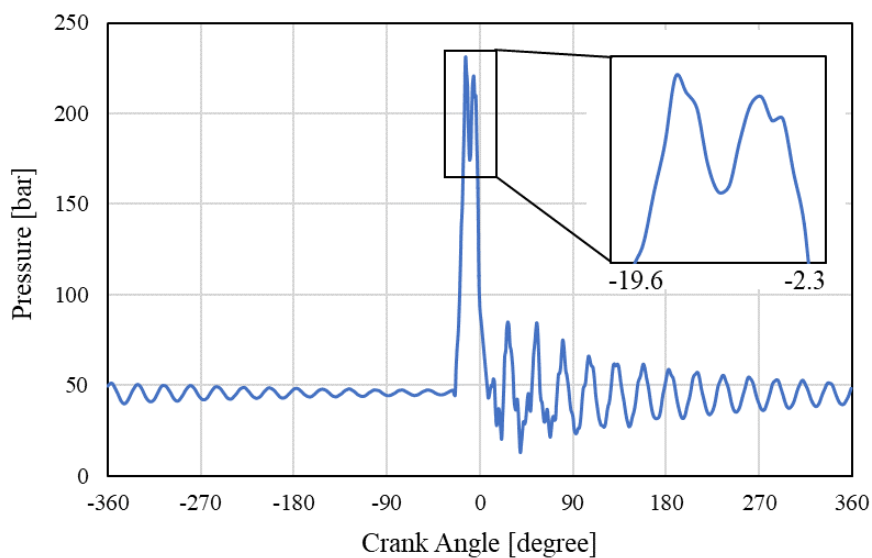


Figure 4.5. Fuel line pressure-crank angle diagram at 2800 rpm

The emission measurements of the test engine were carried out at different speeds. The test engine emits NO_x of 9.95 g/kWh, and CO of 37.57 g/kWh at full load and 2800 rpm. While NO_x emissions increase up to 2000 rpm, then it decreases as the speed increases. CO emission value decreases with engine speed. The lowest NO_x and CO emission is emitted at 3000 rpm (Figure 4.6).

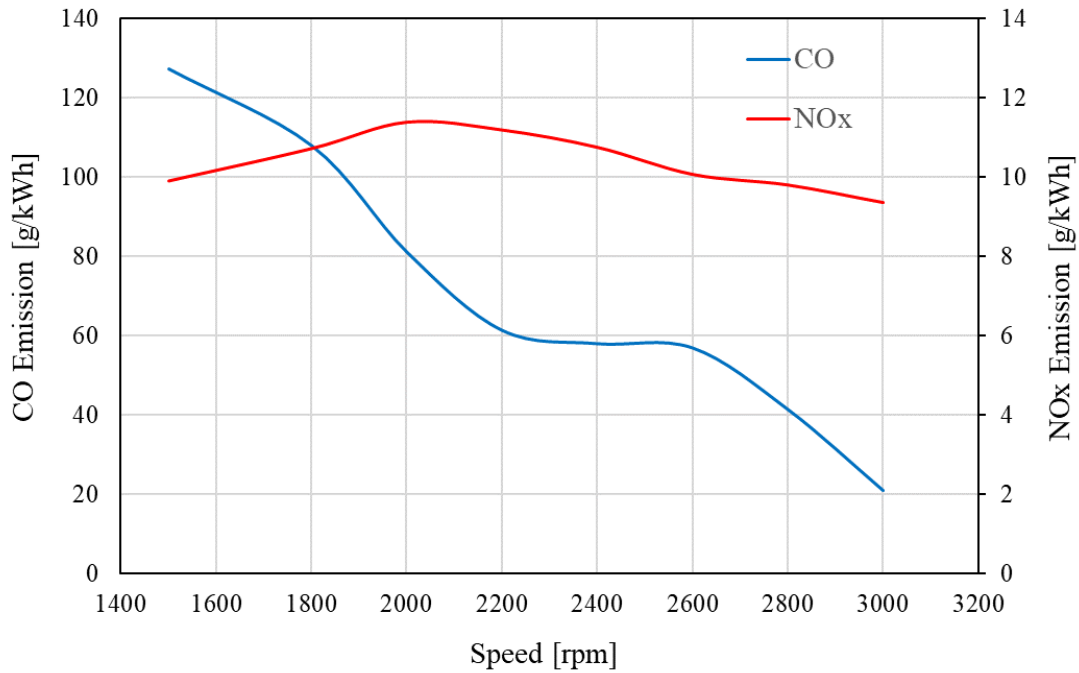


Figure 4.6. The test engine exhaust emissions

4.2. QD Simulation Results for the Baseline Engine

The test engine is modeled as QD using the GT-Suite commercial software (Figure 4.7). Power, torque and BSFC and in-cylinder pressure results of the QD simulations were compared with experimental results at different speeds. In Table 4.2, power, torque and BSFC values of the experimental and the calibrated simulation are shown. As revealed, there is a very good coincidence between the calculated and the experimental values (Figures 4.8, 4.9 and 4.10). In addition, in-cylinder pressure of the test engine was calculated from 1500 to 3000 rpm using QD model (Figure 4.11).

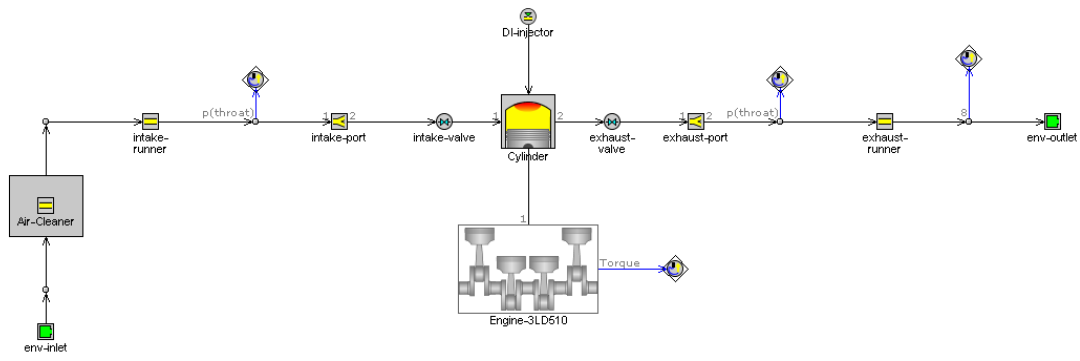


Figure 4.7. GT-Suite QD model of the test engine

Table 4.2. The performance parameters of the test engine QD model

Speed	Torque	Power		BSFC
<i>rpm</i>	<i>Nm</i>	<i>kW</i>	<i>HP</i>	<i>g/kWh</i>
3000	17.61	5.53	7.42	353.54
2800	27.58	8.09	10.85	347.47
2400	30.69	7.71	10.34	330.65
2200	31.48	7.25	9.73	339.22
2000	32.18	6.74	9.04	336.76
1800	33.17	6.25	8.39	355.03
1500	32.65	5.13	6.88	391.87

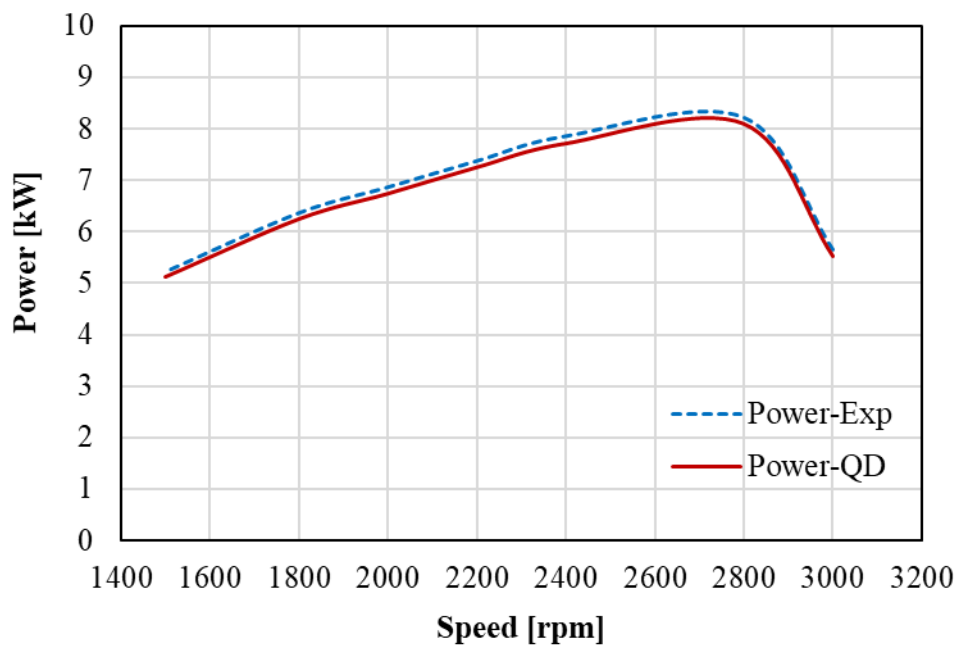


Figure 4.8. Comparison of the power curve of the experimental and QD model

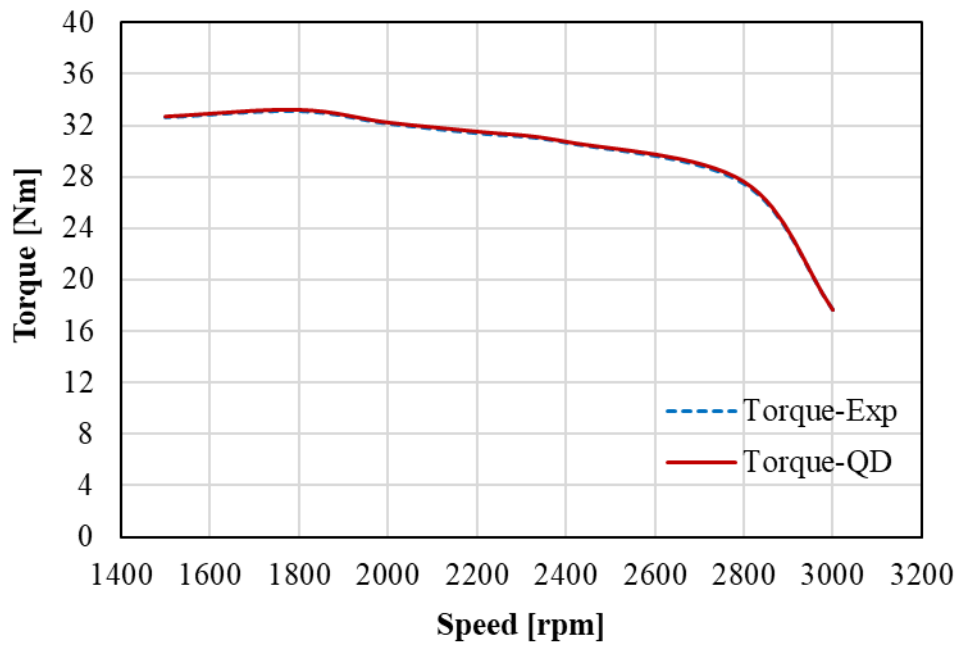


Figure 4.9. Comparison of the torque curve of the experimental and QD model

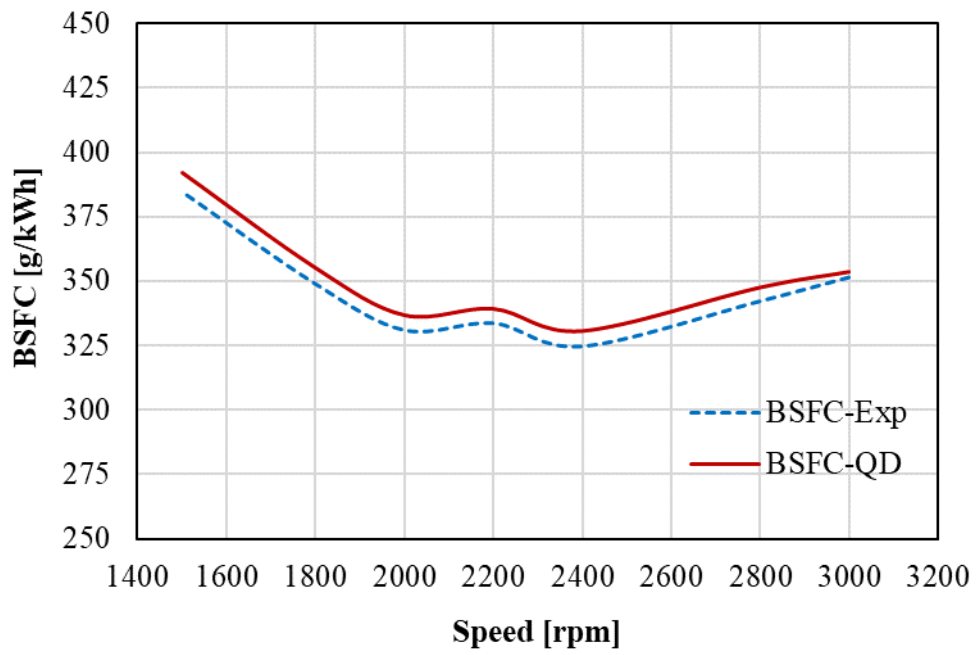


Figure 4.10. Comparison of the BSFC curve of the experimental and QD model

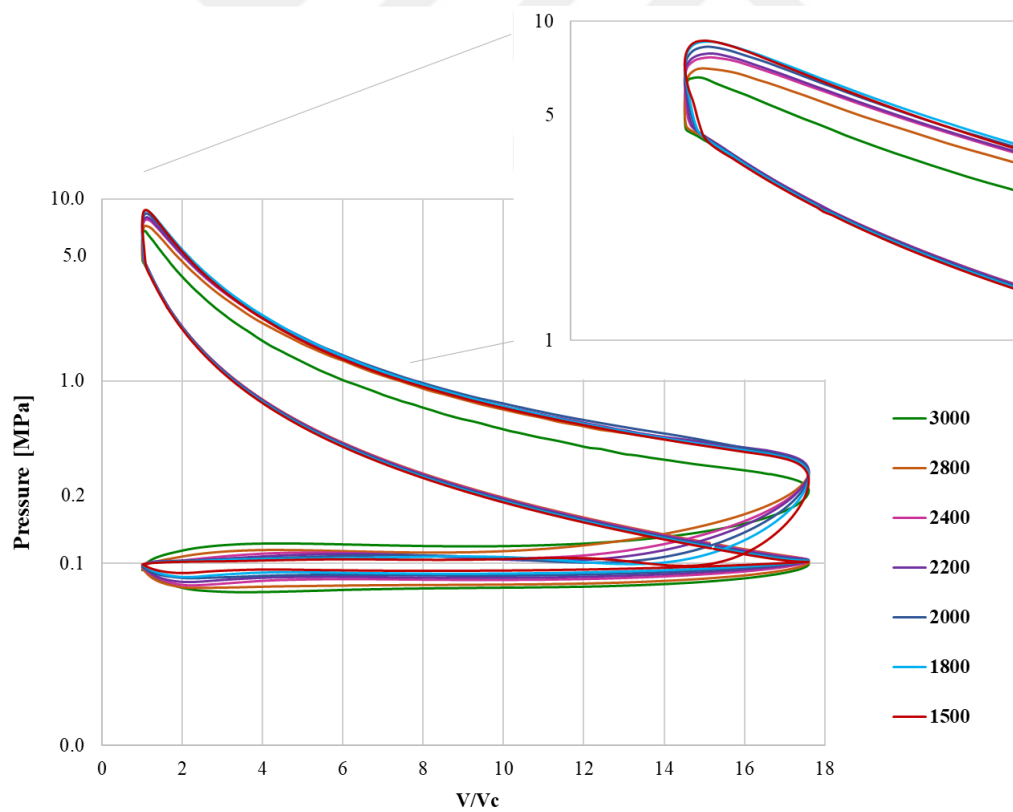


Figure 4.11. In-cylinder pressure-Volume/Clearance volume diagram of QD simulation for different engine speeds

4.3. CFD Simulation Results for the Baseline Engine

The test engine is a single-cylinder, four-stroke, water-cooled naturally aspirated diesel engine. The solid model of the engine was obtained from the engine company. The fluid part of the engine was prepared for CFD simulation. Valve timings and operating parameters of the engine were input. A brief of the engine's operating parameter is listed in Table 4.3. The test engine CFD model is illustrated in Figure 4.12.

Table 4.3. Operating parameter of the test engine

Intake valve closing	-129 CA bTDC
Exhaust valve opening	+137 CA aTDC
In-cylinder pressure at IVC	122.49 kPa
Initial temperature at IVC	376.84 K
Injected fuel mass	33.45 mg/cycle
Injector hole diameter	0.29 mm
Start of injection	-19.6 CA bTDC
Injection duration	17.3 CA
Injection pressure	200 bar
Fuel	Diesel
Compression ratio	17.5:1
Spray angle	120 degree

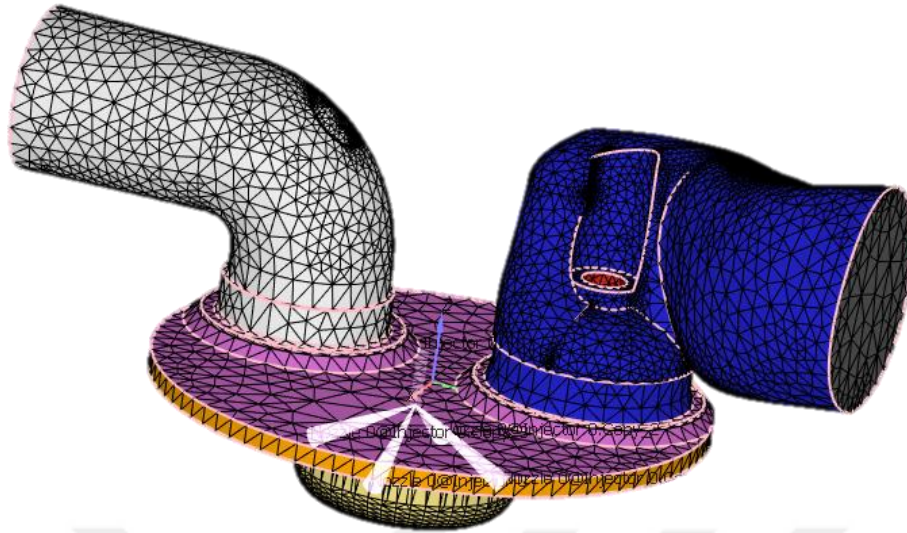


Figure 4.12. Surface of the CFD model at TDC

4.3.1. CFD results for cold flow of the test engine

Firstly, the intake, compression, expansion and exhaust phases of the test engine were examined. The maximum compression pressure was 4.7 MPa (Figure 4.13).

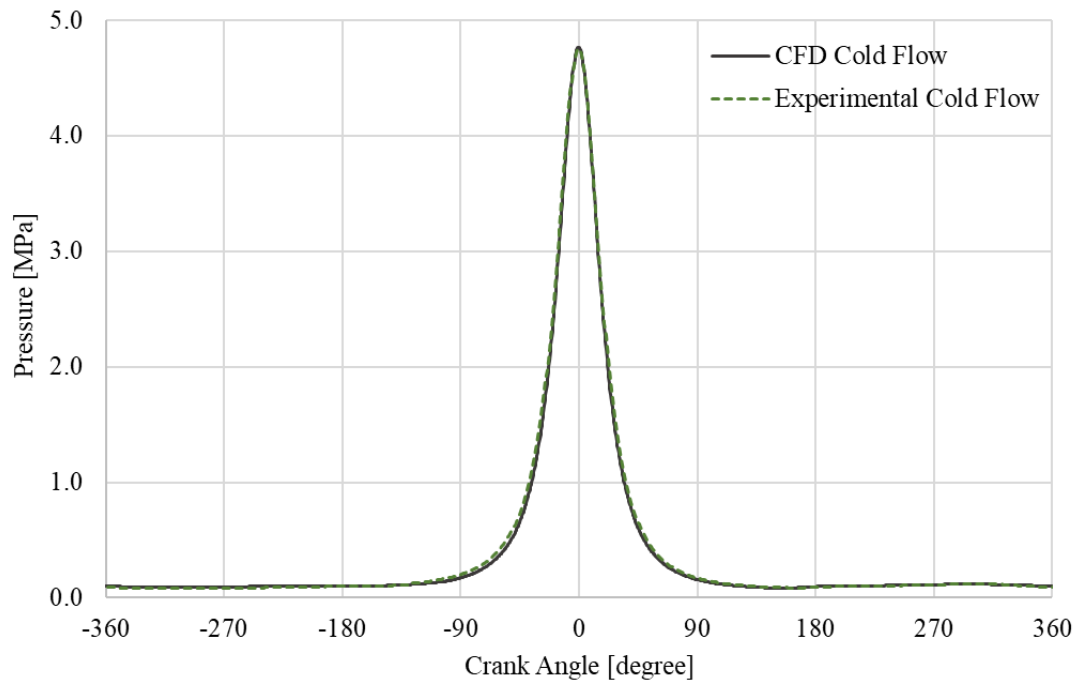


Figure 4.13. In-cylinder pressure curve of cold flow simulation and experimental of the baseline engine

4.3.2. Mesh Independency

The mesh independence test was performed for the base engine. Three different meshes generated as coarse (4-mm grid size), medium (2-mm grid size) and fine (1.5-mm grid size). All operating conditions of three different meshes were the same except the grid size. In-cylinder pressures of the different meshes (i.e. 1.5, 2 and 4-mm) were compared in Figure 4.14. The in-cylinder pressure trends for the three meshes are very similar to each others. The 4-mm mesh produced inconsistent results at high pressures, but the 1.5-mm and 2-mm mesh results were very close. Therefore, the medium size mesh, which has 1.2×10^6 cells and 0.5-mm grid size in the finest zone, is considered for simulation in accordance with the results of independence studies. In addition, Converge CFD uses the adaptive mesh refinement (AMR) method to refine the mesh according to temperature, velocity, species, passive, and boundary and to ensure the convergence.

