PCCI-DI Combustion Simulation for Significant Reduction of NOX and PM for GENSET Engine

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Abstracts: Improvements in engine combustion are required due to the stringent pollution norms. This can be achieved either by making improvements in the combustion or by equipping after-treatment devices to control engine emission levels. PCCI is one of the popular techniques used to enhance the combustion. In this work, Diesel-RK software is used for the simulation. The main and pre-injection timings are altered to give the benefits in power and emissions. Based on a literature survey, the fourth and fifth modes are finalized for PCCI combustion simulation. The amount of total fuel injected was kept the same to compare the performances in DI and PCCI modes. The simulation results show the reduction in soot (PM) and NOx simultaneously with the help of PCCI concept at lower BMEP levels. The results show a decrease in PM by up to 26%, a reduction in NOx by up to 30% and an increase in power by 2%.

Keywords: HCCI, PCCI, Simulation, Emission Reduction, CRDI, Diesel-RK.

1. INTRODUCTION

The health hazard due to the emissions produced by an internal combustion engines is one of the main concerns for leaving beings. This has led to stricter emission regulations around the world. These legislations drive the development of more efficient and non-polluting internal combustion engines.The engine combustion generates exhaust emissions. The existing solution for the reduction of emission levels is done using the after-treatment devices. Diesel Particulate Filter (DPF), Diesel Oxidation Catalyst (DOC), and Selective Catalytic Reduction (SCR) are some types of after-treatment devices used to control emissions. These devices add to the cost of the engine. In view of reducing the cost and improving the emissions within combustion chamber of the engine, various methods are suggested for improvement in the engine combustion itself. Homogenous charge compression ignition (HCCI) is one such technology that reduces the PM and NOx simultaneously.

The correlation between the equivalency ratio (ratio of air-fuel to stoichiometric ratio) and combustion temperature is depicted in Figure 1. Typically, emission levels depend upon said parameters. It also shows the current location of the soot and NOx generation zones. Figure 1 shows HCCI operating zone. The HCCI works in a zone where the PM and NOx formation zones are avoided.

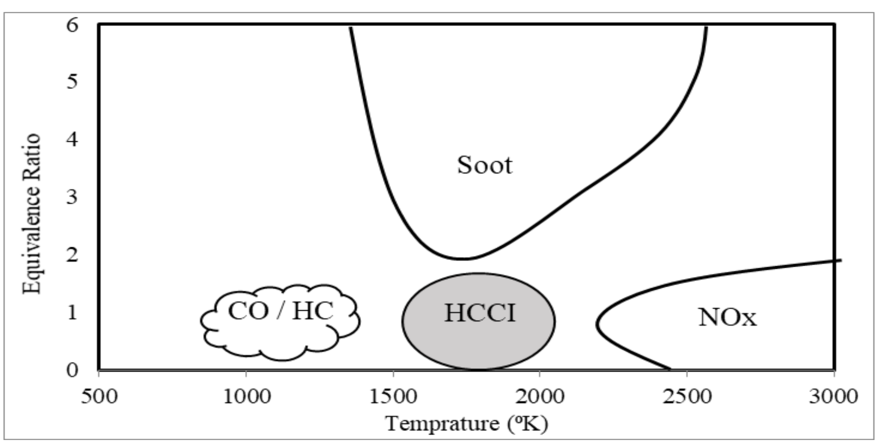

Figure 1. Various zones for emission formation

A generator is usually powered by a diesel engine using an internal combustion engine. Either individual or combined configurations of the above mentioned after-treatment systems are employed to reduce engine emissions. However, using such after-treatment devices increases the base generator set price. Therefore, it is necessary to improve the combustion to reduce the overall cost of the generator set. This can be achieved by using the Homogeneous Compression Ignition (HCCI) approach. In this method of combustion process, the entire charge burns as a uniform mass. Combustion initiation of homogeneous charge depends on the kinetics of the charge chemistry and history time and temperature. Because of this, the start of combustion cannot be directly controlled. The PCCI concept has been proposed to achieve some degree of combustion control.

