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Assessing the Performance of SME and RME Biodiesels through Combustion Simulation for PCCI-DI Constant Speed Engine

Hemant A. Kinikar[1#], Amarsingh B. Kanase-Patil [1], Sukrut S. Thipse [2], Tushar A. Jadhav[1]

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Abstract: The environmental effect of engine exhaust causing environmental pollution has triggered stringent pollution norms. The two ways of achieving the ever-tightening pollution norms are by combustion improvement on the side engine or the use of after-treatment devices after the emissions are already formed inside the engine. NOx and PM emissions are the two engine emitants that form the engine exhaust apart from CO and HC. To limit these emissions, combustion improvement is proposed. This can be one using different fuels, different combustion methodologies and use of higher pressures for fuel injection for better atomization or the external after-treatment devices. This paper studies two aspects of emission alterations through simulation. The first is the use of SME & RME types of bio-fuels and the use of PCCI combustion approach for the emission improvement. The PCCI approach is used as the HCCI is difficult to control. The assessment is done on the constant speed genset engine as the current research is mainly focused on the vehicle engines alone. Diesel-RK simulation software is used for the pre-injection approach for the PCCI and the bio-fuels of SME & RME. The results shows significant reduction up to 85% can be achieved in particulate matter with use of biodiesels. The overall NOx reduction can be achieved with use of B100 SME. However, the B100 RME gives NOx reduction only at higher loads. With biodiesel, the overall engine efficiency deteriorates. This deterioration is significant at lower loads.

***Keywords**: HCCI, PCCI, Simulation, Emission reduction, Bio-Diesel, Diesel-RK*

Nomenclature

aBDC After BDC
aTDC After TDC
bBDC Before BDC
BDC Bottom Dead Centre
BMEP Brake Mean Effective Pressure
bTDC Before TDC
CRDI Common Rail Direct Injection
DI Fuel Injection directly inside the combustion chamber
EGR Recirculation of Exhaust Gases
EGR ratio Ratio of EGR In complete charge
HC Hydro Carbons
HCCI Homogenous Charge Compression Ignition
NOx Oxides of Nitrogen
NTP Nominal Tip Protrusion
PCCI Premixed Charge Compression ignition
PM Particulate Matter (Soot)
RME Rapeseed Methyl Ester
SCR Selective Catalytic Reduction
SFC Specific Fuel consumption
SME Soy Methyl Ester
TDC Top Dead Centre

1 Sinhgad College of Engineering, Savitribai Phule Pune University, Pune-411041, India.
2 Automotive Research Association of India (ARAI), Rambag Coloney, Kothrud Pune - 411 038, India
 # Corresponding Author: hakinikar@rediffmail.com, Mob.no:+91 7276089650

1. Introduction

The ever-tightening emission regulations drive engine improvements. After treatment devices incur an additional cost of the solution. Combustion improvement methods are assessed in this work, Homogenous Charge Compression Ignition (HCCI) is one such method. This gives key benefit is PM and NOx simultaneous reduction. The HCCI is a phenomenon based on the kinetics of chemical reactions and the history of combustion time and temperature, the initiation of combustion is difficult to control. Here the PCCI methods come to help with providing combustion control while retaining HCCI benefits. The main difference between the HCCI and PCCI is the ratio of air and fuel inside the charge before the initiation of ignition. The HCCI is a fully homogenous charge while the PCCI is a partially homogenous charge. This partial homogenous gives the benefits of HCCI combustion phenomenon. However, the mixture air-fuel ratio is not enough to burn till the main injection starts. The PCCI is achieved by pre-injecting the fuel inside the combustion chamber and allowing sufficient time for the formation of some degree of homogeneity inside the charge.

The second aspect of alteration is to assess the use of SME and RME types of biofuels in the PCCI combustion. The constant-speed genset engine is considered for this assessment. Here, the pure diesel is compared with the SME and RME bio diesels. In conclusion, there will be three cases.