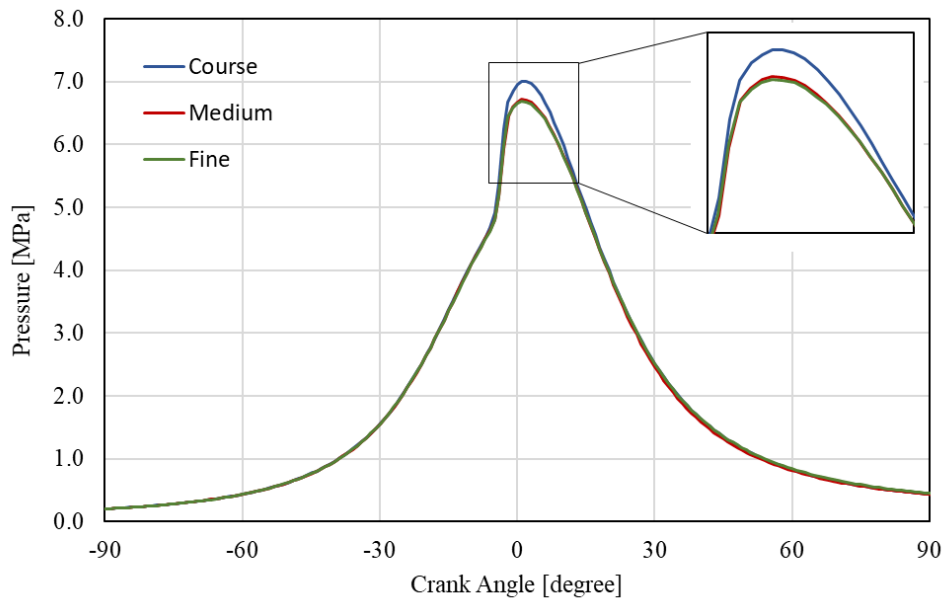


Figure 4.14. Mesh independency result

4.3.3. CFD model validation

In this study, the full engine modeled with intake and exhaust ports. Solid cone and 4-hole diesel injector were used and ECFM-3Z combustion model and RNG k- ϵ turbulence model selected. Results of the simulation and the experiment at 2800 rpm and full-load were compared in Figure 4.15. Rate of Heat release (RoHR) and in-cylinder pressure of the simulation and the experiment have a good consistency and the maximum deviation

is less than 5%. As stated in, the CFD case is considered to be successfully calibrated. Thus, the effects of the bowl shape, the spray angle and injection pressure on the combustion process and emissions are simulated based on the validated model. Besides, optimization studies were carried out using the validated model parameters.

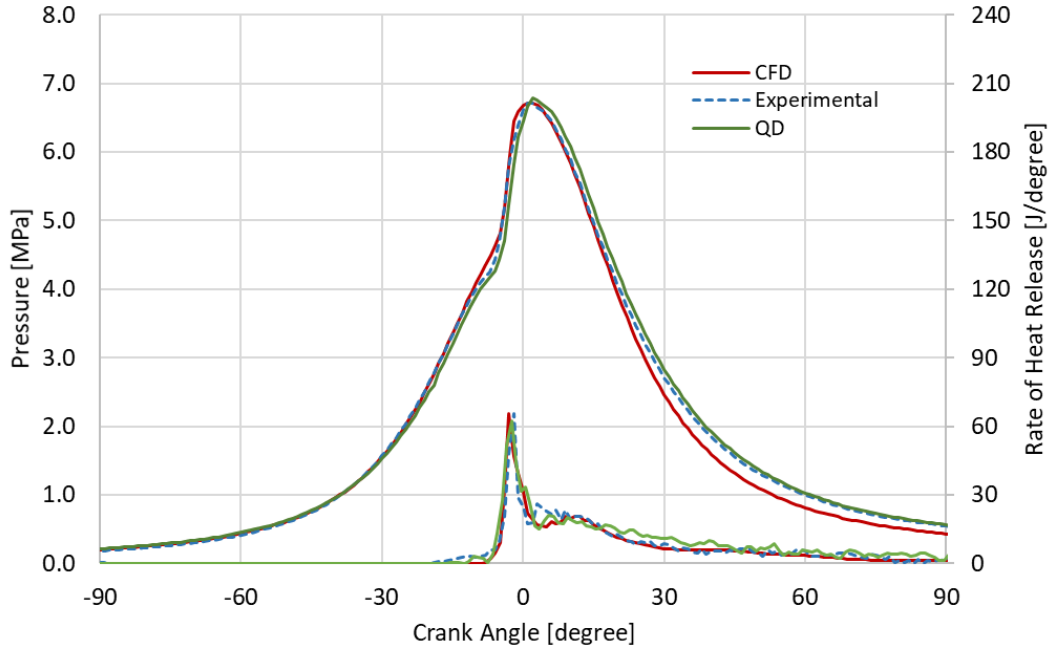


Figure 4.15. Validation of the CFD and QD model with experimental results

4.3.4. Intake process of the test engine

In-cylinder velocity and turbulent kinetic energy (TKE) values were examined at different crank angles, vertical and horizontal cross-sectional areas for the intake phase. The opening of the intake valve and air movements in the cylinder can be seen in Figure 4.16. The intake valve begins to open at -380 CA while reaching a 1.73-mm aperture at -340 CA. The engine has a single intake valve. Intake air flows around the valve upon the intake valve open (Figure 4.17). After -380 CA, the velocity inside the cylinder increases until the intake valve reaches maximum aperture. During the intake valve opens, the piston moves towards the BDC. When the engine reaches -130 CA, the intake valve is fully closed and the compression process starts with air (Figure 4.18).

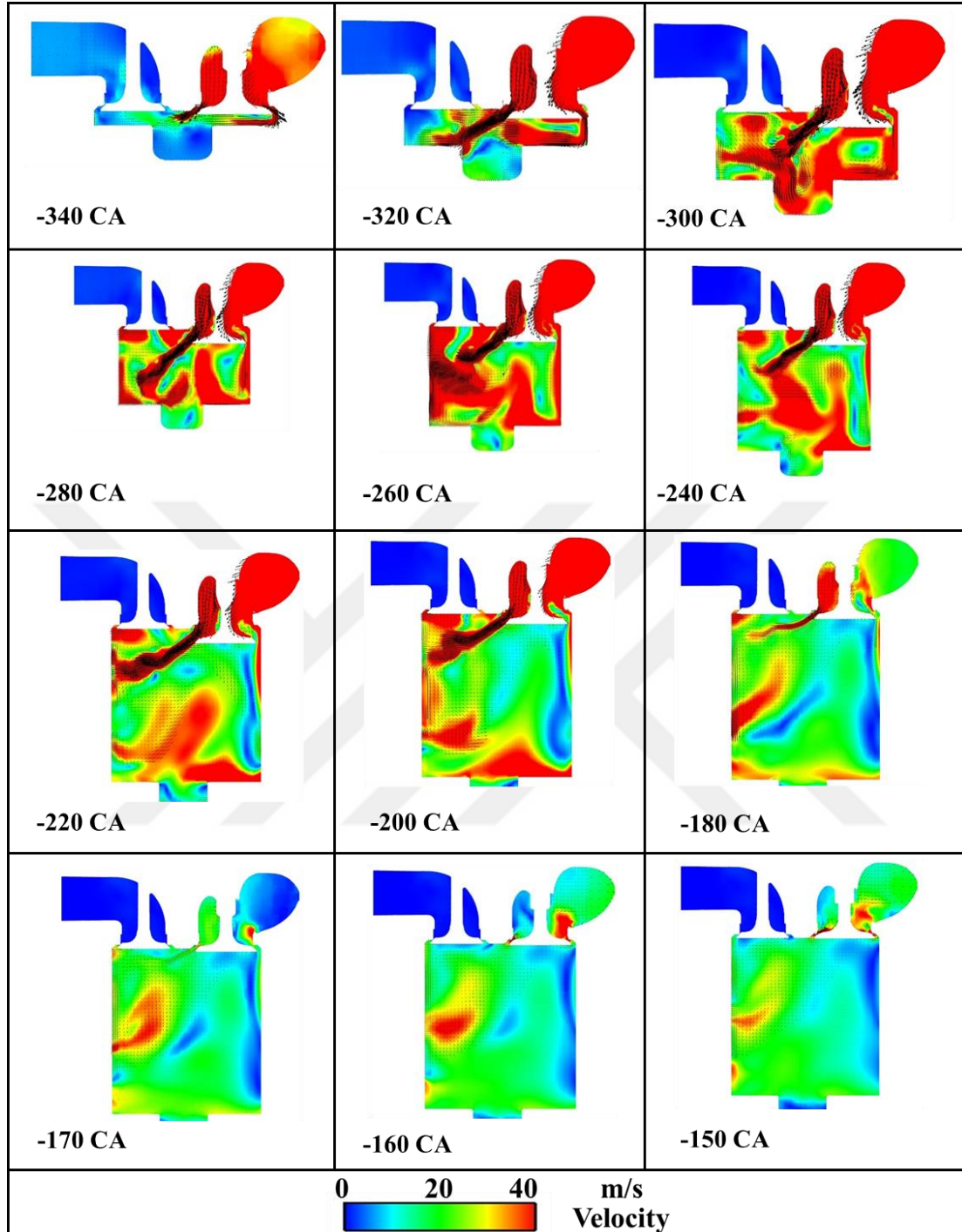


Figure 4.16. Velocity contours of the test engine during the intake process

TKE is the mean kinetic energy per unit mass associated with eddies in the turbulent flow of the in-cylinder air. TKE increases with the opening of the intake valve. With the help of the swirl port, it reaches up to $100 \text{ m}^2/\text{s}^2$ inside the cylinder until the intake valve reaches fully opened. As the intake process ends and the compression process begins, it decreases up to $40 \text{ m}^2/\text{s}^2$ in regions close to the cylinder wall (Figure 4.19).

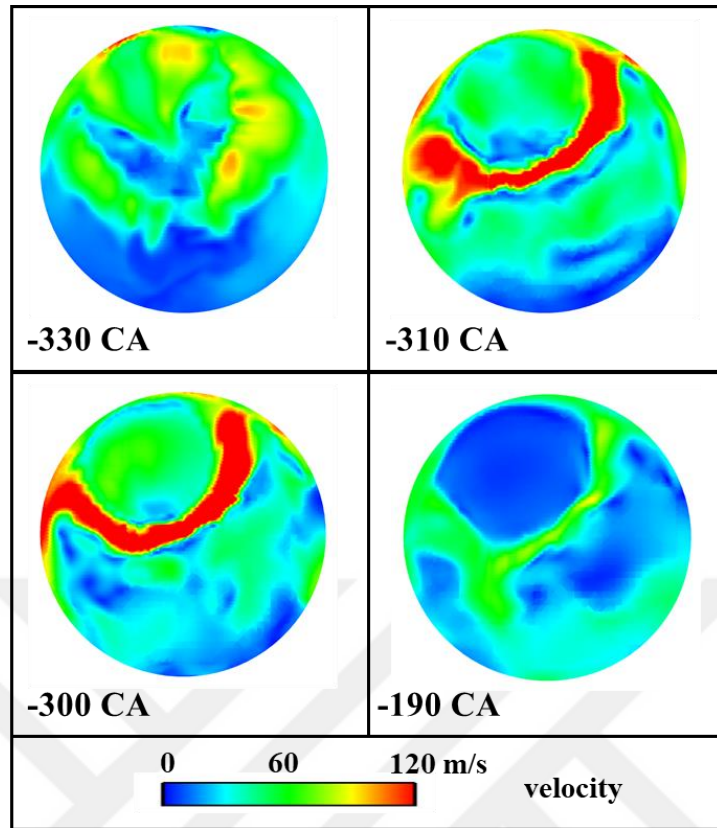


Figure 4.17. Velocity contours of the test engine at horizontal cross-sectional area during the intake process

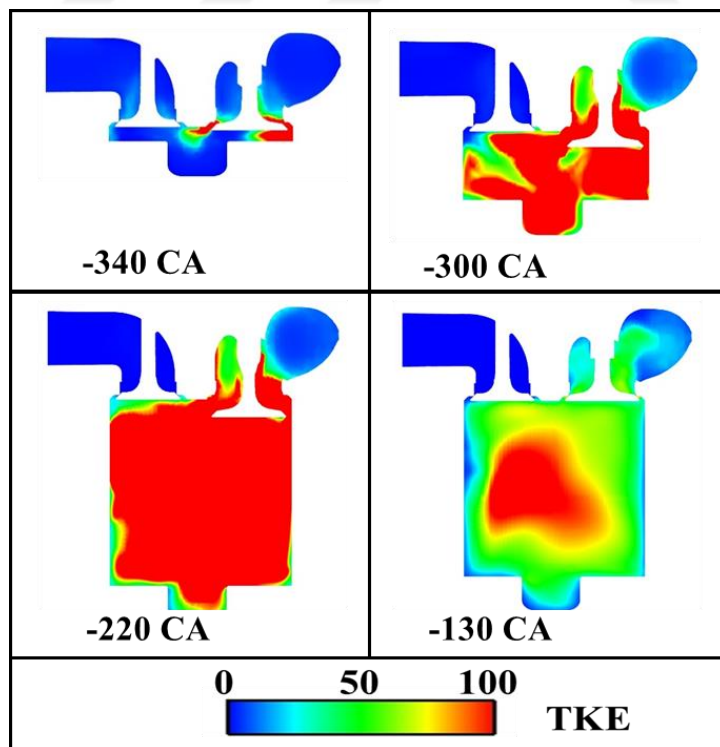


Figure 4.18. TKE contours of the test engine during the intake process

4.3.5. Spray and combustion process of the test engine

The injector characteristics of the test engine were modeled and spray dispersion at different crank angles was examined in this section (Figure 4.19). A 4-hole injector is used in the test engine. The injector location is asymmetrical; the piston bowl is located according to the injector. The injector injects fuel into the cylinder with approximately 200 bar. Fuel reaches up to 97 m/s during the injection.

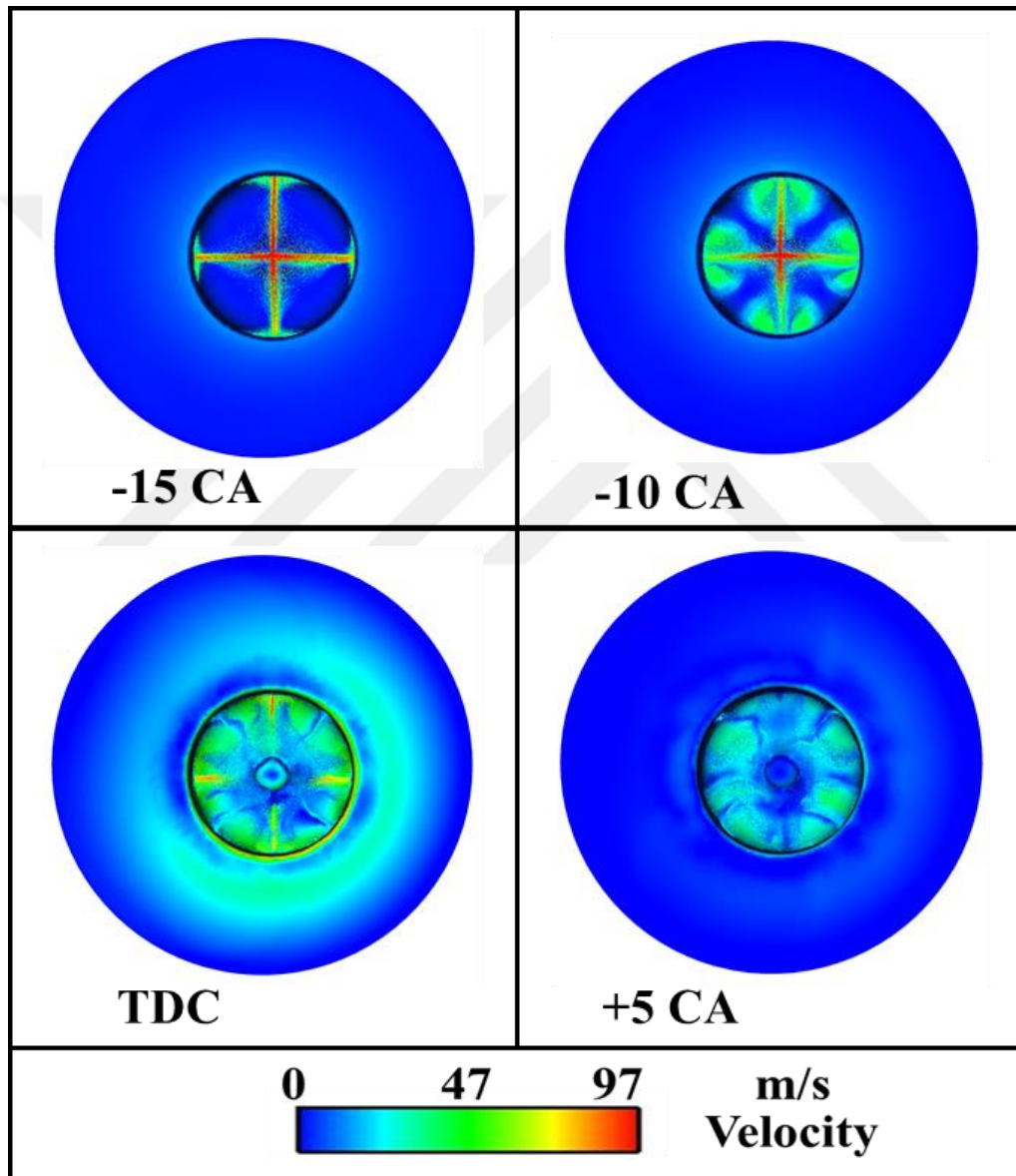


Figure 4.19. Velocity contours of the test engine at horizontal cross-sectional area during the spray process

Spray dispersion, velocity contours, and in-cylinder temperature distribution were examined with the start of combustion (Figures 4.20 and 4.21). The spray angle of the test engine is 120 degrees and the spray cone angle is 10 degrees. The fuel injection starts at -19.6 CA into the cylinder with temperature of 340 K.

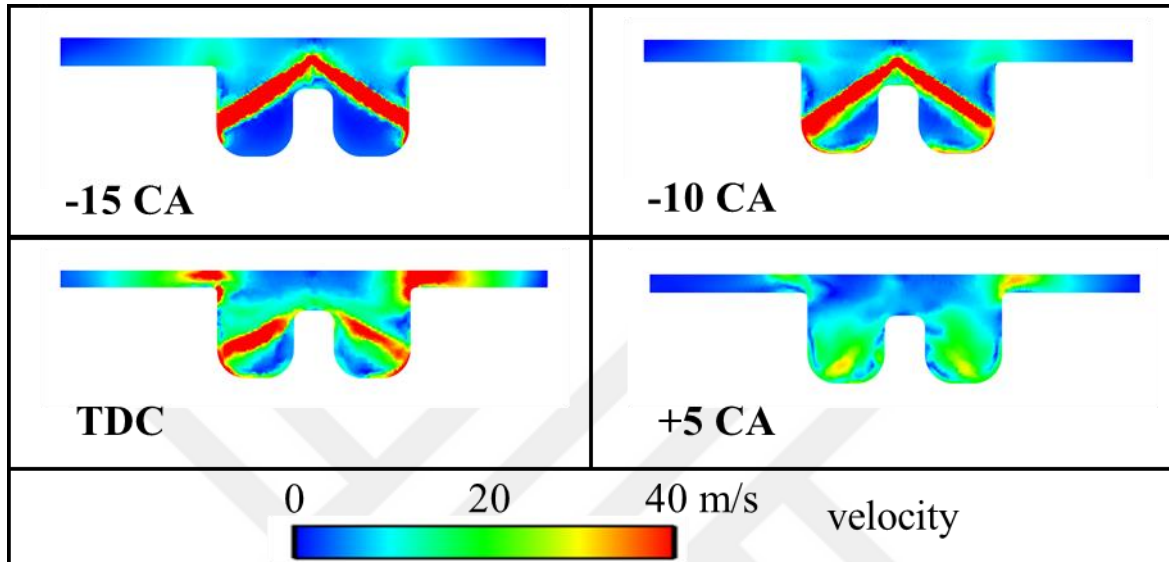


Figure 4.20. Velocity contours of the test engine during the spray process

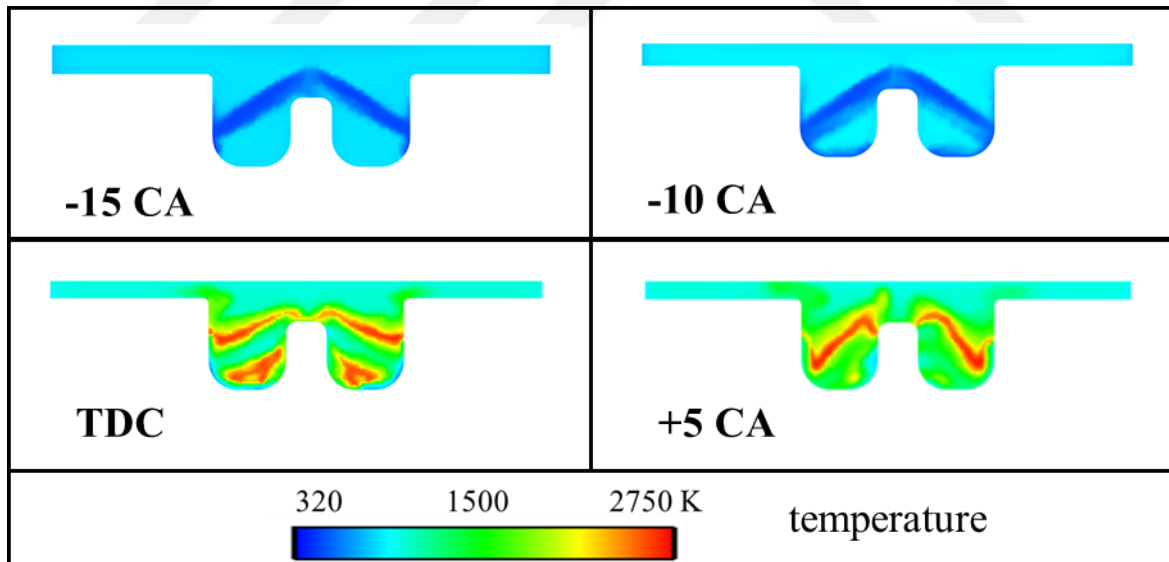


Figure 4.21. Temperature contours of the test engine during the spray process

As can be seen from the Figures 4.20 and 4.21, it is understood that the piston bowl is insufficient to guide the spray effectively. The piston bowl design should be improved to better guide the spray. Soot and HC emissions can be decreased by better steering of the fuel into the cylinder.