PCCI is achieved by injecting a sufficient amount of fuel to allow the charge to achieve some degree of homogeneity [1]. HCCI combustion is characterized by cyclic fluctuations. A flexible fuel injection system is required to reduce these cyclic fluctuations [2]. Along with this flexible system, a robust feedback mechanism is required for combustion control. CRDI (Common Rail Direct Injection) fuel injection systems can provide both flexible control and robust feedback mechanism. Thus, to analyse the above mentioned conditions CRDI engine is proposed.

Several researchers have carried out simulations with various fuels or blends of fuels, such as Diesel, Diesel – Alcohol, Various bio diesel blend and Biodiesel with Alcohol using commercial software's. Kuleshov and Grekhov [3] have analysed the NOx formation in a turbocharged diesel engine with Diesel-RK software. The Multi-Zone Fuel Spray Combustion Model using Multidimensional Optimization was utilized with the inputs of combustion parameters like EGR, temperature pressures and swirl. A 4-D ignition delay period map was developed using detailed chemical simulations in CHEMKIN. The results were correlated for NO emissions, SFC, smoke and power. with the experimental data. Datta and Mandal [4] have also carried out simulation using Diesel-RK software.

The engine under consideration for the simulation was Common Rail Direct injection (CRDI) single cylinder four stroke naturally aspirated, water-cooled diesel engine. The engine speed and timing were kept constant at 1500 rpm and 23°TDC. The experiments were carried out with adding alcohol to analyze it's impact on emissions. The NOx emission observed was more for ethanol blended diesel as compared to diesel-methanol blend. In the case of particulate matter and smoke emission the trend was reversed.

The simulation was carried out in Diesel-RK by Paul et al. [5] for Jatropha Biodiesel. It had yielded in increased brake specific fuel consumption (BSFC). Also, results were verified experimentally using various degrees of blends of Jatropha oil with diesel. The NOx and CO2 emission increases while PM and smoke emission decrease proportional to the amount of Jatropha oil in fuel.

Al-Dawody and Bhatti [6] have conducted a correlation of biodiesel experimental results with simulation in Diesel-RK. As compared to diesel, soybean biodiesel has up to 48.23% lower smoke opacity and 14.65% better sfc. Crude algal oil was compared to croton oil to provide a useful basis for comparing new fuels to other bio-oils and diesel fuels Tsousis et al [7]. Algae oil had lower engine performance and NOx emissions compared to croton oil. It showed higher break specific fuel consumption, particulate matter, and CO2 emissions. The experimental results were then compared with Diesel-RK simulation results and good agreement was reported.

Datta and Mandal [8] analysed different Biodiesel-Alcohol Blends. Methanol and ethanol were added to biodiesel from palm stearin. The reduced NOx was effectively due to alcohol addition in fuel. However, it was found that the PM, and amount of smoke generated were higher with the alcohol-blended fuel. The simulation was also carried out using Diesel-RK for the addition of alcohol in bio-diesel.

The purpose of this work is to simulate diesel combustion at constant-speed Genset engine. The parameters are evaluated in five different modes/load points. The performance with and without the use of PCCI modes is compared for the fourth and fifth modes. These simulation findings will be used as guidelines for engine testing.

2. SIMULATION PCCI-DI ENGINE

Thermodynamic models are used in Diesel-RK software to analyse engine performance parameters and are based on the first laws of thermodynamics. Temperature, pressure, and other parameters are evaluated against crank angle or time. A multi-zone model is used to simulate the combustion process in the engine. [8].

2.1. Modes of PCCI operations for simulation

For the genset engine, the modes are the load points at which the engine emissions get measured. The applicable cycle is ISO 8178 D2 cycle having 5 modes / load points for evaluation. The mode for PCCI implementation is chosen based on the power produced and the BMEP data. According to the literature review [9,10], the fourth mode and fifth mode are used to implement the PCCI method, as shown in Table 1. Based on the existing literature, a BMEP range of 6.5 bar to 1 bar is chosen [9,10].

Table 1. PCCI Mode Selection.

Mode	Weighing (%)	Torque (%)	Power (kW)	BMEP (bar)	Mode of operation
1	5	100	62.9	13.6	Mode - DI
2	25	75	47.1	10.2	Mode - DI
3	30	50	31.4	6.8	Mode - DI
4	30	25	15.7	3.4	Mode - PCCI
5	10	10	6.3	1.4	Mode - PCCI

In Table 1, the weighing factors column indicates the severity assigned to particular modes during the emission test cycle. In view of the same, PCCI is only assessed on the fourth and fifth modes. The necessity of managing emissions at these values is highlighted by the 40% weightage of these modes.