1. Diesel PCCI combustion
2. PCCI Combustion with SME
3. PCCI Combustion with RME

To understand the basics, it is important to understand the basic combustion of HCCI and PCCI. Fig. **1** depicts the relationship between the equivalency ratio (the ratio of air-fuel to stoichiometric ratio) and combustion temperature. For a better understanding, the areas of HCCI and PCCI are highlighted.

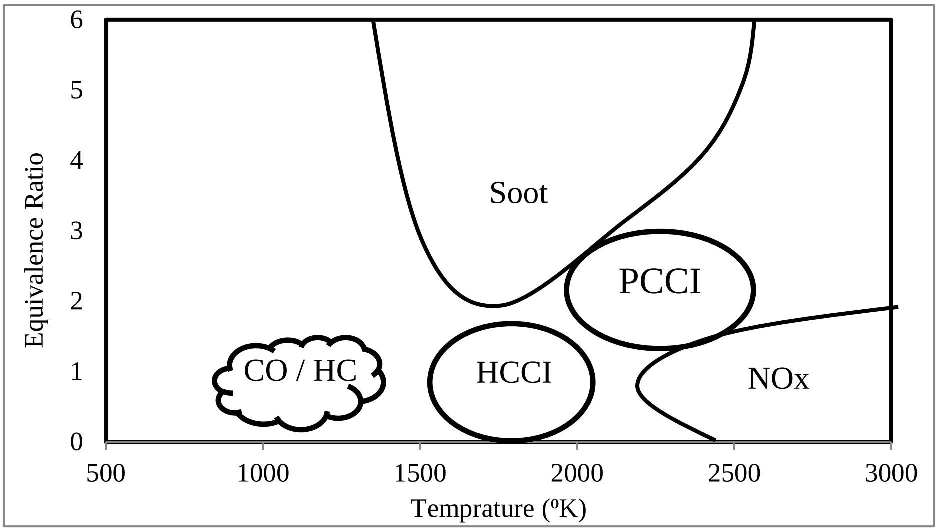

Fig. 1. Various zones for emission formation (Mansoury, Jafarmadar, Talei, & Lashkarpour, 2016)(Liang, Zheng, Zhang, Wang, & Yu, 2019)

1.1. *Simulation need*

HCCI has a high loads knocking and low loads misfiring limits the useful range of HCCI (Juttu, Thipse, Marathe, Babu, & Andersson, 2009). Hence, PCCI- DI is recommended over pure HCCI. With PCCI - DI combustion. Reduced loads PCCI mode is utilized. When subjected to higher loads, DI operation starts. Since, the engine serves two functions, DI and PCCI operations need to be done before the engine testing. Simulation is the ideal way to examine this PCCI-DI combustion.

1.2. *Current research in Biodiesel*

HCCI engine necessitates the use of a flexible fuel injection system to eliminate cyclic variations (Juttu, Thipse, Marathe, & Gajendra Babu, 2007). In PCCI combustion, the fraction of total fuel is injected inside the charge to reach some degree of homogeneity to achieve PCCI (Saxena, 2011). For control over combustion, a reliable feedback mechanism is mandated. CRDI (Common Rail Direct Injection) fuel injection systems can offer variable control as well as a robust feedback mechanism. Hence, the CRDI engine configuration is preferred for PCCI.

Various fuels or fuel blends are simulated by researchers, these can be diesel, diesel-alcohol, various biodiesel mixes, and biodiesel with alcohol. The use of Diesel-RK software is done by Kuleshov and Grekhov (Kuleshov & Grekhov, 2013b) to investigate NOx generation in a turbocharged diesel engine. Multidimensional optimization multi-zone fuel spray combustion model was utilized in the investigation. Combustion parameters like EGR, temperature pressures, and swirl are used as inputs. With chemical simulations in CHEMKIN, a 4-D ignition delay period map was created. The emission and performance parameters are then backed up with the experimental data.

Datta and Mandal (Datta & Mandal, 2016) conducted a simulation with Diesel-RK program. Paul et al. (Paul, Datta, & Mandal, 2014) conducted Jatropha Biodiesel simulation in Diesel-RK. The results indicated an increase in BSFC. Moreover, the simulation results with various degrees of Jatropha oil and diesel mixes were validated experimentally. NOx and CO2 emissions increase while PM and smoke emissions decreases with the increase of Jatropha oil percentage in fuel.