4.3.6. Exhaust process of the test engine

The temperature contours of the exhaust process of the engine are shown in Figure 4.22. The opening of the exhaust valve and air movements in the cylinder can be seen in this Figure. In the model, it can be seen that the exhaust phase, valve, and piston movements are modeled appropriately. The exhaust valve begins to open at +137 CA while reaching a maximum aperture at +260 CA as 9.5-mm. The engine has a single exhaust valve.

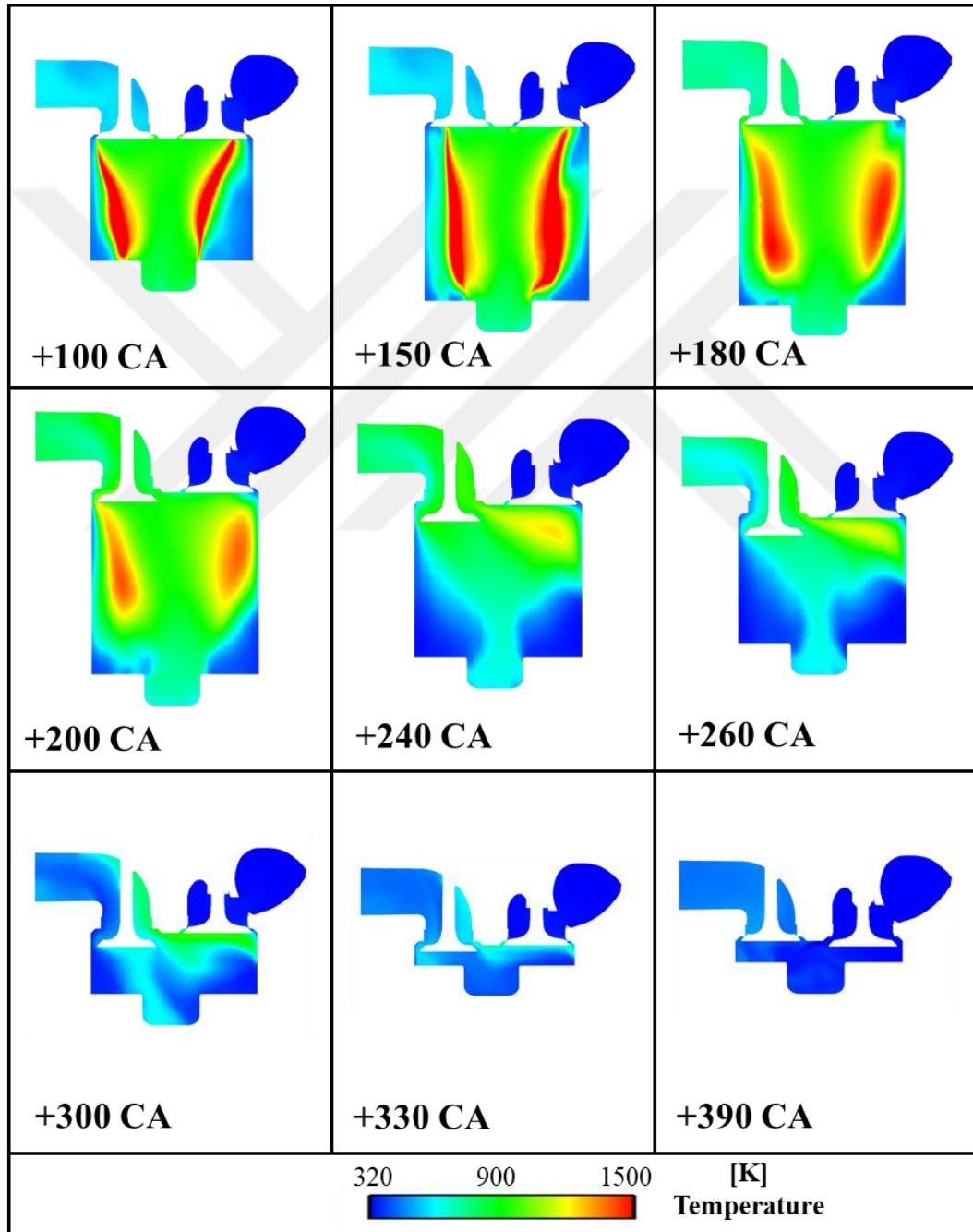


Figure 4.22. Temperature contours of the test engine during the exhaust process

4.4. Parametric Studies using Baseline Case

The simulations have been performed at a constant engine speed of 2800 rpm and full load condition. After validation and mesh independency studies, the model was solved for three cycles. The initial conditions, swirl profile and ratio values of the other cases were taken from -100° bTDC of the last solved cycle, and the other cases were started at this crank angle. The initial in-cylinder mixture was assumed to be fully homogenous and uniform and swirl ratio of 0.827. The swirl profile was assumed as 3.11 (Wahiduzzaman & Ferguson, 1986). The air temperature and in-cylinder pressure were 389.9 K and 170.6 kPa at the start of the simulation, respectively. The initial turbulent kinetic energy and the turbulent dissipation were taken from full engine three-cycle simulation as $29.997 \text{ m}^2/\text{s}^2$, $13545.6 \text{ m}^2/\text{s}^3$, respectively. Wall temperature of piston, liner, head, intake valve and exhaust valve were 525 K, 400 K, 450 K, 450 K, and 550 K respectively. Because the test engine has an asymmetrical combustion chamber, it could not be modeled as a sector. This in turn will increase the solution CPU time. The parameters of the engine's piston bowl, injection pressure, spray angle, SOI, CR, the number of the holes, EGR ratio are simulated. The influence of these parameters on in-cylinder pressure, engine performance and exhaust emissions are examined.

4.4.1. Effect of compression ratio

The compression ratio (CR) is directly related to the combustion inside the cylinder. When the CR increase, the peak firing pressure (PFP) value increases significantly. Of course, when the CR increase, the compression work increases and some of the work produced is spent for compression. The base simulation was run with same parameters except for the CR. As can be observed in Figure 4.23, when increase the CR to 19, rise the maximum pressure up to 7.6 MPa. When the CR is reduced to 16, the maximum pressure drops to 6 MPa. Maximum pressures are critical values for strength and durability.

When the compression ratio increases, NO_x emissions also increase. However, when we reduce the compression ratio, NO_x emissions decrease. Soot and CO emissions, on the other hand, decrease as the CR increases, and as CR decreases, they increase (Figure 4.24).

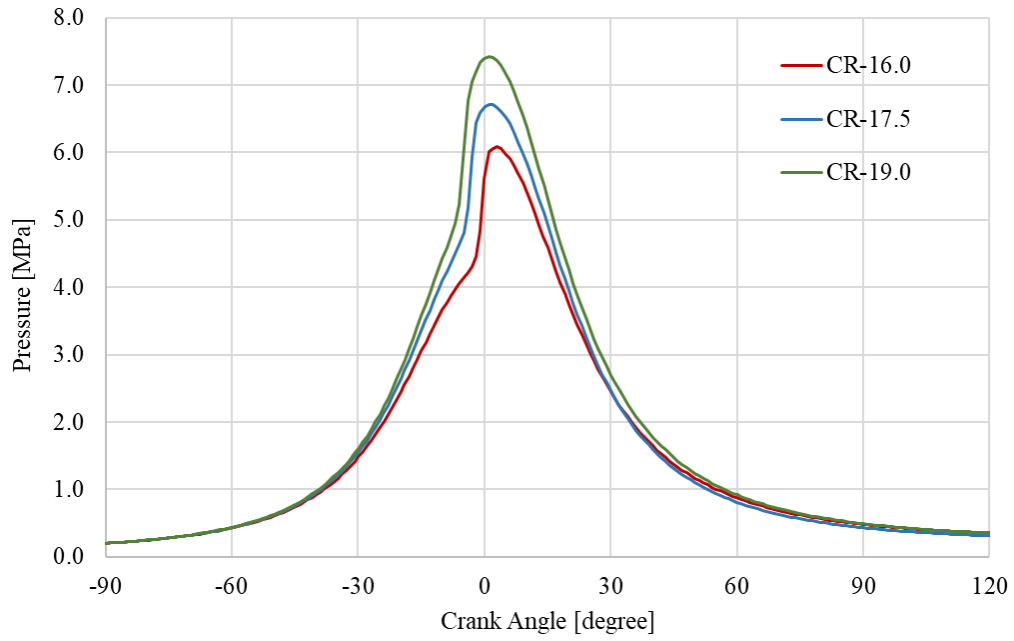


Figure 4.23. In-cylinder pressure values for different compression ratios

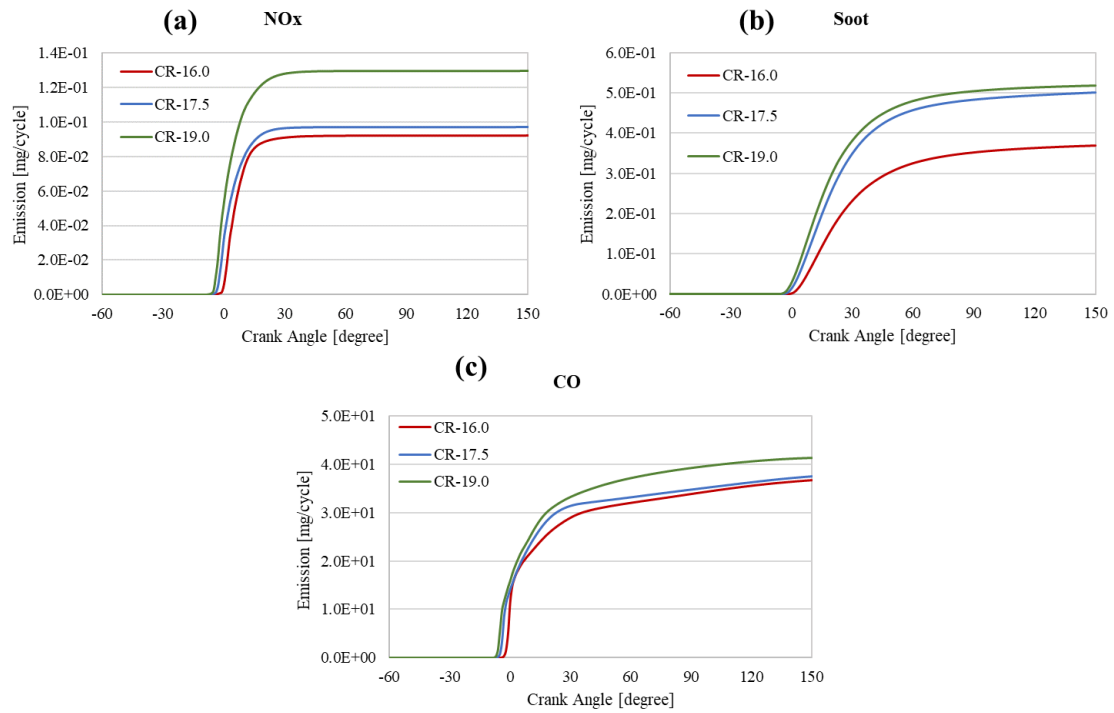


Figure 4.24. Emission values for different compression ratios

4.4.2. Effect of exhaust gas recirculation

The method of sending some amount of exhaust gases into the cylinder, exhaust gas recirculation (EGR), is used to prevent the excessive rising of the internal cylinder temperatures and to control NO_x emissions. In this study, simulations at EGR rates of 0, 4, 8 and 12% were performed. As the EGR ratio increases, the maximum pressures and temperatures inside the cylinder decrease (Figure 4.25).

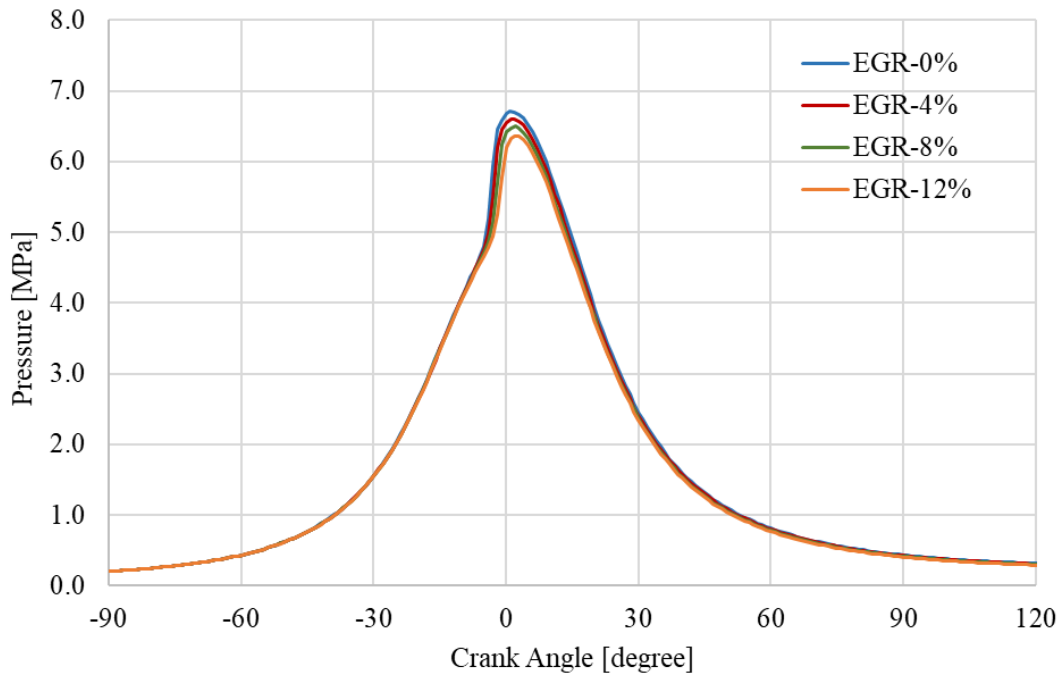


Figure 4.25. In-cylinder pressure values for different EGR ratios

EGR has an important impact on NO_x and soot emissions. Soot and NO_x emissions decrease with increasing EGR rate (Figure 4.26). If the temperature inside the cylinder does not exceed 2300 K, it has been seen in the literature that soot and NO_x emissions decrease with EGR (Li and Ogawa, 2012). CO emissions have slightly increased by the EGR ratio (Figure 4.27).

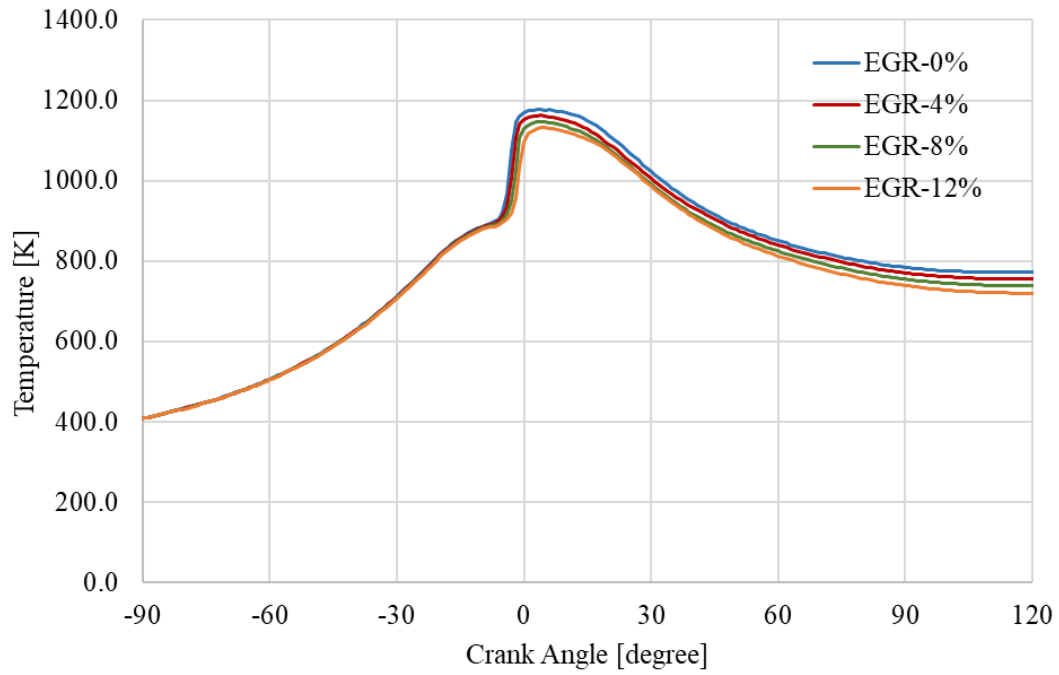


Figure 4.26. Mean in-cylinder temperature values for different EGR ratios

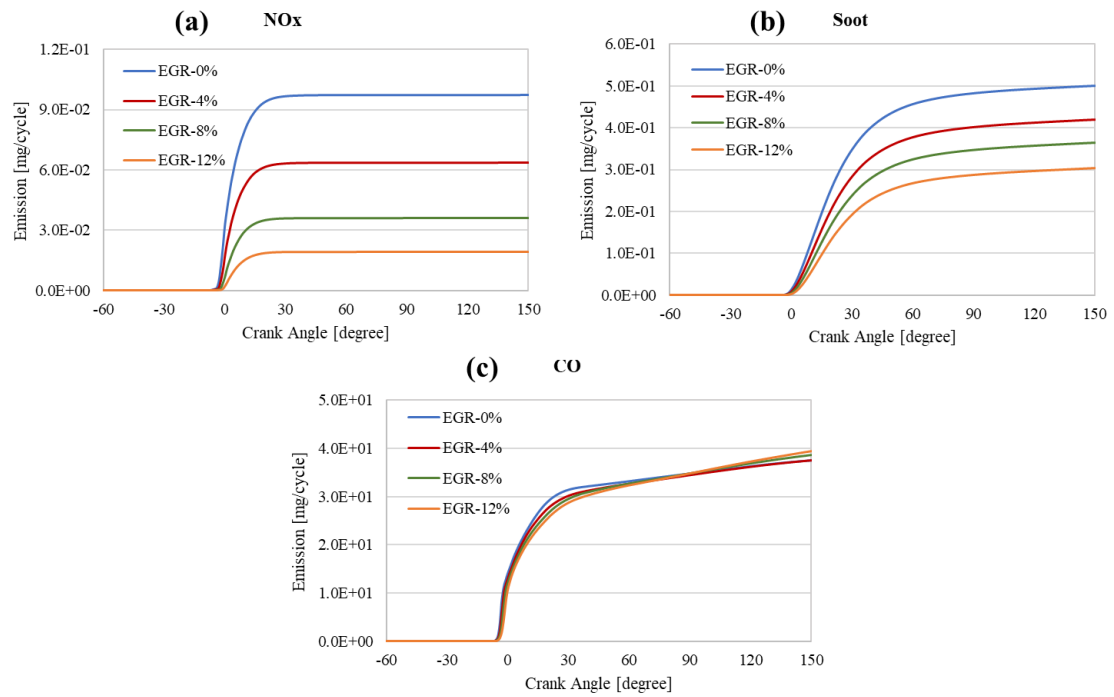


Figure 4.27. Emission values for different EGR ratios

4.4.3. Effect of number of the holes

Increasing the number of injector holes is important as it creates a better mixture in the engines. In this study, the existing 4-hole injector was replaced with a 6-hole injector. The base simulation was run with same parameters except for the number of holes. The 6-hole injector almost did not change the maximum pressure in the combustion chamber but increased the crank angle, which gave the maximum pressure (Figure 4.28). In contrast, the combustion efficiency improved and soot emissions decreased but NO_x emissions increased. It was seen that there was no important change in CO emissions (Figure 4.29).