2.2. Simulation Inputs

The simulation of engine combustion necessitates the identification of many combustion parameters. This section discusses the input parameters used for the simulation. The parameters could be engine design specifications, combustion geometry and fueling values.

The baseline performance is taken in DI configuration. To achieve the PCCI in combustion, the fuel injection pressure and timing are only changed, while the volume of fuel injected into the combustion chamber remains constant. The effect of this PCCI operation is measured in terms of engine performance/power output as well as engine emissions such as NOx, PM, and CO.

2.2.1. Genset engine specifications for simulation

- Bore of 95 mm
- Stroke of 130 mm
- 4 No. of cylinders
- Connecting rod length 230 mm
- Crank through 65 mm
- Cylinder swept volume 921.6 CC
- Ratio of compression 17.5
- Engine speed 1500 RPM
- Rated power - 63 kW

2.2.2. Combustion geometry (bowl) specifications

The piston bowl general parameters are given in Table 2. This mentions the critical bumping clearance (the cylinder head and the piston).

Table 2. Base Engine Clearances and Volumes Details.

Physical Parameters	Required dimension
Min. piston clearance with top surface (Bumping Clearance)	1.733 mm
Total compressed volume	56.7 CC
Compression Ratio	17.5

The simulation software Diesel RK uses the piston bowl geometry as an input to define the combustion chamber. The bowl geometry is specified in the form of 3D CAD data in the simulation as presented in Figure 2.

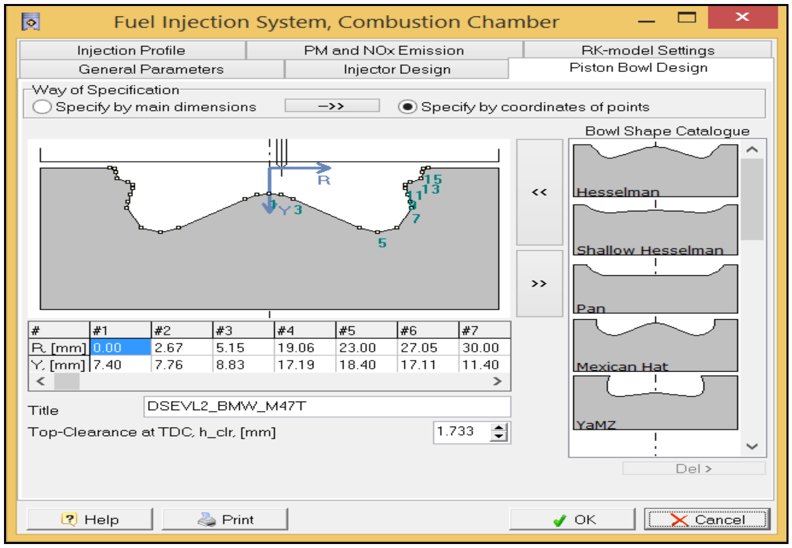

Figure 2. Piston bowl defined in the Diesel-RK software.

2.2.3. Combustion geometry (injection) specifications

The injection profile gives fuel injection spray parameters inside the combustion chamber. The number of sprays and angles made by each nozzle hole with respect to the vertical axis and the reference plane are specified (alpha & beta angles respectively) in Figure 3. There is an offset between the injector and the bowl which is in the 3D CAD data specified as 4.5 mm. Also, the NTP (Nominal Tip Protrusion) of the fuel injector inside the combustion chamber is specified as 1.9 mm along with a hole diameter of 0.115 mm and a nozzle discharge coefficient of 0.66.