Experimental results with Diesel-RK modeling were comparable by Al-Dawody and Bhatti (Al-Dawody & Bhatti, 2014) for emission and performance. Soybean biodiesel offers up to 48.23% lower smoke opacity and 14.65% higher sfc than diesel.

Tsousis et al (Tsaousis, Wang, Roskilly, & Caldwell, 2014) compared crude algal oil to croton oil to provide an adequate base for evaluating novel fuels to other biofuels and diesel fuels. When compared to croton oil, algae oil showed degraded engine performance and NOx emissions. It demonstrated increased break-specific fuel consumption, particulate matter, and CO2 emissions. The experimental data were then compared to the Diesel-RK simulation results, and there was a good agreement.

Datta and Mandal (Datta & Mandal, 2017) investigated methanol and ethanol were an addition to palm stearin biodiesel. The addition of alcohol to the fuel lowers NOx. However, the PM and amount of smoke produced by the alcohol-blended fuel were found to be greater. Diesel-RK was also used in the simulation of alcohol addition to biodiesel.

1.3. *Fuels for simulation*

Diesel - RK simulation software is utilized from the various available softwares based on the availability of software (Kuleshov & Grekhov, 2013a).

Fuels for simulation are as follows

- Diesal
- RME (Rapeseed Methyl Ester)
- SME (Soy Methyl Ester)

These three fuels are altered during simulation for assessing the effect of fuels on performance and emission parameters in DI-PCCI mode.

2. Inputs For Simulation

Table 1 depicts the modes used for Di and PCCI operations. Thermodynamic models, which are based on the basic laws of thermodynamics, are utilized in Diesel-RK software to analyze engine performance metrics. Temperature, pressure, and other variables are compared to crank angle. To simulate the combustion process in the engine, a multi-zone model is employed (Datta & Mandal, 2017).

2.1. *PCCI operation – Mode finalization*

Constant speed genset engines are tested and certified as per D2- 5mode cycle specified under ISO 8178 part 4. BMEP data are utilized to use PCCI mode. Based on literature study (Juttu, Mishra, Thipse, Marathe, & Babu, 2011) (Gowthaman & Sathiyagnanam, 2018). Modes 4 and 5 are employed to carry out the PCCI method, as indicated in Table 1. BMEP range till 6.5 bar for PCCI operation is finalized, This is based on research available on PCCI combustion (Juttu et al., 2011).

Table 1. ISO 8178 part 4 D2- 5 mode cycle

Mode	Power	BMEP	Operating modes	Weightage
	%	bar		%
1	100	13.6	DI Mode	5
2	75	10.2	DI Mode	25
3	50	6.8	DI Mode	30
4	25	3.4	PCCI Mode	30
5	10	1.4	PCCI Mode	10

Table 1 show the severity assigned to each mode during the test cycle of emission certification. The PCCI evaluation is restricted to the fourth and fifth modes. These two modes have an impact on 40% of the total emissions.

2.2. *General specifications*

To simulate engine combustion, many combustion parameters must be specified. The parameters of the simulation span from basic specs to combustion geometry. This section discusses and finalizes the many input parameters for the simulation. These parameters are classified in subcategories listed below.

- General specifications
- Geometry of combustion chamber
- Fuel injection details

The general information and data for any engine is bore (95mm), stroke (130mm), and connecting rod length (230mm) with a compression ratio of 17.5 and swept volume of 921CC. are the main parameters considered here. The genset speed of 1500 RPM is specified for constant-speed genset applications.

2.3. *Specification of Valve Lift*

The inlet and exhaust valve has a maximum valve lift of 11.5 (mm). Fig 2 gives valve timing diagram.