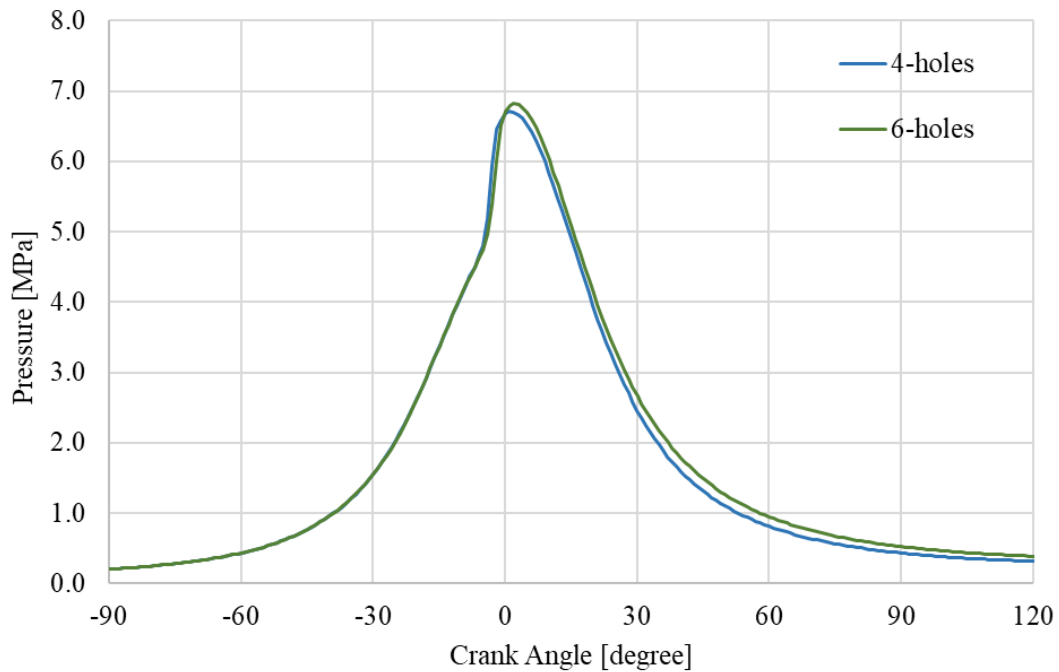


Figure 4.28. In-cylinder pressure values for the injector with 4 and 6 hole

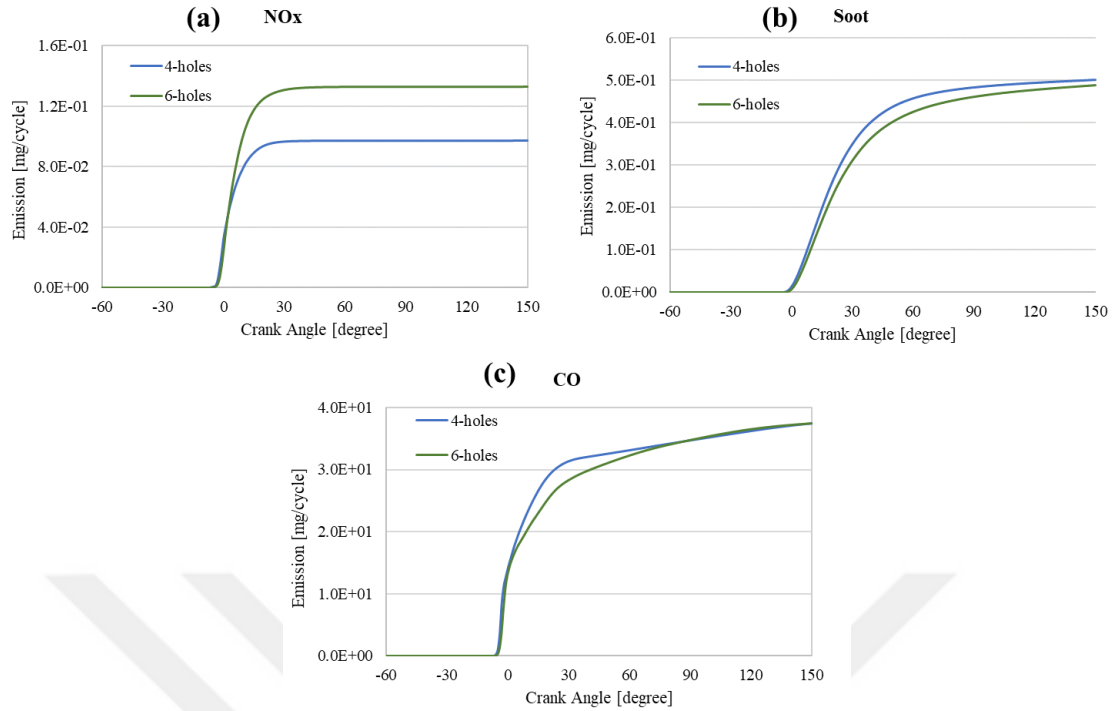


Figure 4.29. Emission values for the injector with 4-hole and 6-hole

4.4.4. Effect of injection pressure

The high injection pressure increases the combustion performance since the fuel is injected into the cylinder more pulverized. By keeping the other parameters constant, simulations were performed at injection pressures of 200, 800, 1000 and 1200 bar. As seen in Figure 4.30, high-pressure injection increases the PFP to 8 MPa levels. It is seen that it increases NO_x emissions approximately 2 times. In contrast, soot emissions have decreased. No significant change was observed in CO emissions (Figure 4.31). The lowest soot and NO_x emission is obtained with injection pressure 1000 bar.

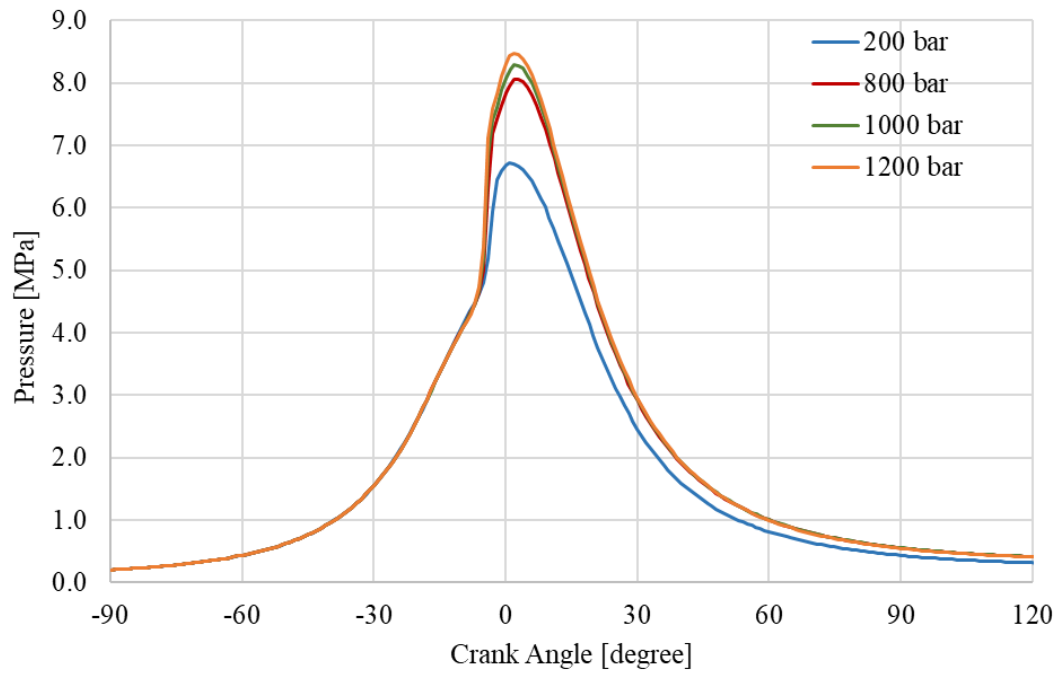


Figure 4.30. In-cylinder pressure values for different injection pressures

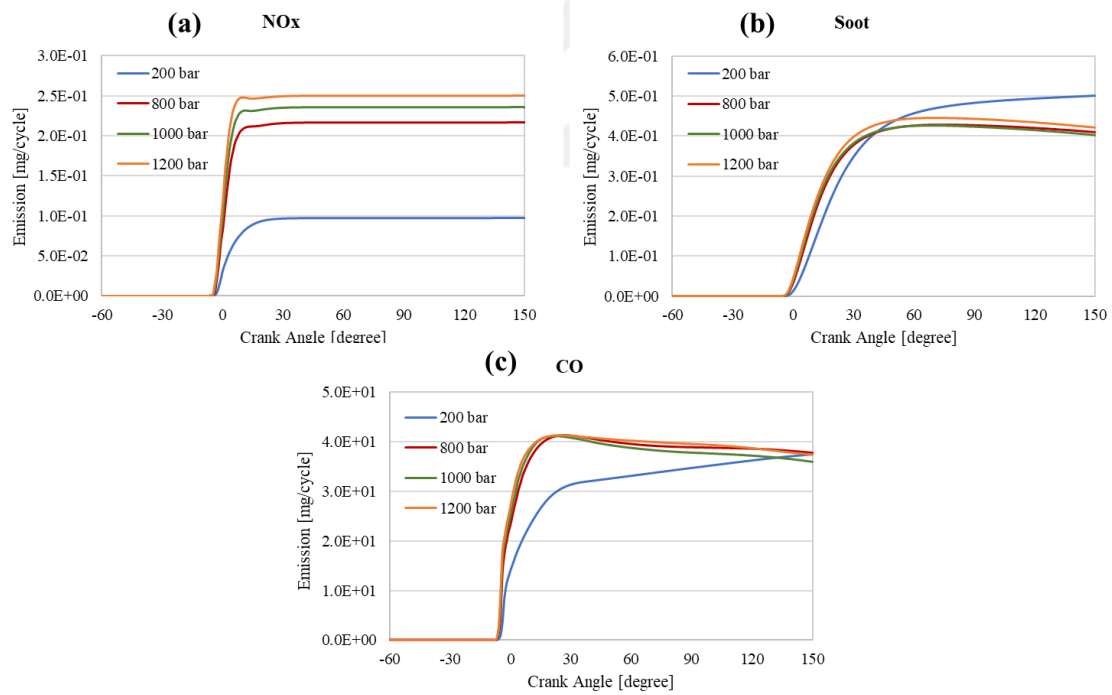


Figure 4.31. Emission values for different injection pressures

4.4.5. Effect of start of injection

The start of injection (SOI) significantly affects the cylinder pressure combustion and emissions. The majority of the injected fuel should burn at 5-10° aTDC and give the maximum pressure in this zone. SOI is chosen to achieve this constraint. Accordingly, the pressure and emission values of the cylinders obtained from simulations that are performed in SOI -25, -20, -15° bTDC are shown in Figure 4.32. NO_x emission increases as SOI is brought forward, and NO_x emissions decrease if SOI is late. Soot emissions, on the other hand, decrease as SOI is brought forward and increase as SOI leaves late. CO emissions are not significantly affected by SOI value (Figure 4.33).

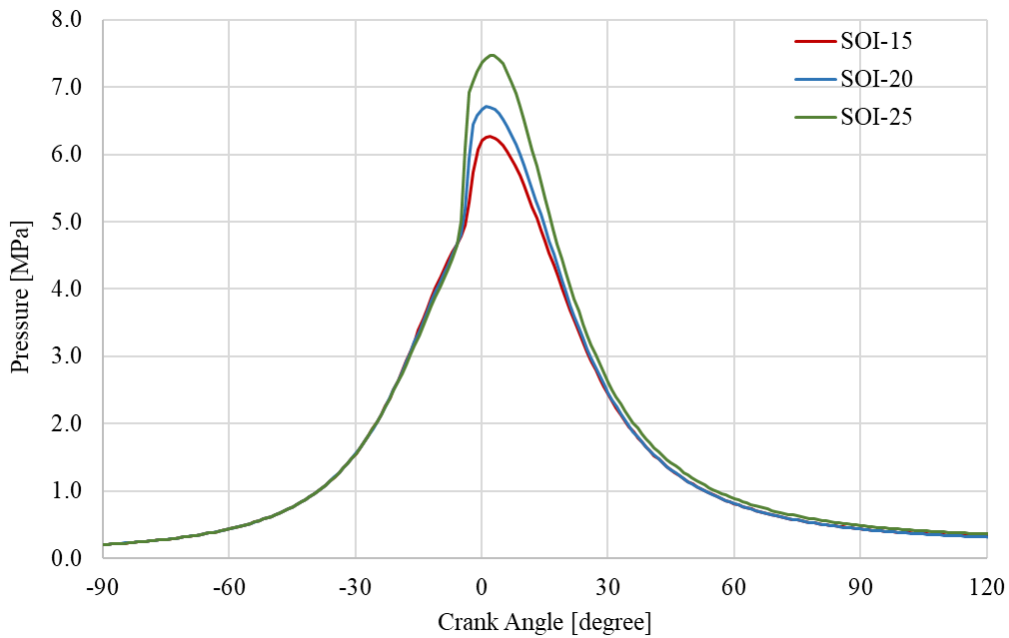


Figure 4.32. In-cylinder pressure values for different SOI

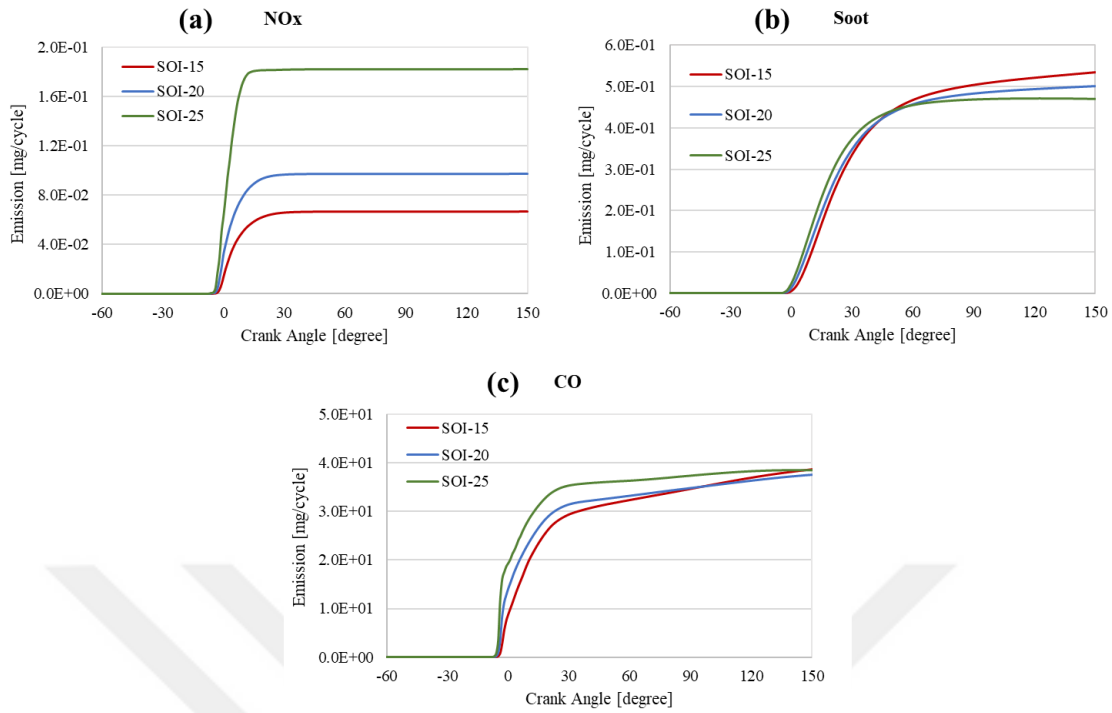


Figure 4.33. Emission values for different SOI

4.4.6. Effect of spray angle

The current spray angle of the injector of the engine is 120°. The bowl design and spray angle parameters should be studied together. In this thesis, simulations were performed for the spray angle of 100°, 120°, 140°, 150°, while all other parameters were constant for the test engine. It was observed that when the injection pressure increased, the pressure inside the cylinder increased for the spray angle of 120°, 140°, and 150°. With spray angle of 100°, a pressure value close to spray angle of 150° was observed (Figure 4.34). Accordingly, NO_x emissions were higher at spray angle of 100° and 150°. It produced lower NO_x emissions at 120° and 140° spray angles. Soot emissions were highest at 120° and lower at 100°, 140° and 150°. For CO emissions, the lowest value was determined at 150°. CO emissions increase as the spray angle decreases (Figure 4.35).

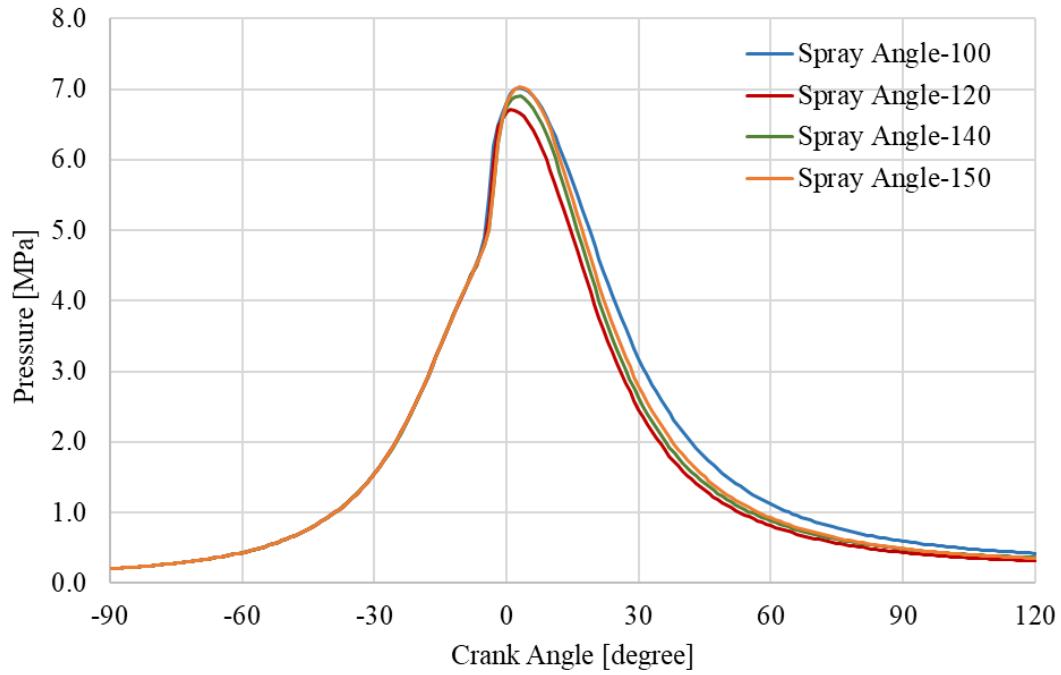


Figure 4.34. In-cylinder pressure values for different spray angle

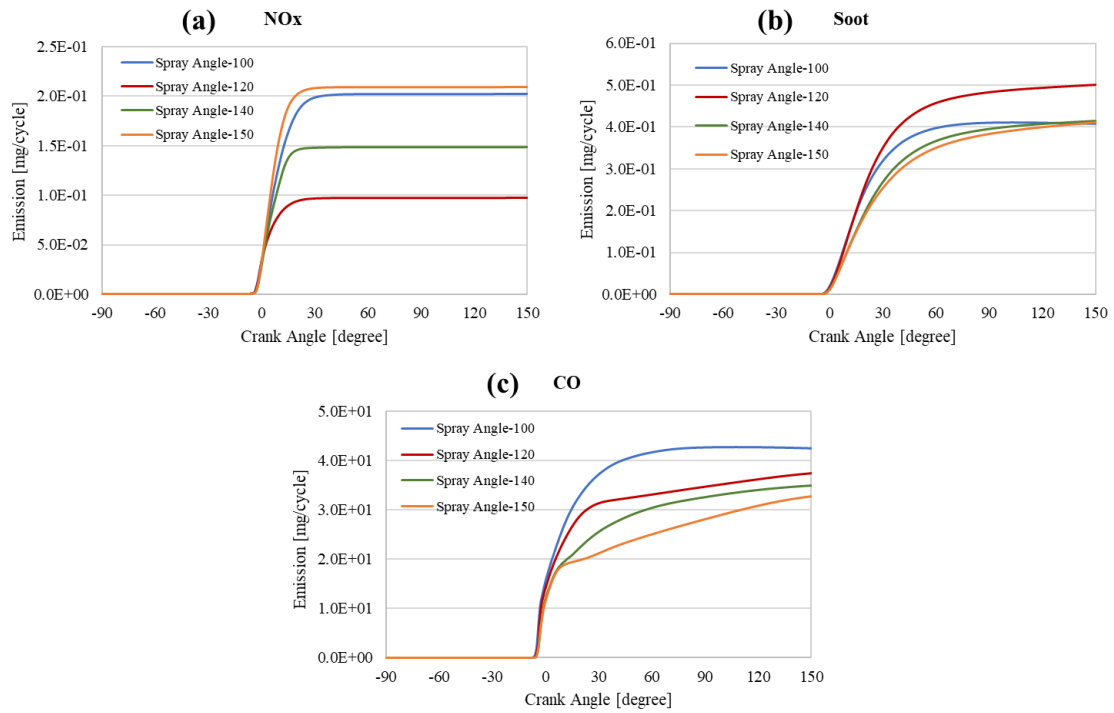


Figure 4.35. Emission values for different spray angle

4.5. Modified Engine with Different Piston Bowl Geometries

Changes in the design of combustion chamber directly affect the engine performance and exhaust emissions. Bowl geometries influence the air/fuel mixing formation and squish in the cylinder. Reentrant bowl (RB), double swirl bowl (DSB) and multi swirl bowl (MSB) geometries have been simulated to be able to improve the mixture of air/fuel and increase combustion efficiency in this thesis. Figure 4.36 illustrates the geometries of the piston bowl used in the simulations. All other conditions were kept the same when making changes in geometry. The spray parameters, the amount of fuel and the compression ratio of the engine were kept constant.