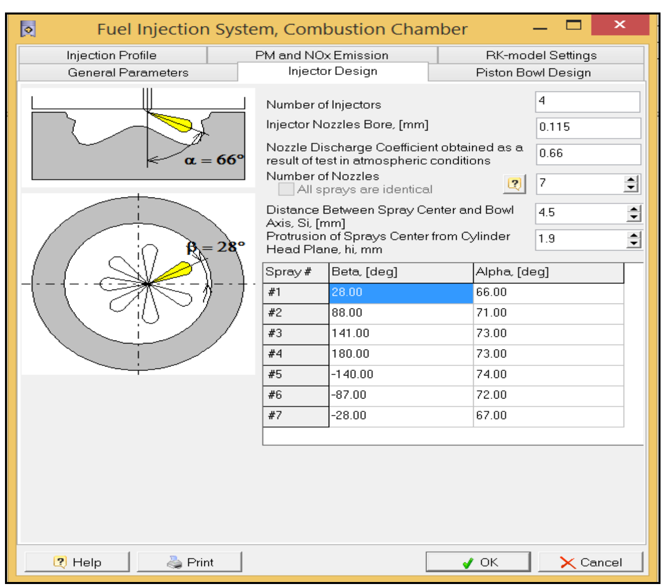

Figure 3. Fuel Injection Nozzle Details in Diesel-RK Software

These factors are the most influential parameters in a simulation analysis as they decide the details of the spray and the atomization of the spray. The combustion depends on these basic injection details. Hence, this is the main input in the simulation.

2.2.4. Combustion geometry (inlet and exhaust port) specifications

Figure 4 and Figure 5 shows the gas exchange parameters for the exhaust and inlet port.

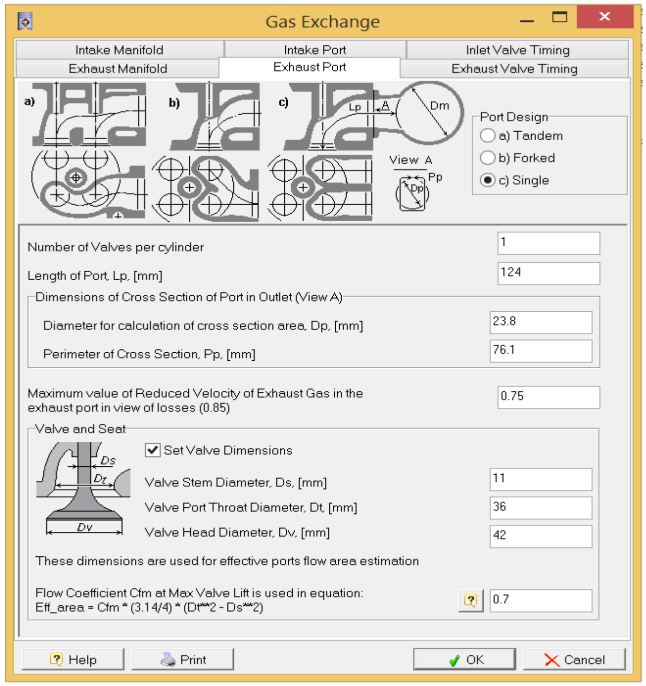

Figure 4. Diesel-RK software gas exchange parameters – Exhaust port

The details of the exhaust port and the configuration of the exhaust port give the basic restriction caused to the exhaust during the discharge from the cylinder head.

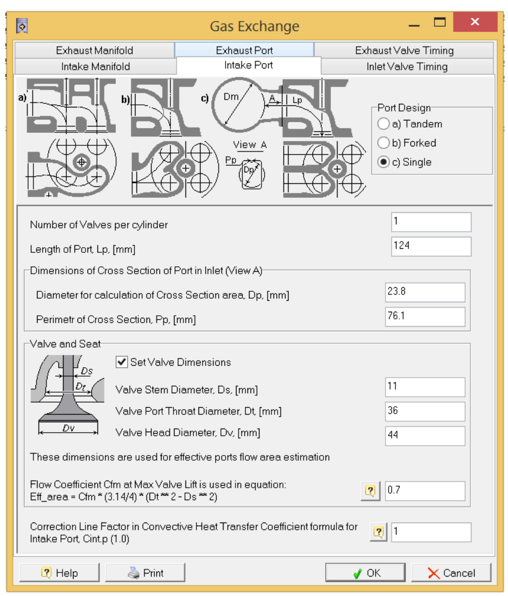

Figure 5. Diesel-RK software gas exchange parameters – Intake port

The details of the intake port and the configuration of the intake port give the basic restriction caused to the air intake during the suction into the cylinder head.