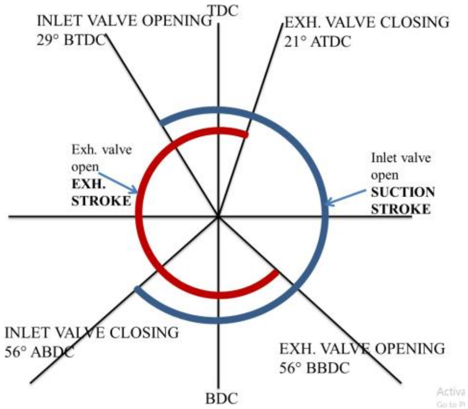

Fig 2. Valve timing diagram

Table 2 shows the general specifications of the piston bowl. This refers to the crucial bumping clearance (the cylinder head and the piston).

Table 2. Base engine clearances and volumes details

Physical Parameters	Value
Minimum clearance between piston with the top surface (Bumping Clearance)	1.7 mm
Total compressed volume	57 CC
Compression Ratio	17.5

The piston bowl shape is used as input by the modeling program Diesel RK to create the combustion chamber. The bowl geometry is supplied in the simulation as 3D CAD data, as seen in Fig 3.

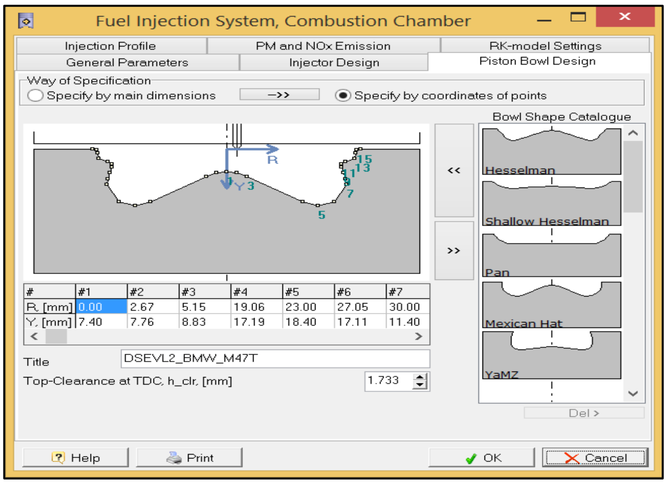

Fig 3. Diesel-RK software piston bowl definition

The injection profile specifies the spray parameters for fuel injection inside the combustion chamber. Sprays and angles formed by each nozzle hole about the vertical axis and the reference plane (alpha and beta angles, respectively) are shown in Fig 3. There is a 4.5 mm offset between the injector and the bowl, which is defined in the 3D CAD data. In addition, the fuel injector's NTP (Nominal Tip Protrusion) inside the combustion chamber is defined as 1.9 mm, with a hole diameter of 0.115 mm and a nozzle discharge coefficient of 0.66.

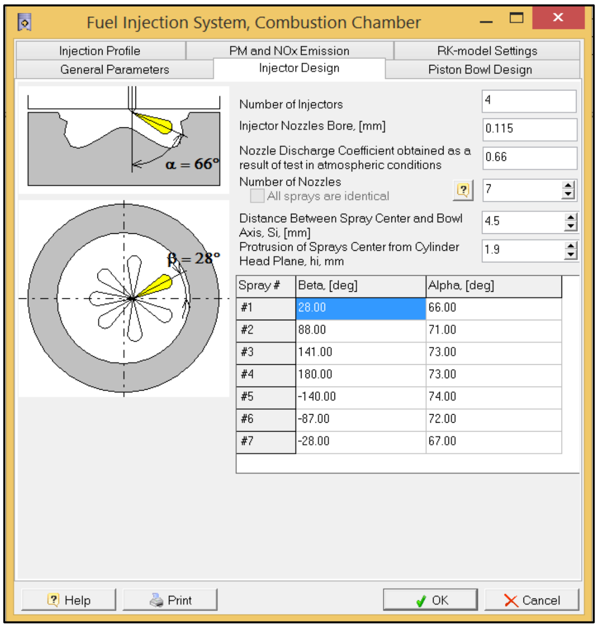

Fig 4. Diesel-RK software fuel spray definition

They are the most important factors in a simulation study since they determine the spray's details and atomization. These crucial injection details govern combustion. As a result, this is the primary input in the simulation. Fig 5 and Fig 6 show the gas exchange parameters for the exhaust and inlet port.