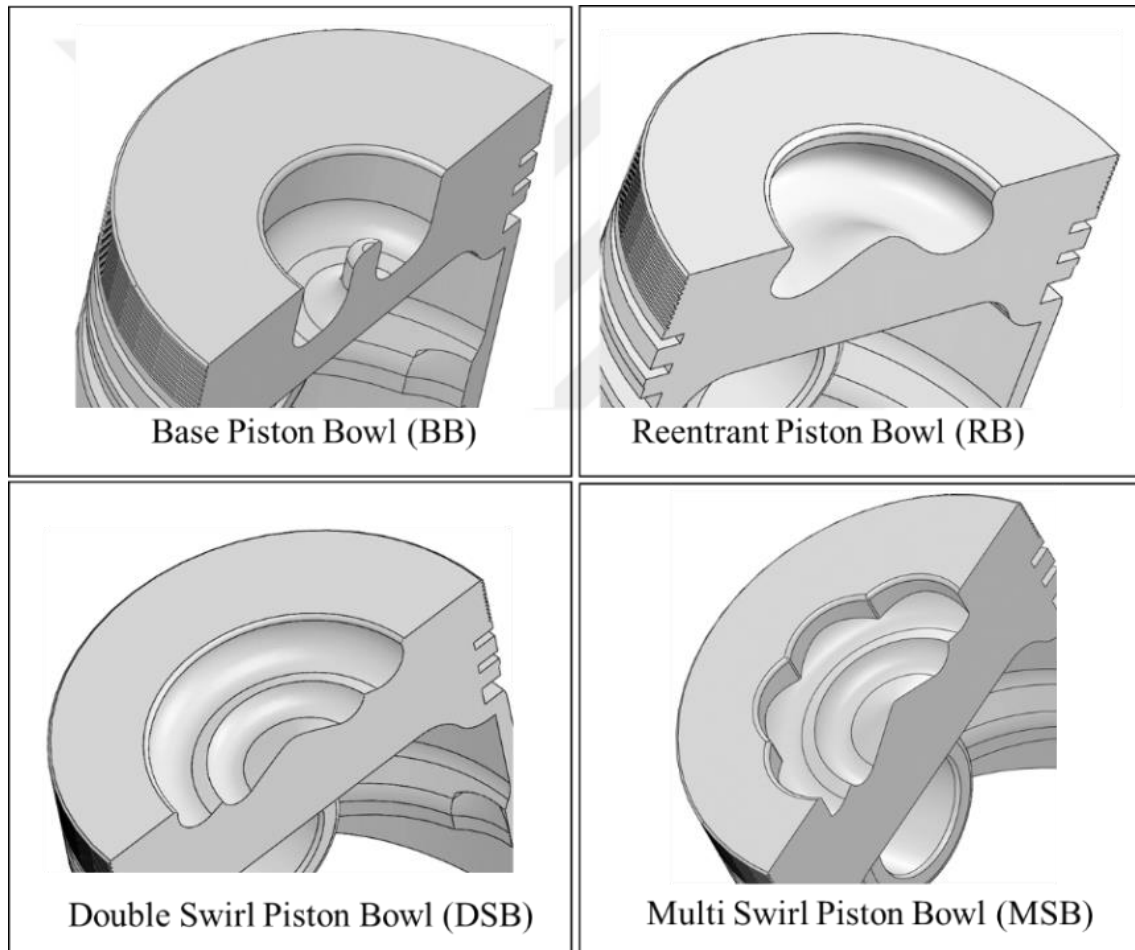


Figure 4.36. The piston bowl types used in the simulations

The DSB and the MSB are two wall-guided flow piston bowl geometries. The injection targeting of the DSB and the MSB are shown horizontally in Figure 4.37. In this DSB piston bowl type, the fuel collides with the vertical convex edge and splits into two swirl eddies in the inner and outer chambers, which accelerates the process of fuel/air mixing

and combustion. The MSB has also a lateral convex edge. When the fuel hits the lateral convex edge, the spray divides into two swirl eddies and develops along the lateral convex edge, which accelerates the mixing of fuel/air mixing inside the cylinder. Besides the advantage of the MSB with multiple swirls, it disrupts the main swirl of the engine.

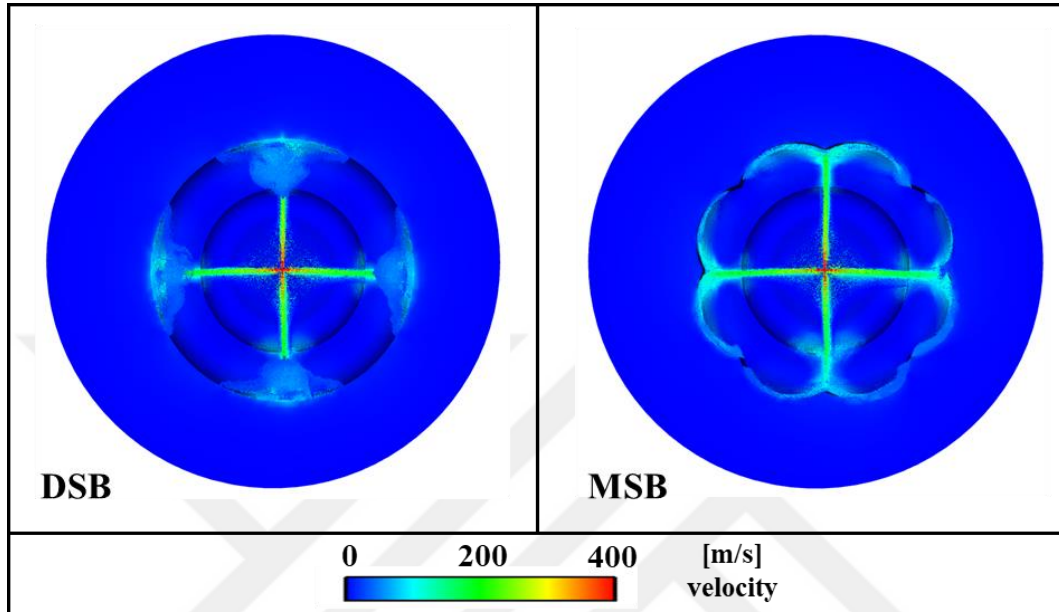


Figure 4.37. Velocity contours of the DSB and MSB bowl at horizontal cross-sectional area at -10 CA

In-cylinder pressure values for BB, RB, DSB, and MSB are compared at the spray angle of 120, 140 and 150 degrees under full load operation as shown in Figure 4.38, in order to understand the combustion process. It has been found that the in-cylinder pressure values of MSB and DSB are higher than BB and RB. This situation is attributed to better mixing and faster evaporation of fuel due to its bowl shape. MSB and DSB have a similar trend. MSB has reached slightly higher peak pressures at the spray angle of 140, while DSB has gained higher peak pressures at the spray angle of 150. BB has the lowest in-cylinder pressure in all cases. Since the in-cylinder pressures are directly linked to the performance of the engine, MSB and DSB will achieve higher power.

Figures 4.39, 4.40 and 4.41 compare the emission of the four piston bowls at varied spray angle. The piston bowl shape affects emissions significantly. With increasing spray angle, NO_x emission values of BB and DSB are directly proportional, whereas the NO_x emission values of RB and MSB are inversely proportional. BB has the lowest NO_x emission, but also it has the lowest thermal efficiency. DSB has the lowest CO emission

at the spray angle of 120 degrees, but with the rise in the spray angle, the CO emission of the BB is getting lower. The CO emissions of MSB are reduced with high injection pressure, yet, CO emissions have been not effected considerably with the high injection pressure for other bowls. DSB produce less soot emission at the spray angle of 150 degree. The design that produces the least soot emission is DSB.

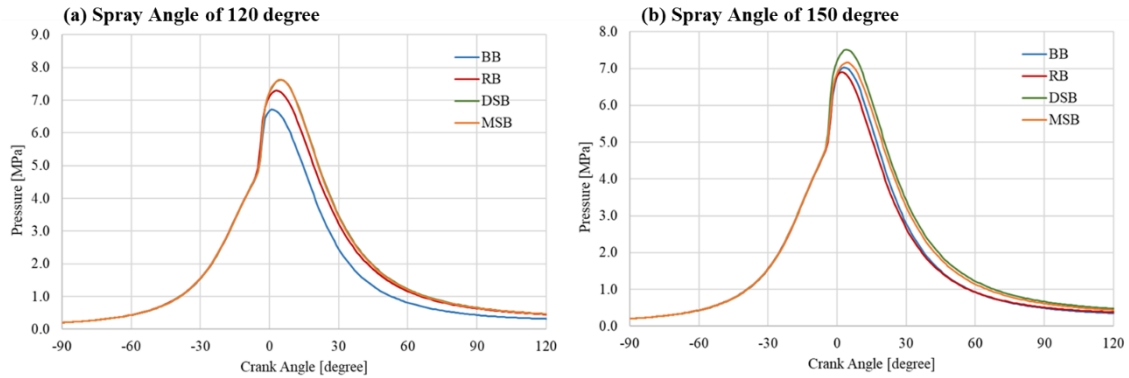


Figure 4.38. In-cylinder pressure values of different bowl designs

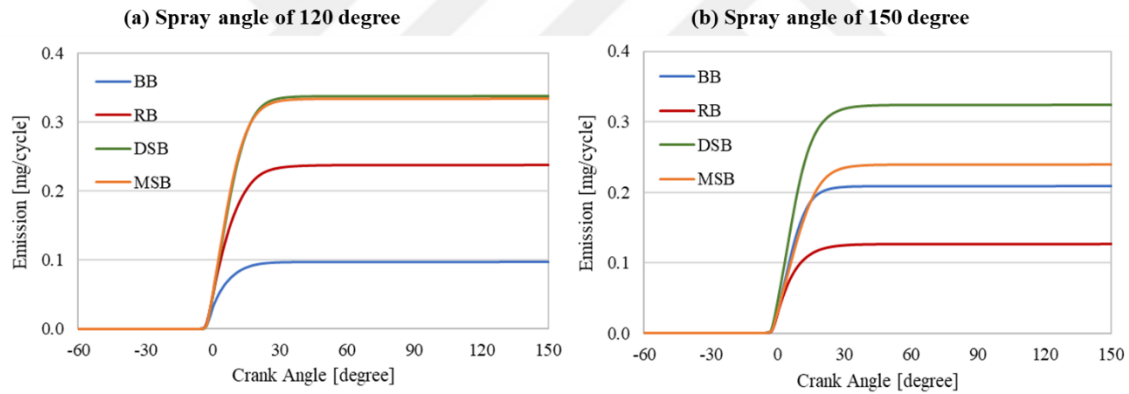


Figure 4.39. NO_x emissions of different bowl designs

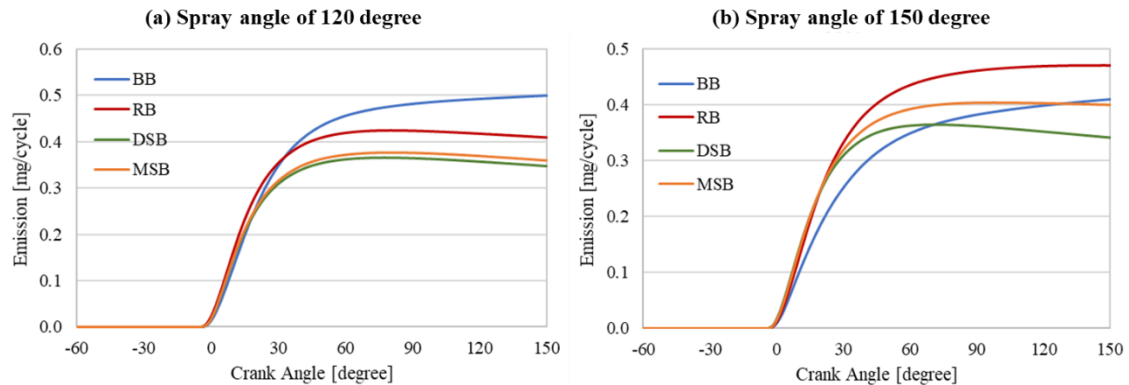


Figure 4.40. Soot emissions of different bowl designs

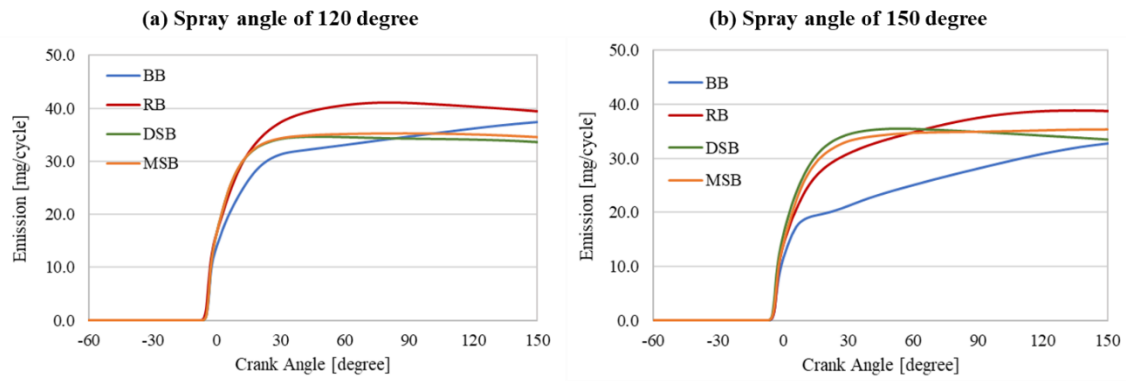


Figure 4.41. CO emissions of different bowl designs

The air/fuel mixing process and evaporation of fuel are related to piston bowl geometry. The in-cylinder velocity distribution at 10° bTDC, TDC and 10° aTDC are presented in Figures 4.42, 4.43 and 4.44 for four bowls and at different spray angles. The DSB and MSB design could not be fully utilized at the spray angle of 120 and 140, because the fuel spray could not reach the convex edge of DSB and MSB. If the spray hits the convex edge, the swirl vortices are formed on the bowl sides. In-cylinder swirl increases the fuel diffusion area (X. Li et al., 2017). Accordingly, it can be observed that the ideal angle for reaching the spray to the convex edges of DSB and MSB and for achieving very good mixing is the spray angle of 150 degrees (Figure 4.44) (Sener, Yangaz, & Gul, 2020). It can be seen that the velocity on the sides of the convex edge is greater. RB with less complex shape has relatively a better mixture compared to BB.

The in-cylinder temperature distribution at 10° aTDC for the spray angle of 120, 140 and 150 illustrated in Figures 4.45, 4.46 and 4.47. At the spray angle of 150, MSB and DSB achieve more homogeneous temperature distribution inside the piston bowl. This may be due to more mixing of air-fuel and more swirl formation by better use of convex surfaces of MSB and DSB. There are high-temperature zones on both sides of the convex edge of these bowls. Due to the shape of the DSB and the MSB, the temperature can rise in the cylinder head. The fuel hits the convex surfaces, a large portion of the fuel moves upwards and a high concentration of the fuel-air mixture is formed near to the cylinder head. When the mixture burns, the temperature and the thermal load of the cylinder head increases. A similar scenario occurs in RB, but this effect is more significant for DSB and MSB (Figures 4.45, 4.46 and 4.47).

Figure 4.48 shows the equivalence ratio of the bowls for different spray angles. MSB has a very homogeneous fuel-air mixture within the cylinder; therefore, the equivalence ratio

is approximately the same in each region. It can be seen there are lesser high equivalence ratio regions in MSB compared to other bowls. Regions with high equivalence ratio are responsible for incomplete combustion and higher soot emissions (Khan, Panua, & Bose, 2018). Accordingly, it can be seen that relatively good results are obtained with RB. But the best results are obtained with MSB.