2.2.5. Details of Valve Lift and timing diagram

The valve lift is 11.5 mm for the inlet and exhaust. Regardless of load, the engine needs set valve timings. The valve train mechanism opens the valves mechanically. The opening and closing of the inlet and exhaust valve are shown in Table 3.

Table 3. Valve Timing Details.

Valve status	Timing	
Opening of inlet valve	29	°bTDC
Closing of inlet valve	56	°aBDC
Opening of exhaust valve	56	°bBDC
Closing of exhaust valve	21	°aTDC

2.2.6. Fueling Specifications

Table 4 shows the inputs for the operating modes. In Diesel-RK software, every mode's simulation is conducted individually. Several studies [3,11] employed this software to predict diesel combustion in an internal combustion engine. It has also been used to predict the combustion behaviour of other fuels [4–8]. This investigation begins by using the ISO 8178 D2 cycle with the five modes testing set points. It then examines the two PCCI modes of the fourth and fifth modes. Since modes 4 and 5 are altered to operate on PCCI.

Table 4. Fuel injection timing in DI mode.

Mode	Power (kW)	Main Injection timing (°bTDC)	Injection Pressure (bar)	Main Injection mass (%)	Fuel-injected (gms/stroke)	Pre Injection mass (%)	Pre Injection timing (°bTDC)
1	62.9	1.5	1063	97.8	0.0681	2.2	17
2	47.1	1.5	952	97.1	0.0522	2.9	
3	31.4	1.5	918	96.1	0.0380	3.9	
4	15.7	1	877	93.3	0.0226	6.7	
5	6.3	0.5	800	88.8	0.0134	11.2	

2.3. Boundary conditions of simulations

The following steps describe the process for evaluating the engine in PCCI mode.

- DI operation values
- PCCI operation values for the selected modes

The engine is first simulated in its current state using the DI mode of operation. This serves as the benchmark for comparing changes caused by PCCI operation.

To obtain the PCCI mode engine, several engine parameters can be altered. In this simulation, the injection timing and fuel quantity are changed to achieve PCCI mode. It is analyses best fuel injection settings. To fulfil the lowered NOx requirements, the fuel is bifurcated between pre-injection and main injection. The post-injection is not employed since it is mostly used for soot burning in the combustion chamber. For back-to-back comparisons of the DI and PCCI modes, the fuelling for the PCCI mode is the same as the fueling for the DI mode. This assists in providing an accurate comparison of the DI and PCCI combustion regimes. Engine simulation results are measured in terms of engine emission and performance characteristics.

2.4. Simulation in PCCI-DI Mode – Parameters summary

The simulation is carried out using Diesel-RK software with various parameters as presented in Table 5. These parameters are the key parameters to analyse the results for drawing conclusion.

Table 5. Performance values.

Parameter	Unit	Mode 1	Mode 2	Mode 3	Mode 4	Mode 5	Mode 4	Mode 5
Combustion type	DI/PCCI	DI	DI	DI	DI	DI	**PCCI**	**PCCI**
Power	kW	62.9	47.1	31.6	15.8	6.3	16.0	6.4
Engine efficiency (Indicated)	bar	0.47	0.48	0.47	0.46	0.43	0.46	0.43
Engine efficiency	Fraction	0.44	0.43	0.40	0.34	0.23	0.34	0.23
Max. Cylinder Pr.	bar	138	120	92	71	60	80	66
Injected Fuel Mass	g/stroke	0.068	0.052	0.037	0.0218	0.013	0.0218	0.013
sfc	kg/kWhr	0.195	0.199	0.211	0.249	0.372	0.246	0.364
Start of Combustion	°bTDC	10.44	9.94	9.35	8.67	8.06	11.12	6.58
Ignition Delay Period	CAD	6.56	7.06	7.65	8.33	8.94	8.88	7.42
Intake Air flow	kg/s	0.1030	0.0901	0.0761	0.0640	0.0588	0.0762	0.0640
Lambda	Ratio	2.091	2.391	2.839	4.048	6.233	4.822	6.793
Fraction of wet NOx	PPM	1953	1700	1247	560	211	390	168
PM emission	g/kWh	0.0723	0.1023	0.1445	0.1951	0.6014	0.1531	0.4425

The simulation did not include an EGR ratio. Since this paper's goal is to evaluate the impact of PCCI engine modes during this evaluation.