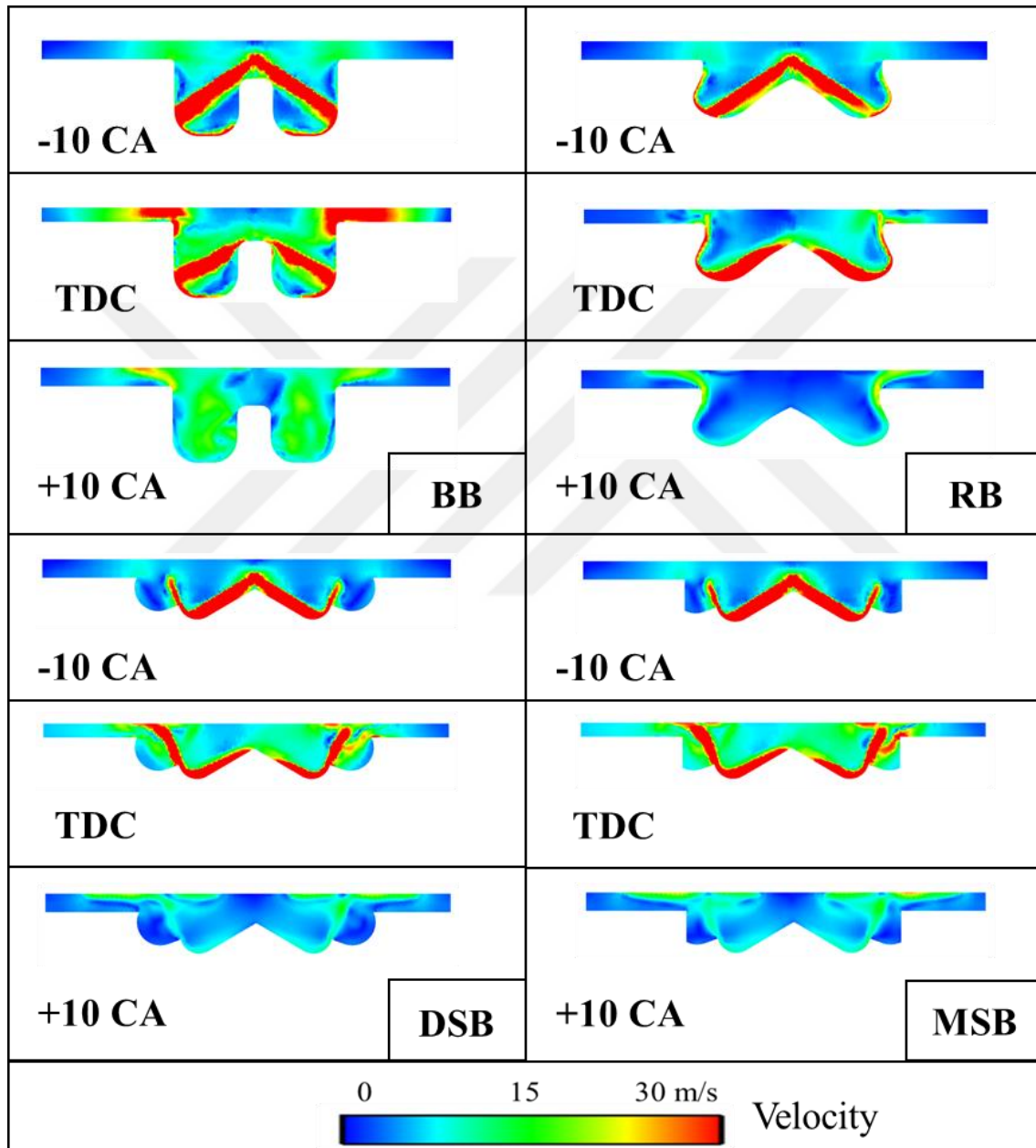


Figure 4.42. In-cylinder velocity for 120 spray angle

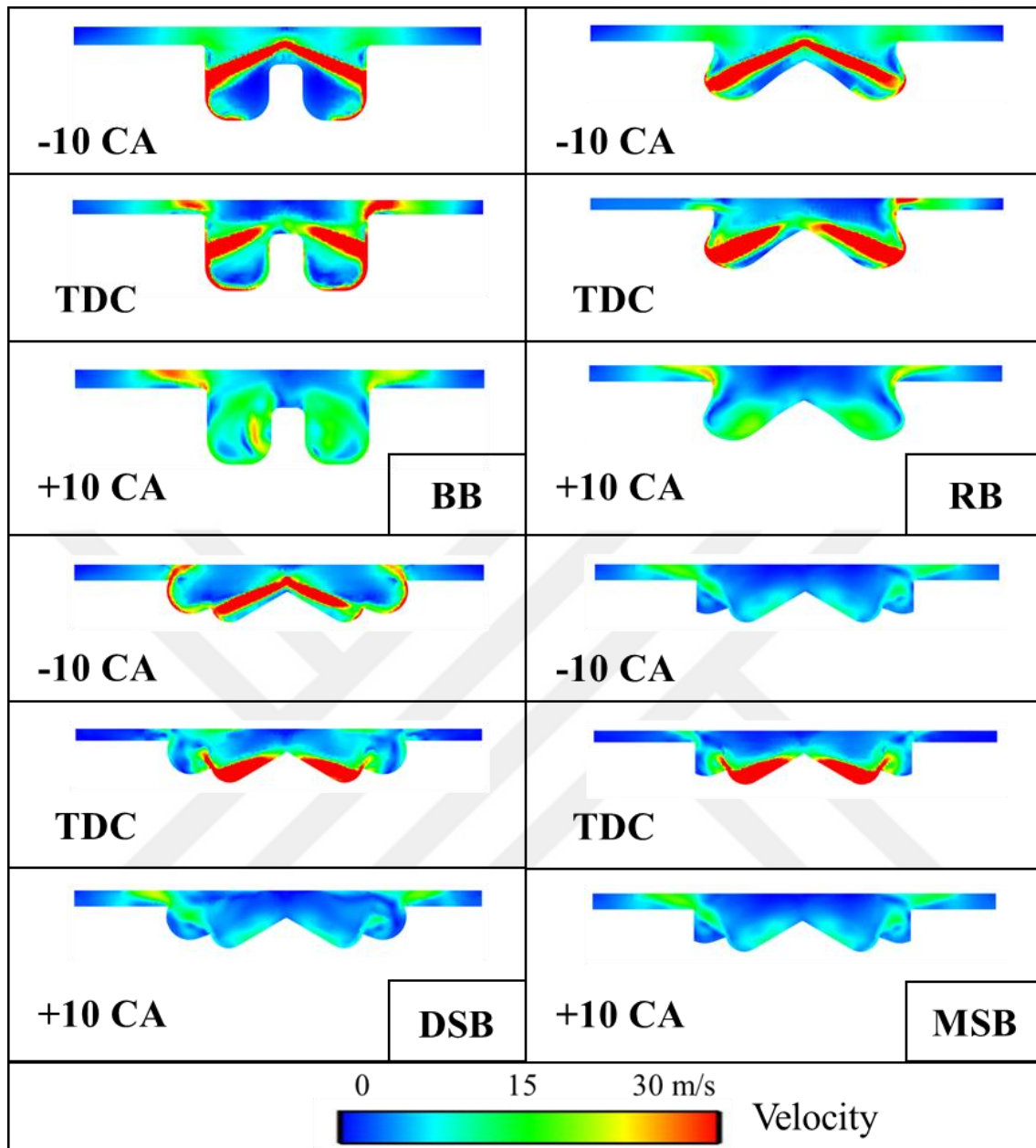


Figure 4.43. In-cylinder velocity for 140 spray angle

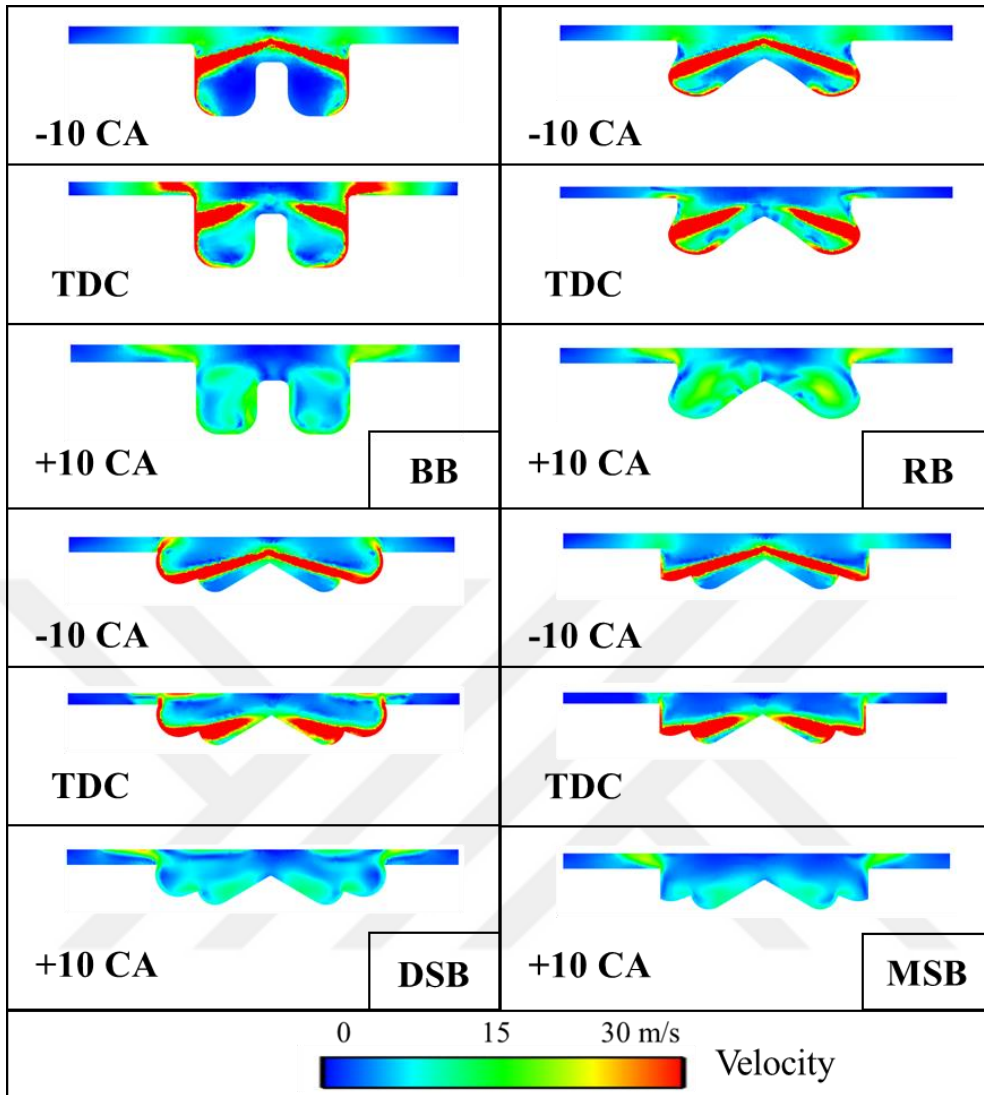


Figure 4.44. In-cylinder velocity for 150 spray angle

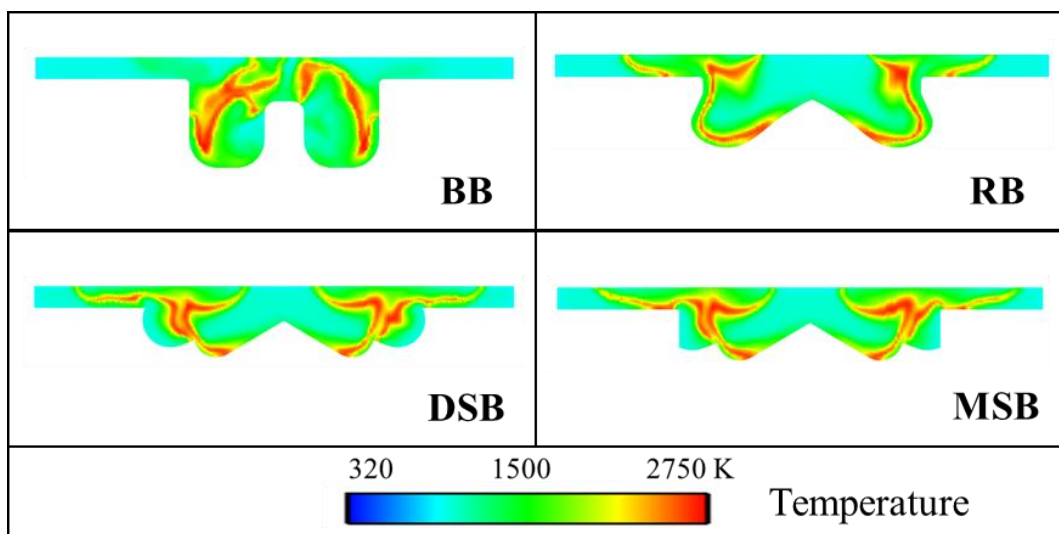


Figure 4.45. In-cylinder temperature distribution at 10 CA aTDC for 120 spray angle

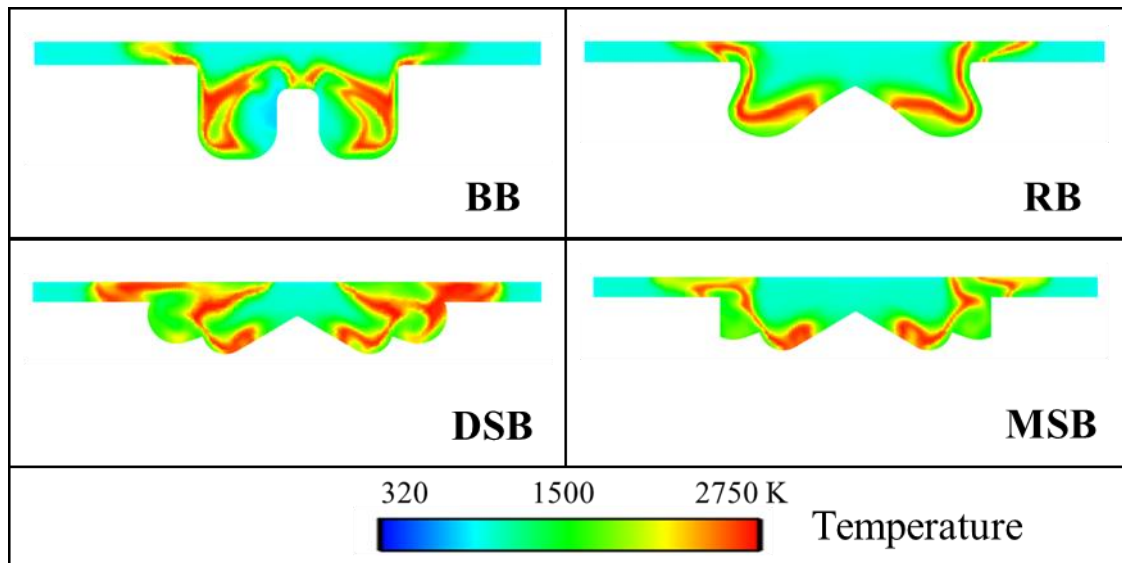


Figure 4.46. In-cylinder temperature distribution at 10 CA aTDC for 140 spray angle

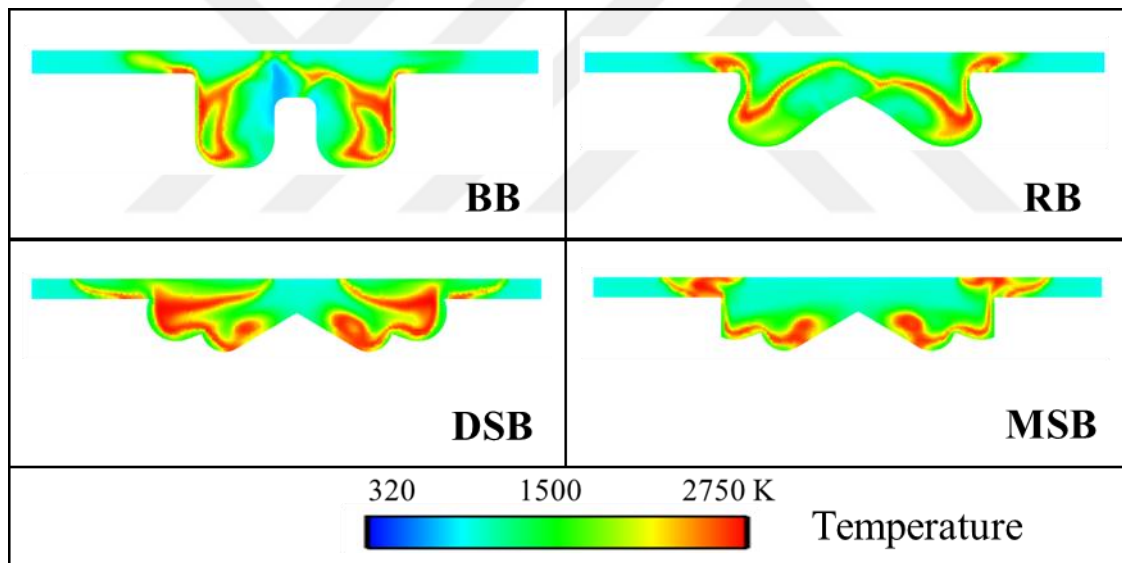


Figure 4.47. In-cylinder temperature distribution at 10 CA aTDC for 150 spray angle

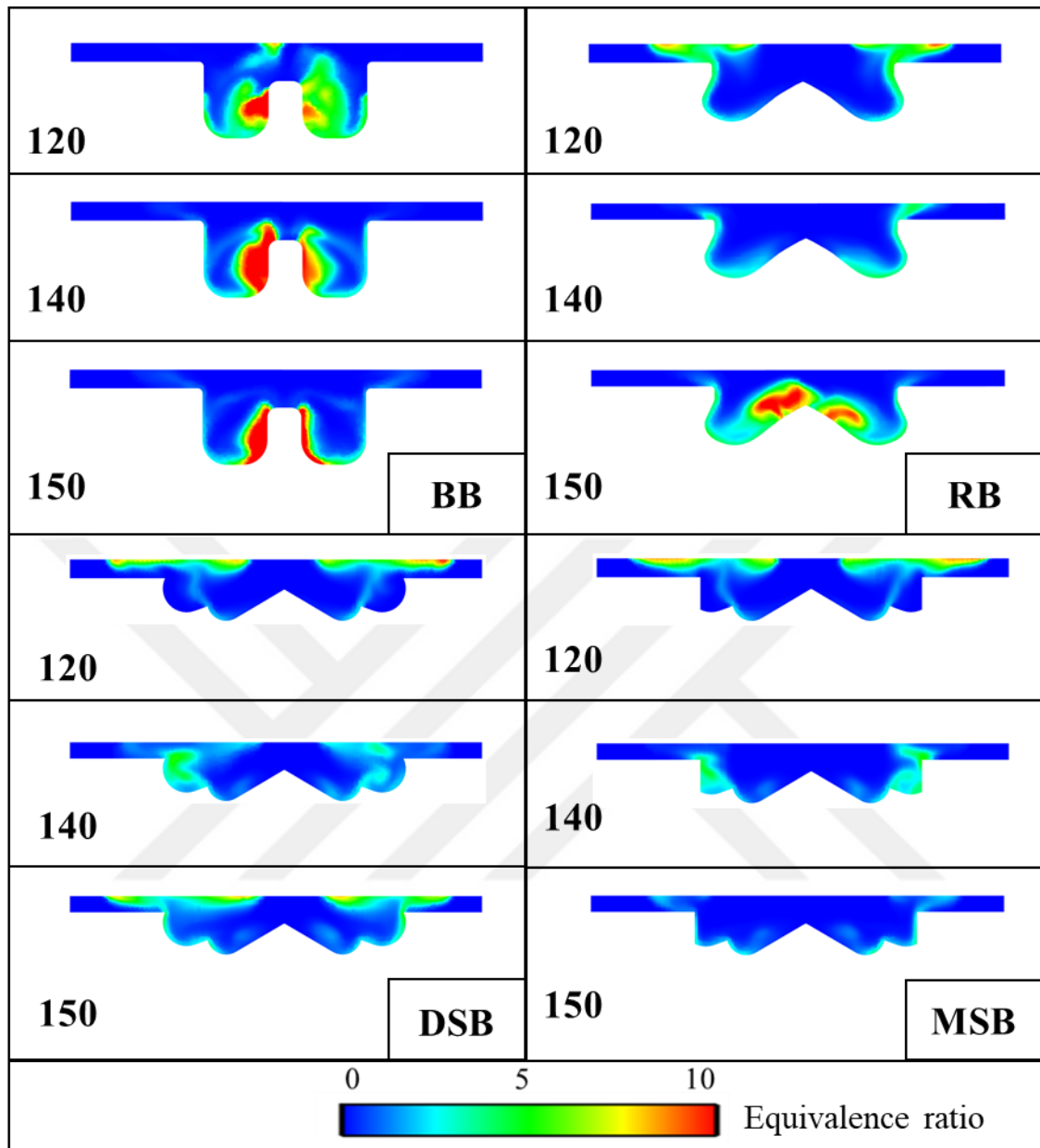


Figure 4.48. In-cylinder equivalence ratio at 10 CA aTDC for different spray angle

4.6. QD Model Optimization Studies

Optimum valve timing and injection parameters were found using Genetic Algorithm. Optimization cases were performed using GT-Suite optimization tool with NSGA-II method.

4.6.1. Valve Lift Optimization

4.6.1.1. Valve lift optimization case for NO_x minimization

IVO, EVO, IVC and EVC values optimization is studied in order to minimize the emission. Firstly, total 250 iterations were solved using the validated QD model. Exhaust timing from 100 to 155 CA and intake timing from 309 to 364 CA resolved. It gave the lowest emission value with almost same brake power at exhaust timing of 132 CA and intake timing of 340 CA.

4.6.1.2. Valve lift optimization case for EGR

In order to decrease NO_x emission in the test engine, EGR is proposed. However, since the EGR system is complex, it is proposed to regulate valve lifts according to the less evacuation of residual gases by regulating exhaust and intake valve timings. According to the total 530 iteration optimization studies, when the exhaust timing is determined as the exhaust timing of 345 CA and the intake timing of 135 CA, the exhaust and intake valve lifts are narrowed by 10%, the residual gas of 12% remains in the cylinder (Figures 4.49 and 4.50).

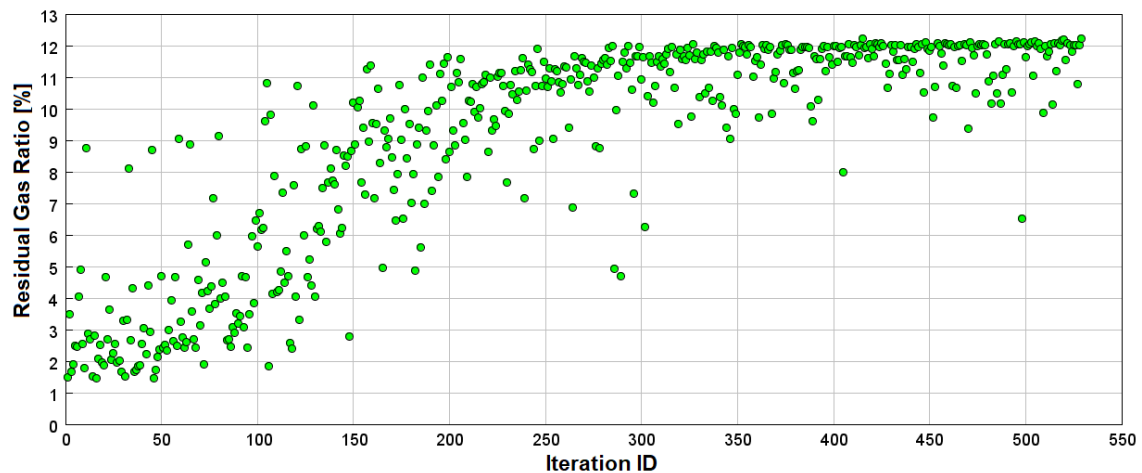


Figure 4.49. Residual gas ratio variation relative to valve timings

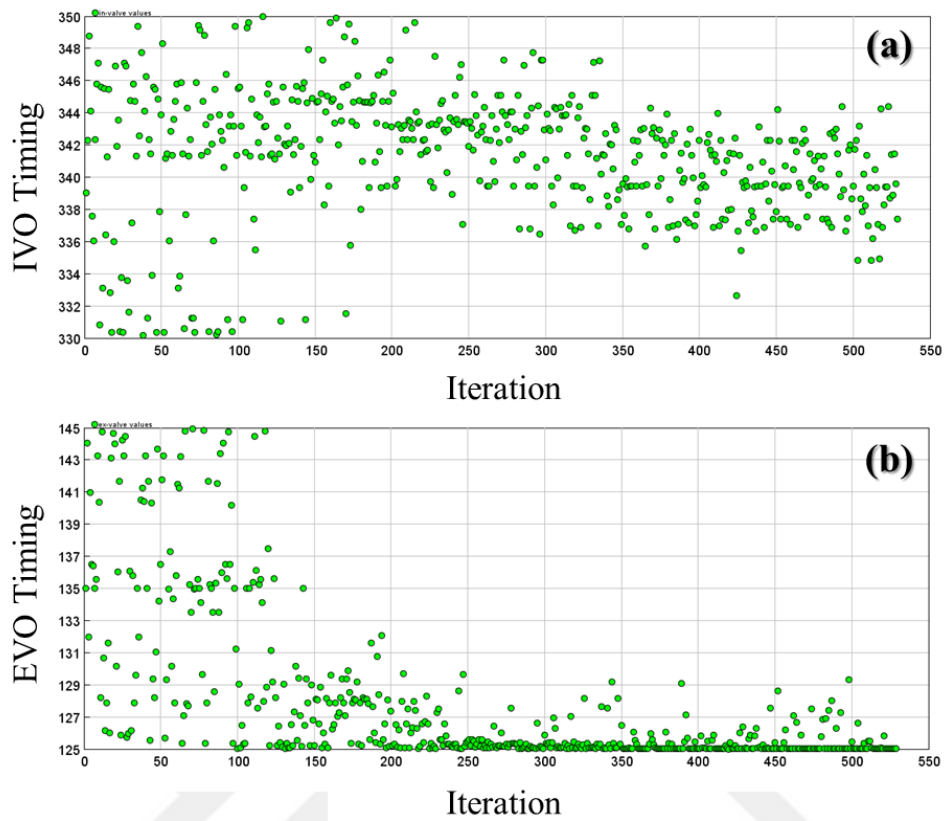


Figure 4.50. Valve timings for a) intake and b) exhaust during optimization process

4.6.2. Injection Strategy Optimization

4.6.2.1. Injection Strategy Optimization case for NO_x minimization

SOI and injection duration values are optimized in order to minimize the emission. A total of 480 iterations was solved using the validated QD model (Figure 4.51). SOI from -20 to -5 CA bTDC and injection duration from 10 to 30 CA resolved. According to the optimization cases, it is predicted that when SOI -15 CA bTDC and injection duration are set to 18 CA, it will give minimum NO_x emission with almost the same brake power (Figure 3.52 and 3.53).