3. RESULTS AND DISCUSSIONS

The Simulation Findings Were Separated Into Two Categories: Performance And Emissions. These Were Explored in the Tabular And Graphical Representations In The Following Sections.

3.1. Comparison of performance under PCCI-DI Mode

The DI mode engine simulation model study was performed using existing engine data. The foundation for comparing changes is this initial data analysis. The engine's baseline data are shown in Table 6.

Table 6. Base engine data and power improvement in PCCI mode.

Mode	Speed	Load	Power		Increase (improvement)
	RPM	%	kW (baseline)	kW (PCCI)	% (Variation)
1	1500	100	62.9	NA	NA
2	1500	75	47.1	NA	NA
3	1500	50	31.6	NA	NA
4	1500	25	15.8	16.0	1.33
5	1500	10	6.3	6.4	2.12

The two modes 4 and 5 are modified to work on PCCI. As a result, the performances in these two modes have been altered. Table 7 and Table 8 show the differences in fuelling and injection time between modes 4 and 5. This fuelling adjustment resulted in the improvements shown in Table 7 and Table 8.

Table 7. Fuel bifurcation in DI and PCCI for mode 4.

Mode	Power	Pre Injection			Main Injection			Total fuel
	kW	% of total fuel	mg	°bTDC	% of total fuel	mg	°bTDC	mg
4 DI	15.8	7	1.53	17	93	20.27	1	21.8
4 PCCI	16	13	2.83	20	87	18.97	-2	

Table 8. Fuel bifurcation in DI and PCCI for mode 5.

Mode	Power	Pre Injection			Main Injection			Total fuel
	kW	% of total fuel	mg	°bTDC	% of total fuel	mg	°bTDC	mg
5 DI	6.3	11	1.43	17	89	11.57	0.5	13
5 PCCI	6.4	22	2.86	14	78	10.14	-1	

The usage of PCCI mode reduces the NOx emissions produced by the engine. With a 25% load, the fourth mode achieves a 30% reduction in NOx from 560 PPM to 390 PPM. The fifth mode with 10% load produces a 20% reduction in NOx from 211 PPM to 168 PPM.

The use of PCCI mode reduces the PM emissions produced by the engine. The fourth mode, with a 25% load, reduces PM from 0.195 g/kWh to 0.153 g/kWh, a 22% decrease. The fifth mode with a 10% load produces a 26% reduction in PM emissions, decreasing from 0.601 g/kWh to 0.443 g/kWh. Fuel bifurcation refers to variations in pre-injection quantity and injection timing. Table 7 and Table 8 compare fuel bifurcation in DI and PCCI modes for mode 4 and mode 5, respectively.

3.2. Comparison of Emission under PCCI-DI Mode

In line with the change in performance, the emissions also changed. It shows the absolute and percentage changes in power, NOx, and PM levels in % wise.

- The engine power is increased by a small amount of 1.3% to 2.1 %.
- NOx is reduced significantly due to PCCI to 30% and 20%.
- PM is reduced by 22% and 26%.

Table 9. Engine DI-PCCI delta change PCCI mode performance values.

Mode	Power		Improvement	NOx		Reduction	PM		Reduction
	kW	kW	%	PPM	PPM	%	g/kWh	g/kWh	%
	DI	PCCI		DI	PCCI		DI	PCCI	
4	15.8	16.0	1.3	560	390	30	0.195	0.153	22
5	6.3	6.4	2.1	211	168	20	0.601	0.443	26

3.3. Simulated results for Genset engine

Graphical visualization of results was presented in this section for better understanding. The output of the simulation was given below in graphical form.

- Fuel injection against CAD graph -Figure 6
- NOx (PPM) against CAD graph - Figure 7

Figure 6 exhibits the information on fuel-injected for the various modes of DI and PCCI operation. It depicts the spray velocity as a result of injection timing and pressures specified as input parameters. For the 25% and the 10% load DI operation, pre-injection timing and the quantity remain similar. The fuel quantity is changed in the main injection for catering to different loads. In the PCCI mode of operation, the pre-injection quantity and timings are required to be altered to produce charge homogeneity. The main injection methodology remains the same, but the timing is optimized considering the effect of pre-injected fuel.

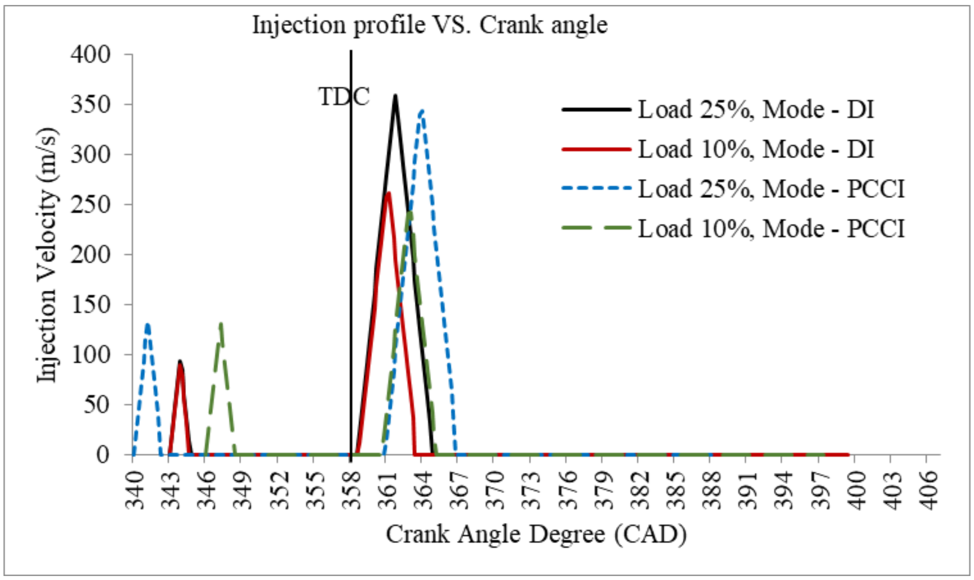

Figure 6. Fuel injection velocity at different crank angles

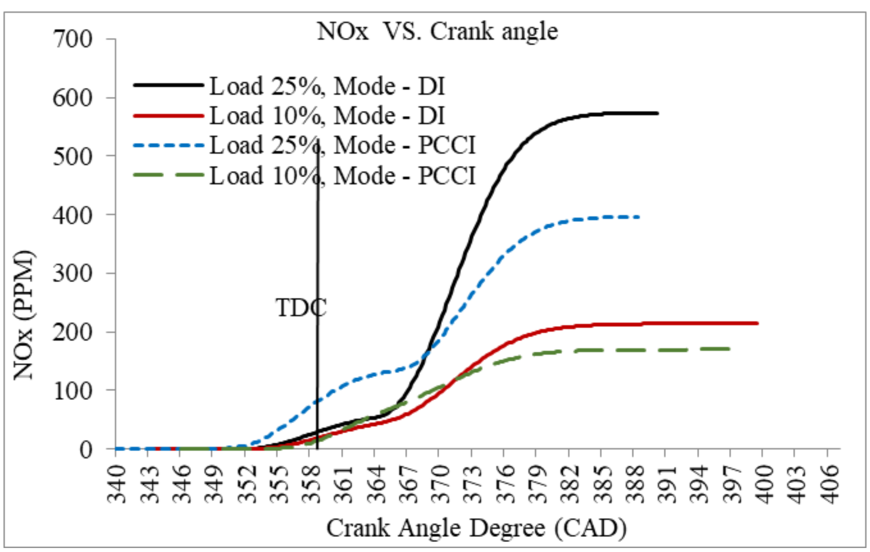

Figure 7. Crank angle and NOx formation correlation.

Figure 7 shows the NOx formation process in the combustion chamber. The PCCI modes produce less NOx than the DI modes as shown. In DI and PCCI NOx formation trends are different. The NOx formation in DI is steeper than in the PCCI mode. The maximum value of NOx is also high. This characteristic is basically a result of higher peak cylinder temperatures in DI combustion as compared to PCCI. This can be observed in Figure 8.