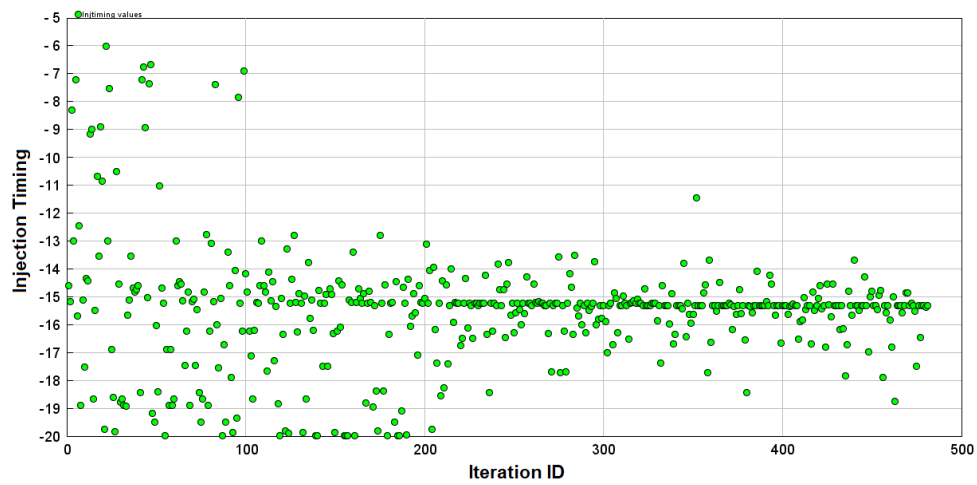


Figure 4.51. Injection timings during optimization process

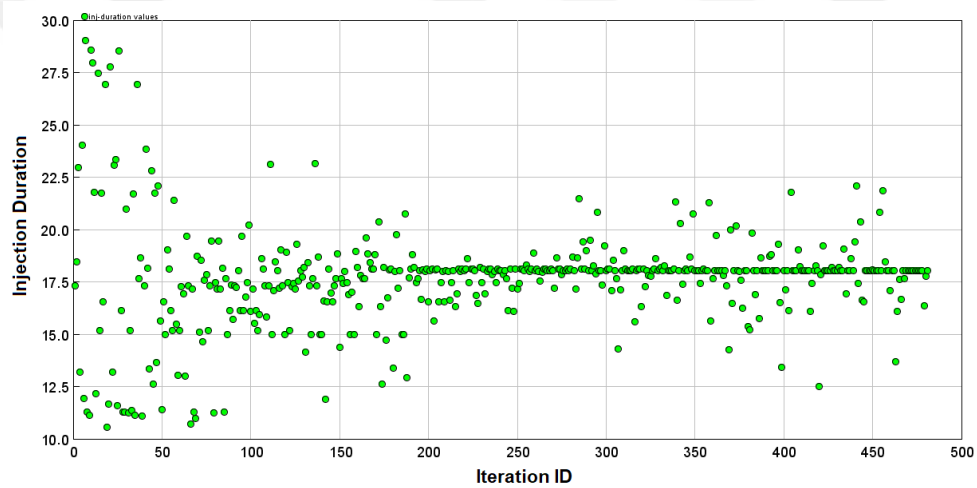


Figure 4.52. Injection duration during optimization process

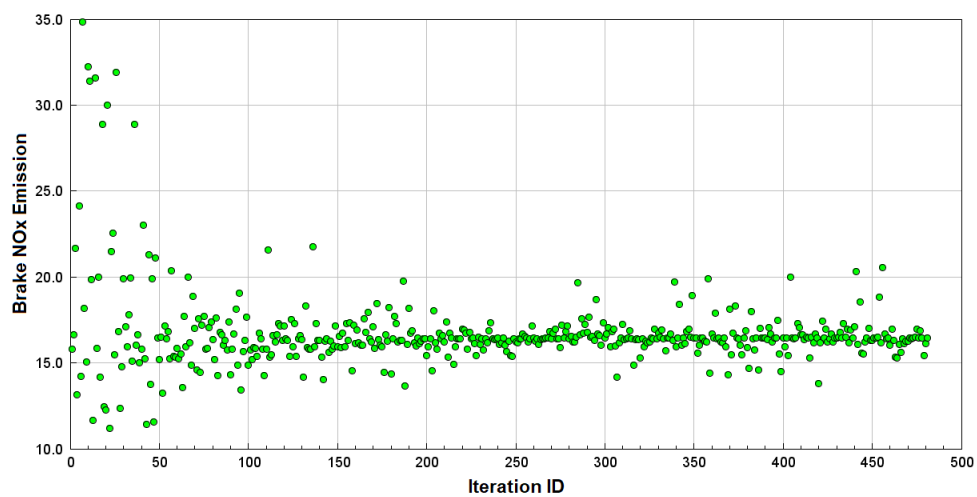


Figure 4.53. Brake NO_x emission variation relative to injection timings and durations during optimization process

4.7. CFD Optimization Studies

The piston bowl geometry has been parameterized to find the optimum design. Optimization studies were performed with parameterized double-swirl piston bowl (DSB) according to better results it gave in previous parametric studies. Bowl height, radius-1, radius-2 and bowl radius values were changed and resolved parametrically (Figure 4.54) using CAESES and Converge software. Dakota MOGA method was used to find the optimum design. A total of 104 CFD simulations have been solved. Results were evaluated according to NO_x , Soot emissions, PFP, indicated power and ISFC. Figures 4.55 and 4.56 show the NO_x and soot emissions according to solved cases, respectively. NO_x versus soot emissions of the designs shown in Figure 4.57. It can be seen from this graph that the soot and NO_x have a trade-off. Figures 4.58 and 4.59 show the changes in emissions according to the design parameters. Therefore, 12 designs that give minimum emission and ISFC and maximum power were recommended according to the MOGA method from the design pool (Table 4.4 and Table 4.5). The recommended 12 designs evaluated with in-cylinder velocity and temperature distribution (Figures 4.60 and 4.61). According to this design pool, the design-101 was chosen as the optimum design. While several designs have acceptable results, the design-101 gave minimum NO_x and soot, and ISFC and maximum power. Since these parameters are trade-off with each other, one design must be selected according to the thesis purpose.

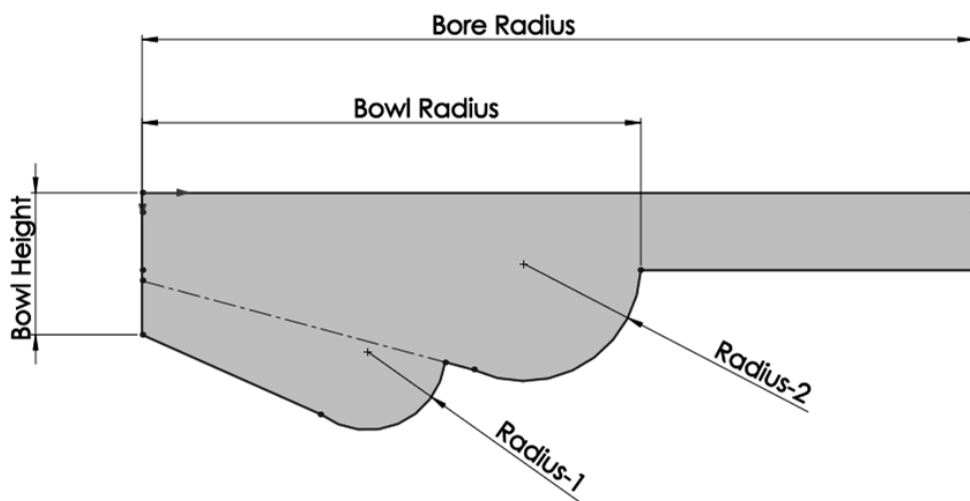


Figure 4.54. Locations of the optimization design parameters

Table 4.4. Parameters of the optimum designs

	Radius-1	Radius-2	Bowl Radius	Bowl Height	NO_x Emission	Soot Emission
Design 28	2.87982	1.81796	27.3667	4.90854	7.11E-08	6.90E-09
Design 35	2.77630	1.52617	26.8506	4.80114	7.81E-08	5.55E-09
Design 37	2.84179	1.50163	26.8785	4.79675	7.74E-08	5.69E-09
Design 46	2.68072	1.91601	27.3696	4.85415	7.33E-08	6.50E-09
Design 49	2.96661	1.82839	27.4188	4.75344	7.18E-08	6.83E-09
Design 50	2.71838	1.49028	26.8407	4.89645	7.66E-08	6.15E-09
Design 54	2.95593	1.65545	27.4683	4.87658	6.94E-08	8.21E-09
Design 56	2.98517	1.85989	27.4653	4.96759	6.98E-08	7.20E-09
Design 74	2.82025	1.58724	26.8744	4.84399	7.69E-08	5.71E-09
Design 77	2.74047	1.45265	26.4903	4.90753	7.80E-08	5.68E-09
Design 87	2.90753	1.65947	27.4904	4.87210	6.95E-08	8.14E-09
Design 101	2.70141	1.52553	26.8186	4.95624	7.50E-08	6.36E-09

The minimum NO_x region is radius-1 between 2.7 and 3 mm, radius-2 between 1.2 and 1.7 mm, bowl radius between 15 and 15.5 mm, and bowl height between 2.7 and 3 mm. The minimum soot region is radius-1 from 1 to 2 mm, radius-2 from 3 to 4 mm, bowl radius from 16 to 19 mm, and bowl height from 3.5 to 5 mm. It is anticipated that NO_x and soot emissions will be minimized when this range of parameters is selected in this range (Figure 4.59 and 4.60). Of course, minimum soot and NO_x emission regions are different. It is necessary to choose according to these values.

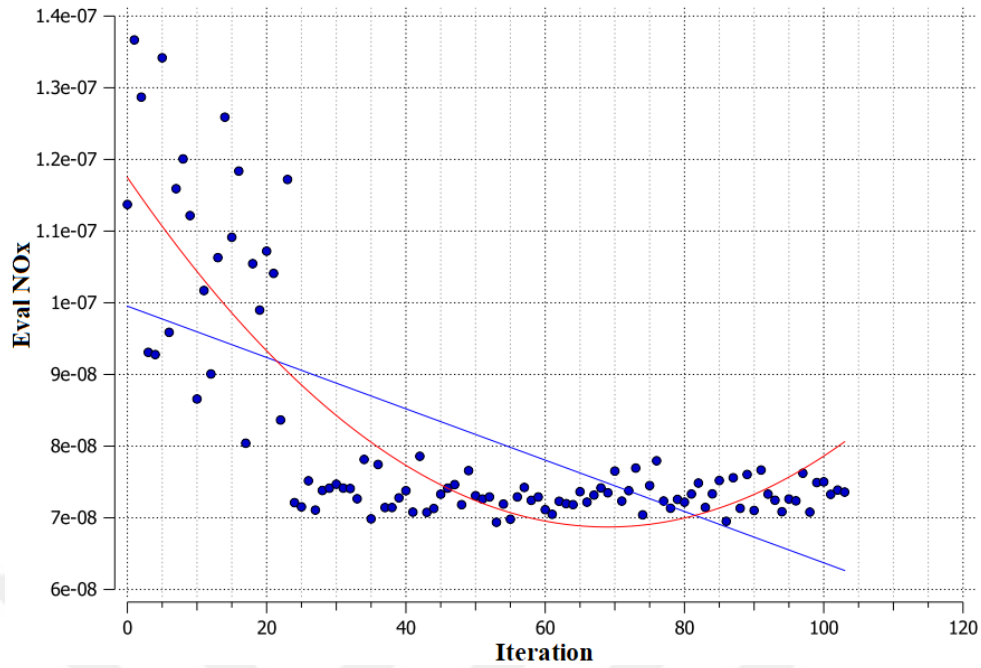


Figure 4.55. Result pool of the optimization studies according to NO_x emission

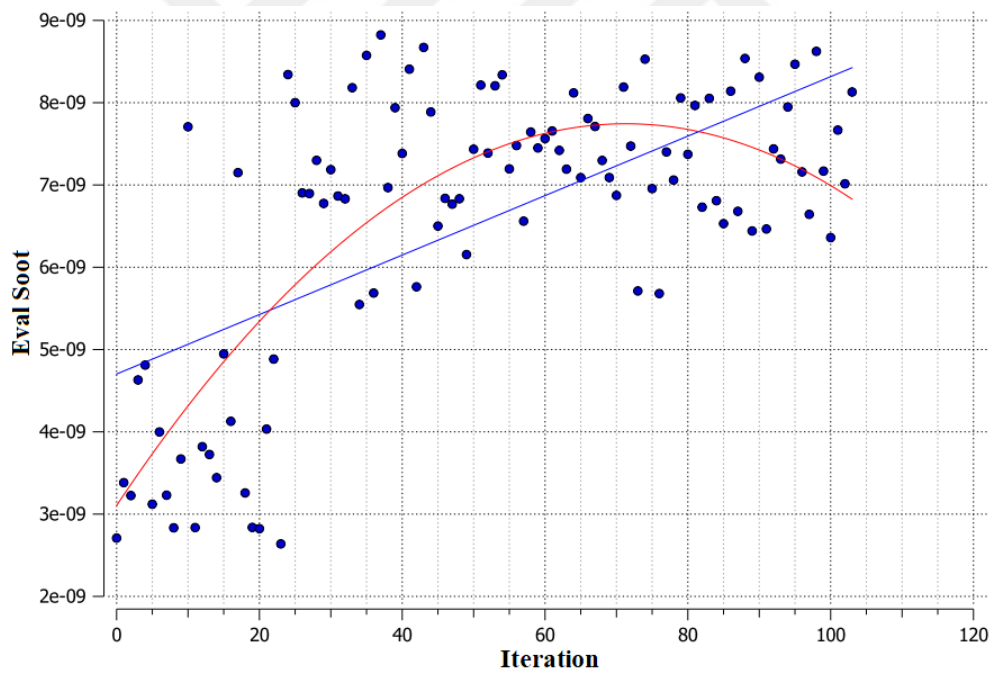


Figure 4.56. Result pool of the optimization studies according to soot emission

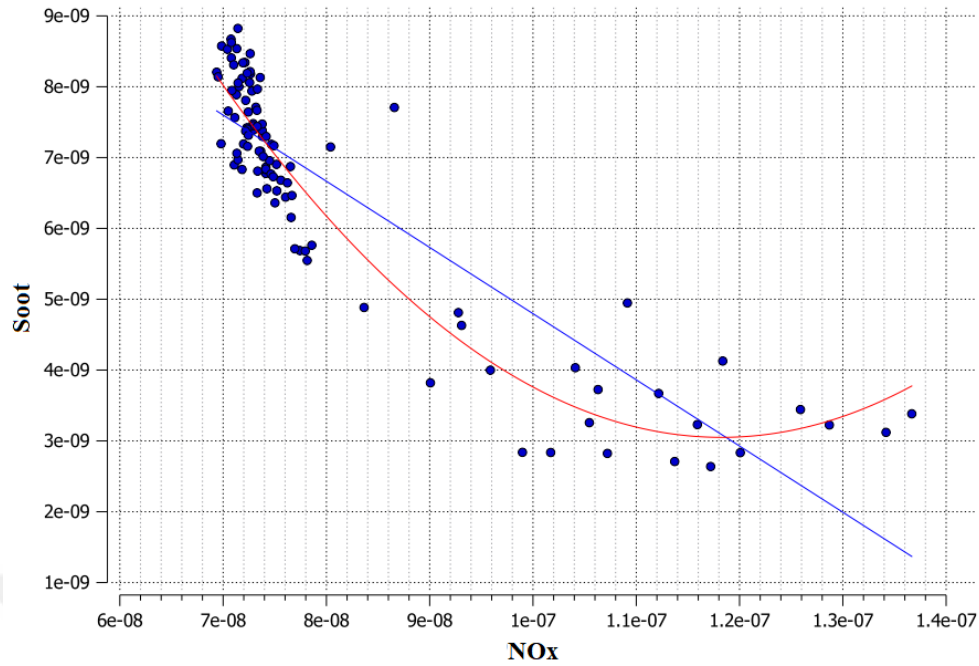


Figure 4.57. Soot emissions versus NO_x emissions according to the optimization studies

Table 4.5. Performance and Emission Parameters of the optimum designs

	NO _x	Soot	PFP	Indicated Power	ISFC
Design 28	7.11E-08	6.90E-09	7.7115	10.97	153.16
Design 35	7.81E-08	5.55E-09	7.9024	11.10	151.32
Design 37	7.74E-08	5.69E-09	7.8930	11.10	151.39
Design 46	7.33E-08	6.50E-09	7.7311	10.99	152.92
Design 49	7.18E-08	6.83E-09	7.7183	10.96	153.31
Design 50	7.66E-08	6.15E-09	7.8851	11.07	151.72
Design 54	6.94E-08	8.21E-09	7.7195	10.91	153.96
Design 56	6.98E-08	7.20E-09	7.6779	10.91	153.93
Design 74	7.69E-08	5.71E-09	7.8707	11.09	151.48
Design 77	7.80E-08	5.68E-09	7.9445	11.12	151.02
Design 87	6.95E-08	8.14E-09	7.7159	10.91	153.96
Design 101	7.50E-08	6.36E-09	7.8717	11.06	151.84

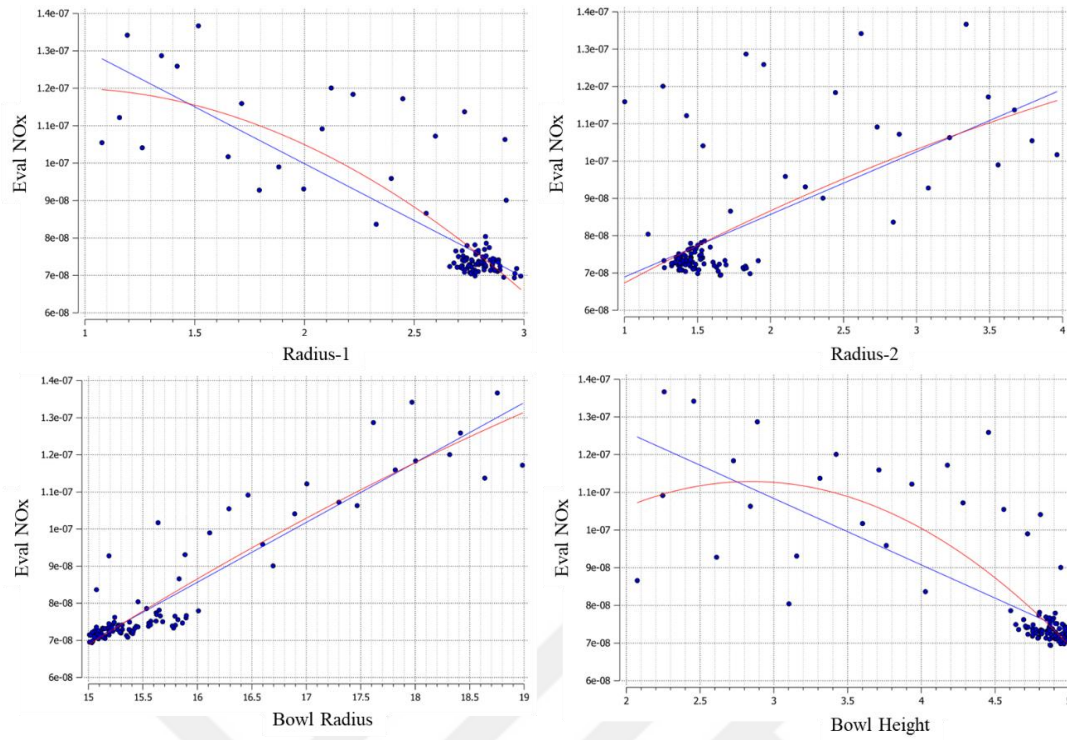


Figure 4.58. Result pool of the optimization studies according to NO_x emission versus design parameters

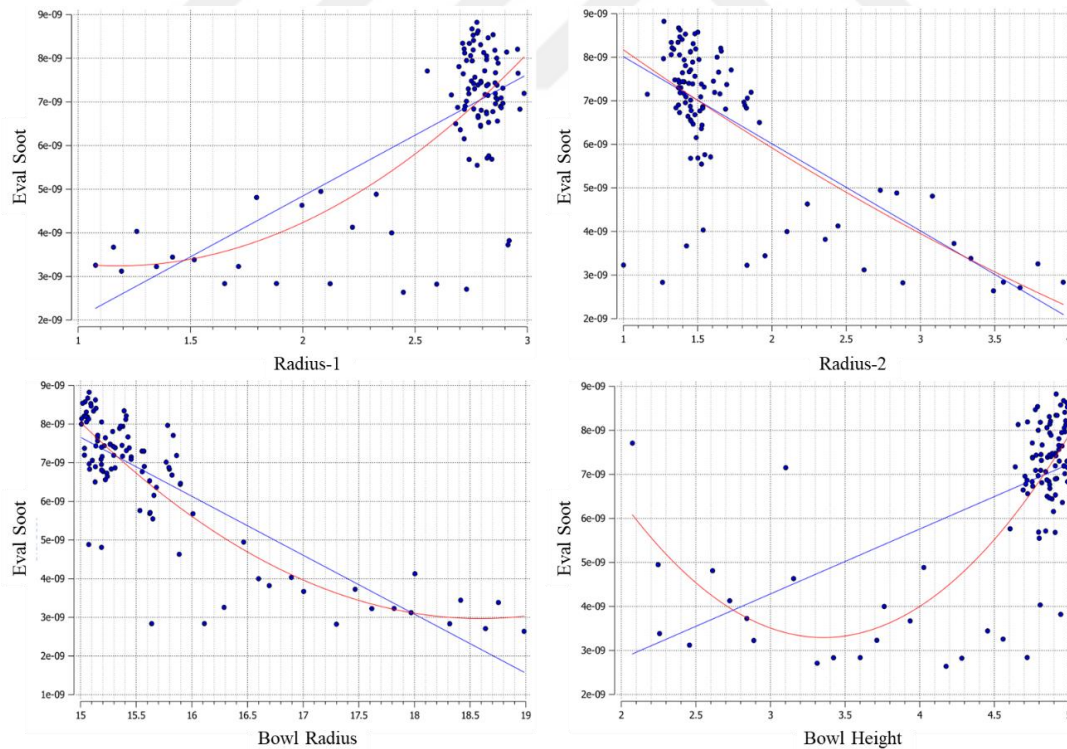


Figure 4.59. Result pool of the optimization studies according to soot emission versus design parameters