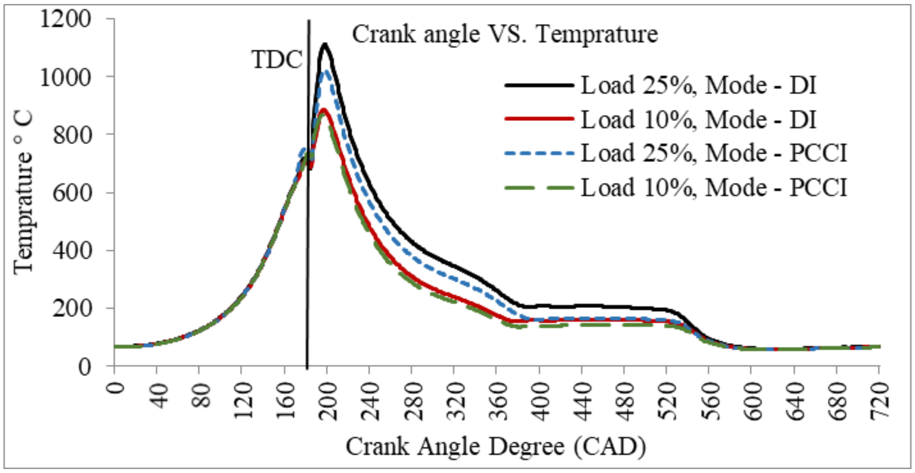

Figure 8. Instantaneous temperature of charge at different crank angles

In mode 4 and mode 5 the PCCI is forming lesser soot than DI. Table 10 gives the exact amount of soot formed in these two modes when compared between PCCI and DI modes. This reduced soot formation in PCCI mode is a result of mixture homogeneity as air for combustion is readily available. However, in DI mode the diffusion flame plays a key role in soot formation.

Table 10. Soot values in DI and PCCI modes.

Mode	Engine	Soot Concentration in the cylinder (g/m^3)
4	DI	0.1951
	PCCI	0.1531
5	DI	0.6014
	PCCI	0.4425

3.4. Inferences of results obtained

In PCCI mode the amount of pre-injected fuel is increased to 13% and 22% for the 4th and 5th modes, respectively, while the main injection stays close to TDC, injecting the remaining fuel into the combustion chamber. Since the fuel is pre-mixed in PCCI modes, rapid combustion occurs, resulting in a greater rate of heat release per CAD. This leads to peak cylinder pressures raising in PCCI modes. The increased cylinder pressures resulted in a small increment in power with the same quantity of fuel being injected (Table 9).

The amount of fuel burnt in the main injection in PCCI is lower as compared to DI causing a lesser maximum temperature. This reduced temperature also reduces NOx formation. However, the soot reduction (Table 9) is the result of homogenous mixture formation making more availability of oxygen around the burning fuel droplets.

4. CONCLUSION

A constant-speed DI-PCCI genset engine's performances in various modes are investigated via simulation. The main objective was to have a basic comparison of DI and PCCI combustion. The simulation findings led to the following conclusions:

The comparison of DI and PCCI engine through simulation predicts improvements in NOx and PM for the genset engine. This is in line with the other research in the field of PCCI for vehicular engines.

The NOx is reduced by 30% and 20% for the 4th and 5th modes respectively. While the PM/soot is reduced by 22% and 26% for the 4th and 5th modes respectively.

With PCCI combustion, the engine power is slightly increased by 1.33% and 2.12% for the 4th and 5th modes respectively. This is due to higher peak pressure formation in PCCI mode.

The fourth mode's comparison of the DI and PCCI modes predicts a fuel pre-injection timing of 20°bTDC and pre-injection fuel percentages of 13% of the total fuel. The remaining fuel is delivered to the cylinder at 2°aTDC as the main injection.

The fifth mode's comparison of the DI and PCCI modes predicts a fuel pre-injection timing of 14°bTDC and pre-injection fuel proportions of 22% of the total fuel. At 1°aTDC, the main injection occurs by injecting the remaining fuel.

By predicting performance parameters before engine testing on the test bed, simulation supports in shortening the experimental validation period and lowers the number of trials.

Conflict of Interest

Conflict of interest is not available.

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