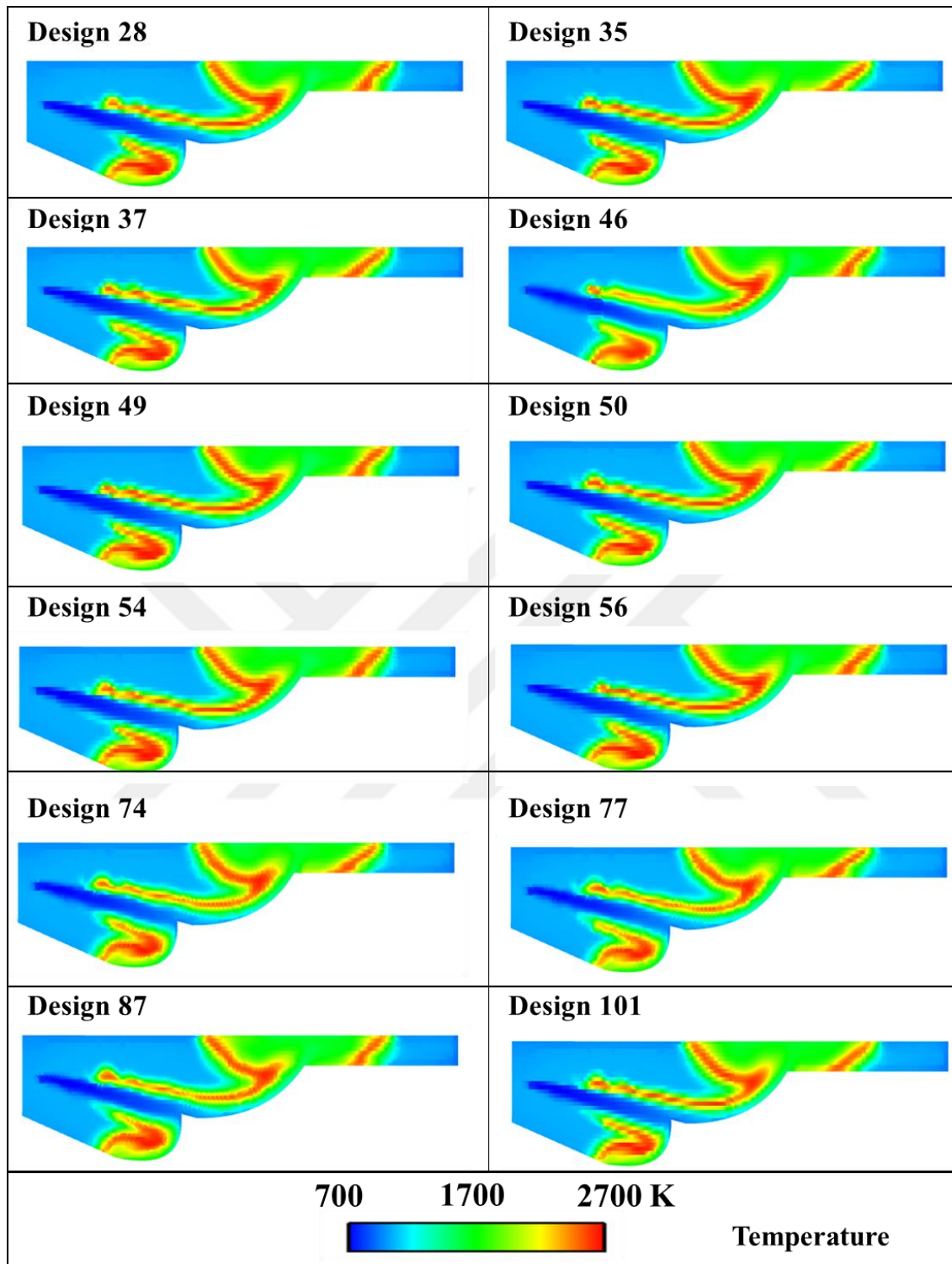


Figure 4.60. Temperature distributions of the result pool designs at TDC for DSB

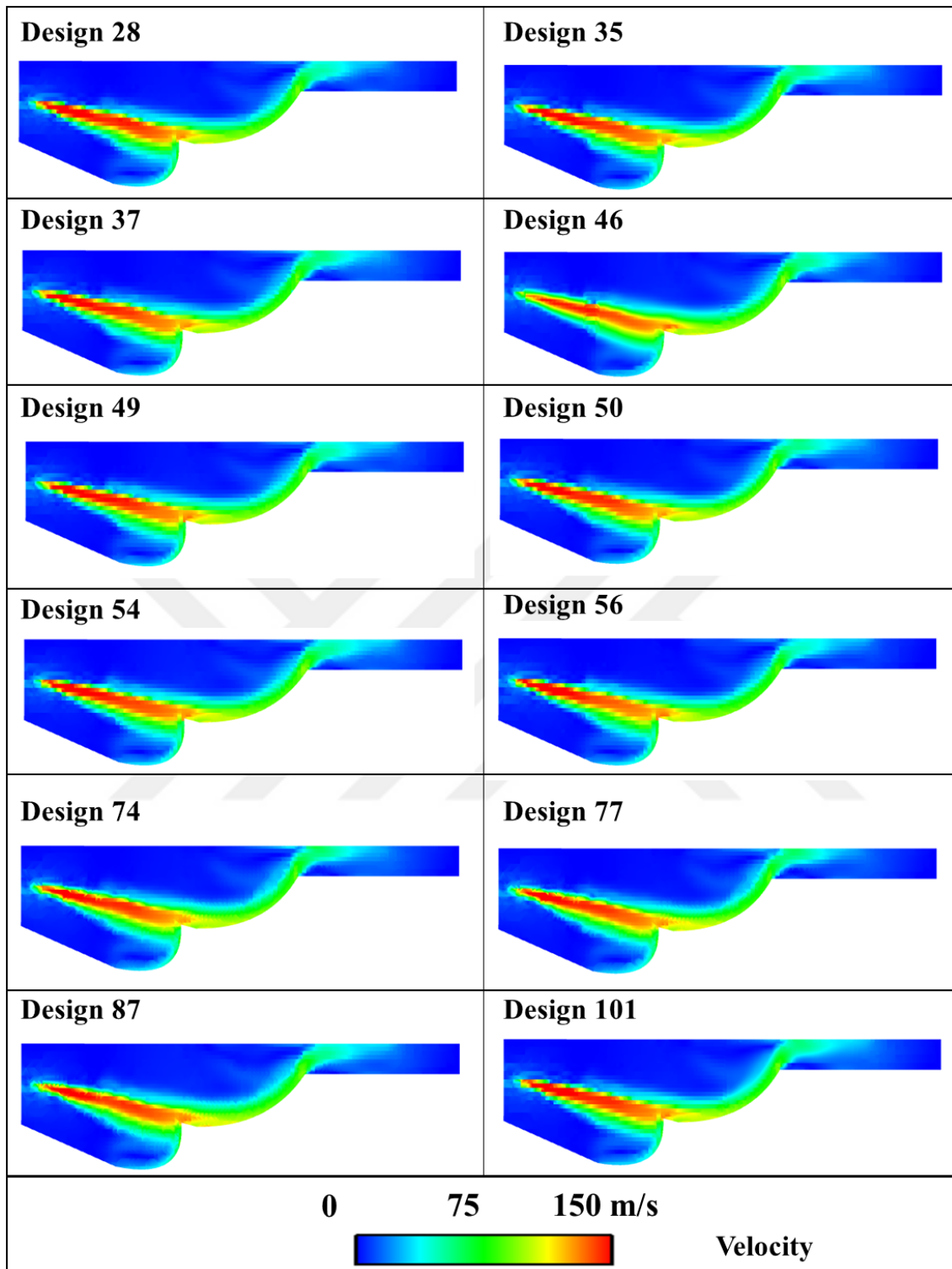


Figure 4.61. Velocity distributions of the result pool designs at TDC for DSB

4.8. Optimized Engine Final CFD Simulation Results

The optimum design has been simulated using Converge CFD as full engine geometry and three-cycle. According to the first parametrical studies, the optimum engine parameters to minimize the emission and ISFC have been studied by keeping the engine performance nearly the same. The optimized DSB bowl geometry and injector with six holes, the spray angle of 150° , the injection pressure of 1000 bar were applied. SOI of -15° bTDC and injection duration of 17.3 CA was used as injection parameters. The compression ratio was kept constant. The amount of fuel injected has been reduced to achieve the almost same power and in-cylinder maximum pressure as the baseline engine. The EGR of 12% was implemented to control NO_x emissions. EGR ratio could be achieved with the EGR valve or by optimizing the valve timing to obtain this ratio. It was determined that this EGR ratio can be achieved according to the valve timing optimization study. With these operating parameters and optimum bowl design, combustion efficiency is improved. NO_x and soot emissions are minimized. When the simulation is performed with these parameters, PFP values remain the same as the base engine (Figure 4.62). It can be predicted that the engine strength and durability will be the same. The crank angle at which the maximum pressure was obtained increased by 2° compared to the baseline engine. This is a positive condition for engine performance and also the elimination of diesel knock.

The optimized engine produces 2 times less NO_x emissions, 34 times less soot emission, and 12 times less CO emission than the baseline engine (Figure 4.63). Besides, the BSFC decreased significantly and the power increased slightly (Table 4.6). It can be concluded from these results that it significantly improves combustion efficiency.

Table 4.6. Comparison of the baseline and the optimum engine

	The baseline engine	The optimized engine	Improvement
Brake Power [kW]	8.21	8.52	+3.8 %
Indicated Power [kW]	9.81	10.12	+3.2 %
Brake Torque [Nm]	27.46	29.1	+6.0 %
IMEP [bar]	8.24	8.50	+3.2 %
BMEP [bar]	6.90	7.16	+3.8 %
BSFC [g/kWh]	342.26	197.27	-42.4 %

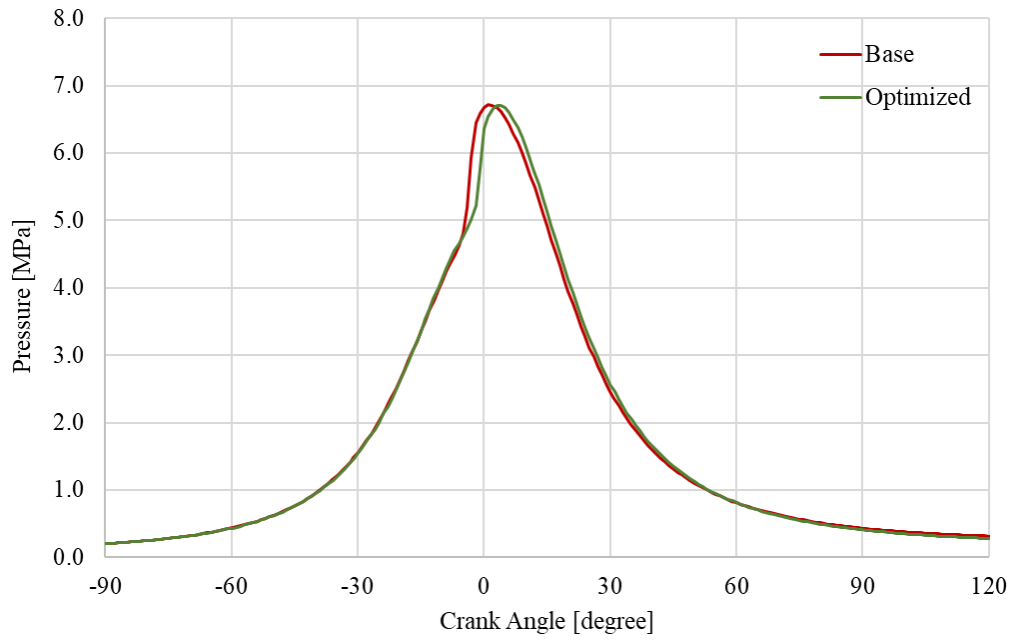


Figure 4.62. In-cylinder pressure comparison of optimized and base engine

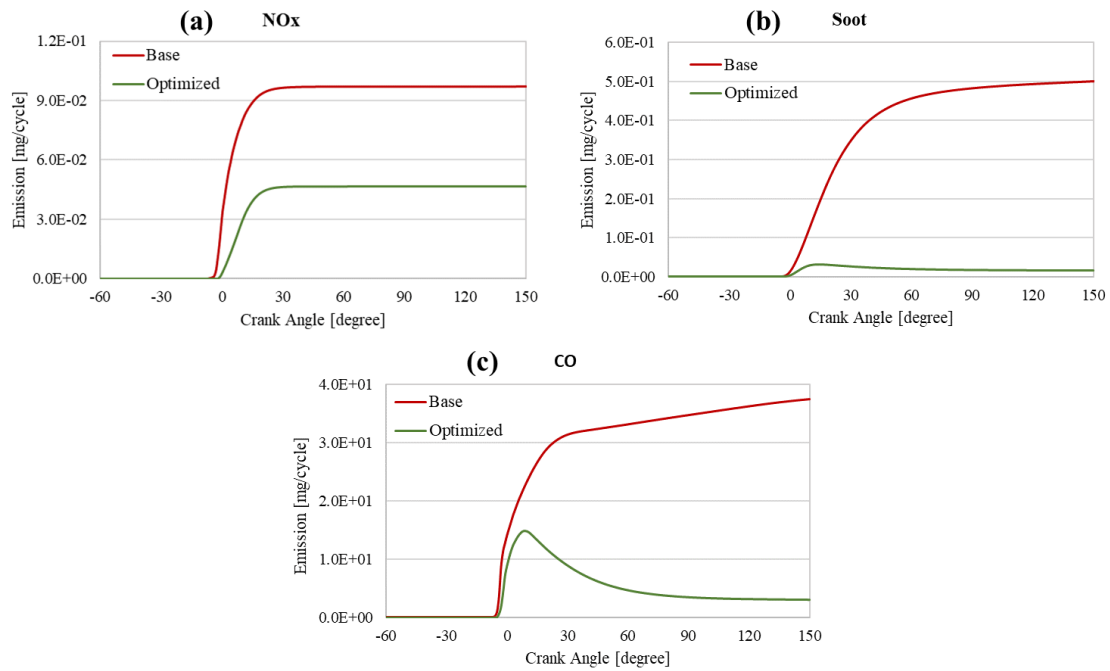


Figure 4.63. Exhaust emission comparison of optimized and base engine

The optimized engine has experienced considerably fewer emissions, moreover, engine performance has not been compromised. Table 4.7 shows the results of the optimized and base engine compared to the NRE-v/c-2 emission standard. With the studies conducted

according to these results, it is seen that the optimized engine will meet the NRE-v/c-2 emission standards.

Table 4.7. Comparison of optimization results with NRE-v/c-2 standards

	Soot	NO_x	CO
base CFD [g/kWh]	5.07	9.95	37.57
best CFD [g/kWh]	0.16	4.75	3.20
improvement [%]	-97	-52	-91
NRE-v/c-2 standards	0.40	7.50	6.60

The temperature distribution inside cylinder of the optimum design illustrated in Figures 3.64 and 3.65. The homogeneous temperature distribution is observed inside the cylinder with combustion. As seen in Figure 4.66, uniform distribution of fuel is provided with the help of the edges of the piston bowl during the injection. The spray impingement position is precisely on the convex edges. The edges guide the fuel/air mixing. The fuel is evenly distributed inside the cylinder. Consequently, the equivalence ratio in the cylinder is homogeneous (Figure 4.67). The contribution of this situation to combustion efficiency and thus emissions is noteworthy.

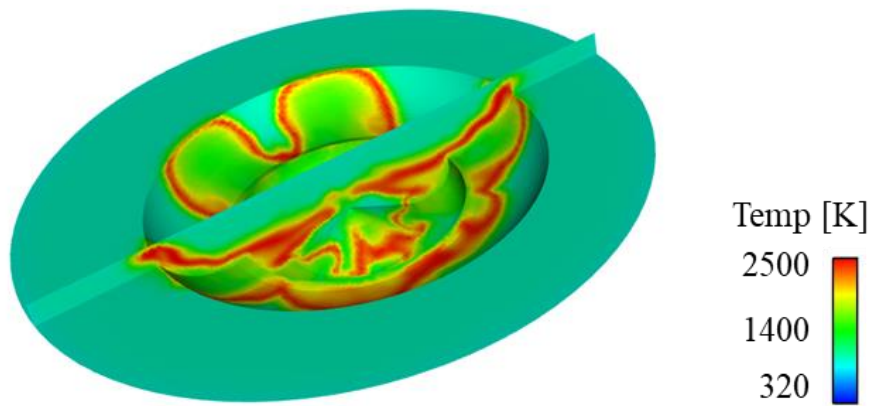


Figure 4.64. Temperature distribution of the optimum design at +5 CA

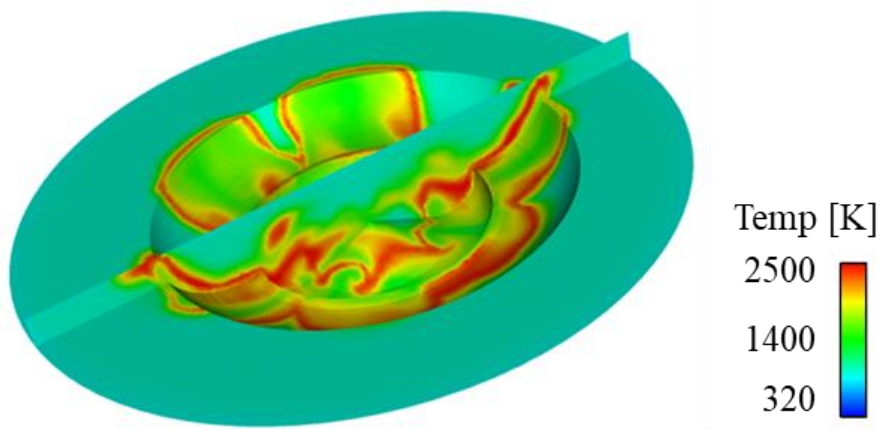


Figure 4.65. Temperature distribution of the optimum design at +10 CA

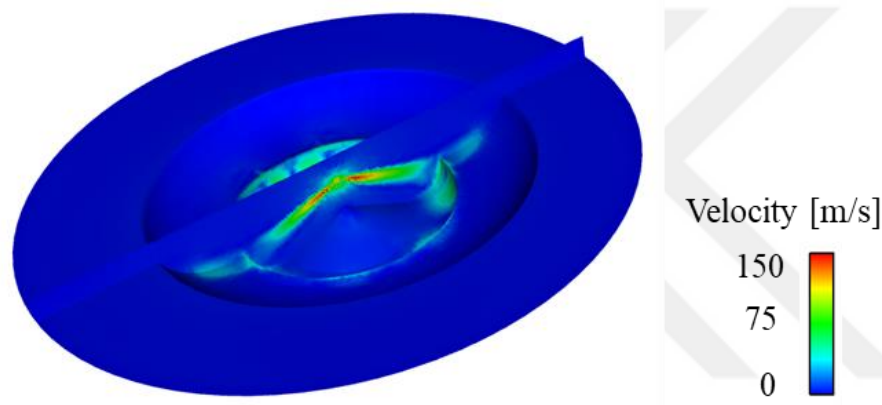


Figure 4.66. Velocity distribution of the optimum design at -5 CA

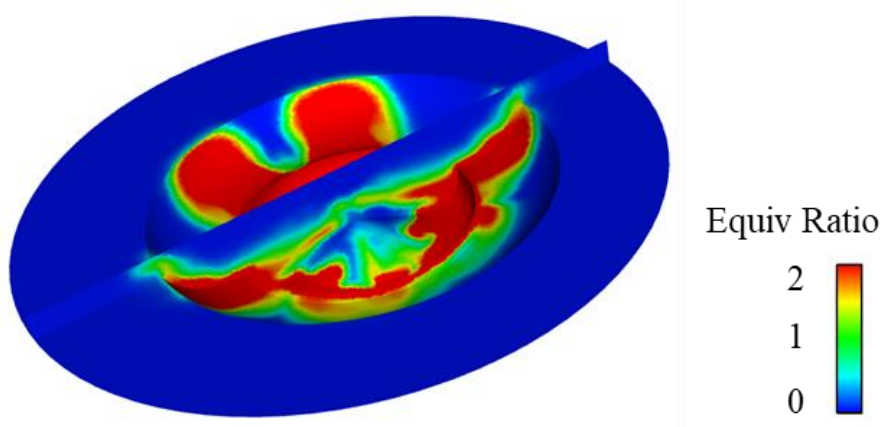


Figure 4.67. Equivalence ratio distribution of the optimum design at +5 CA

5. CONCLUSIONS

The exhaust emissions and engine performance were investigated for a single-cylinder diesel engine. In order to eliminate the major disadvantage of the diesel engine, which is the release of many hazardous gases, experimental methods, QD, and CFD simulation techniques were used in this thesis. CFD and QD models were validated with experimental results. Parametric studies and optimization studies were carried out using the validated QD and CFD models.

Parameters affecting combustion, engine performance, and exhaust emissions were studied to improve combustion efficiency and to minimize exhaust emissions. These parameters were piston bowl geometry, compression ratio, the SOI, injection pressure, spray angle, the number of injector holes, EGR ratio.

Combustion chamber geometry, spray angle, and injection pressure are important parameters influencing fuel/air mixing, combustion, and emission. DSB and MSB improve the air/fuel mixing formation among four bowls in the test engine. These piston bowl geometries reduce the fuel-rich regions. MSB and DSB, which guide the movement of the fuel inside the cylinder, ensure high thermal efficiency and low soot emissions. Based on the simulation results, it can be understood that the MSB and DSB combustion chambers can be used especially for decreasing soot emissions in diesel engines. Significant improvements in exhaust emissions and combustion characteristics can be obtained by modifications like optimizing injected fuel mass, the SOI and injection duration. Despite its simpler geometry, the DSB achieves better results in the most present cases.

A correlation cannot be established about the effect of the spray angle on performance and emissions. This value also varies depending on the combustion chamber geometry. As the injection pressure increases, soot and CO emissions decrease, while indicated thermal efficiency increases. Increasing the compression ratio significantly increases PFP and NO_x emissions. By using EGR, NO_x emissions can be controlled. With the high injection pressure, combustion efficiency improves as it is ensured the better-pulverized fuel injection.

The piston bowl geometry has been parameterized to find the optimum design. Optimization studies were performed by using CFD simulation and MOGA method with parameterized DSB according to better results it gave in parametric studies. The main objective of the optimization study was to reduce exhaust emissions.

Injection parameters and valve timings were optimized with the validated QD model and NSGA-II method. EGR method was proposed to decrease NO_x emissions in the test engine. Because of the complexity of the EGR system, valve lifts were changed according to the less evacuation of residual gases by regulating exhaust and intake valve timings. Furthermore, SOI and injection duration were optimized to minimize the emission using the validated QD model.

The engine operating parameters were determined to obtain minimum emissions with these optimization studies. According to these studies, the final full engine simulations were performed with optimized combustion chamber design and operating conditions. Comparing the optimized engine with the baseline engine, a substantial reduction in soot, NO_x and CO emissions were observed. There was an increment in the engine performance and a significant decrease in BSFC value. Combustion efficiency and engine performance were critically improved using the optimum piston bowl geometry and optimizing injection parameters. This consequence can be achieved quickly and efficiently with the genetic algorithm method. In this way, the engine will be environmentally friendly and very economical. This engine will be able to meet today's emission standards.

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CURRICULUM VITAE

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Selected Publications:

1. Sener, R., Yangaz, M. U., & Gul, M. Z. (2020). Effects of injection strategy and combustion chamber modification on a single-cylinder diesel engine. *Fuel*, 266, 117122.
2. Yangaz, M. U., Özdemir, M. R., & Şener, R. (2020). Combustion performance of hydrogen-enriched fuels in a premixed burner. *Environmental technology*, 41(1), 2-13.
3. Şener, R., Özdemir, M. R., & Yangaz, M. U. (2019). Influence of piston bowl geometry on combustion and emission characteristics. *Proceedings of the Institution of Mechanical Engineers, Part A: Journal of Power and Energy*, 233(5), 576–587.
4. Şener, R., Özdemir, M. R., & Yangaz, M. U. (2019). Effect of the geometrical parameters in a domestic burner with crescent flame channels for an optimal temperature distribution and thermal efficiency. *Journal of Thermal Engineering*, 5(6), 171-183.
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