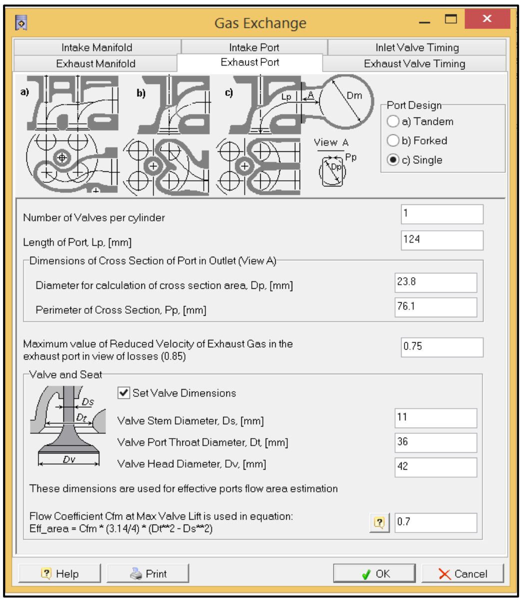

Fig 5. Exhaust port exchange parameters in Diesel-RK software

The exhaust port features and layout provide the primary restriction caused to the exhaust during discharge from the cylinder head.

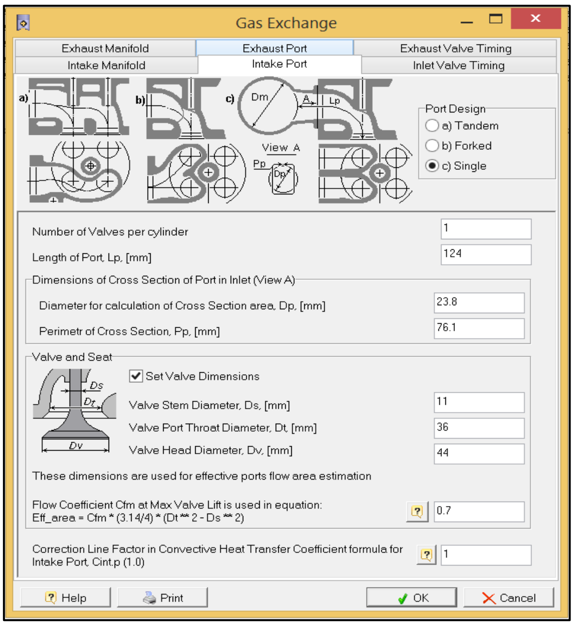

Fig 6. Intake port exchange parameters in Diesel-RK software

The features of the intake port and its configuration provide the basic limitation to air intake during suction into the cylinder head.

Table 3. Simulation run is performed independently in the Diesel-RK program for each mode. At the beginning of this study, emission testing points at the

2.4. *Fueling table*

The primary fuelling inputs are given in

five different genset modes are employed. Then it considers the implications of utilizing different fuels instead of diesel.

Table 3. Fuel injection table

Operating Mode	Load	Pre-Injection		Main Fuel Injection		Injected Fuel	Inj. Pr.
	%	%	°b TDC	%	°b TDC	gms/stk.	bar
1	100	2.2		97.8	1.5	0.0681	1063
2	75	2.9		97.1	1.5	0.0522	952
3	50	3.9	17	96.1	1.5	0.0380	918
4	25	6.7		93.3	1	0.0226	877
5	10	11.2		88.8	0.5	0.0134	800

The EGR is not considered in the assessment because the research's objective is to examine the influence of biofuels in the simulation.

3. Results And Discussions

This data is used as a reference for analyzing the different biofuels performances. Fuel chemistry is the only difference for the different biofuels used, which does not necessitate any changes to the diesel engine. The simulation findings are grouped into two categories: performance and emissions. They are addressed in tabular and graphical form in the sections that follow.

3.1. *Simulation results – Performance and emission comparison*

Initially, DI mode performance is analyzed using a simulation model. This basic data analysis provides a basis for changes comparison. Fig. **7** depicts the variance in engine power caused by fuel changes.

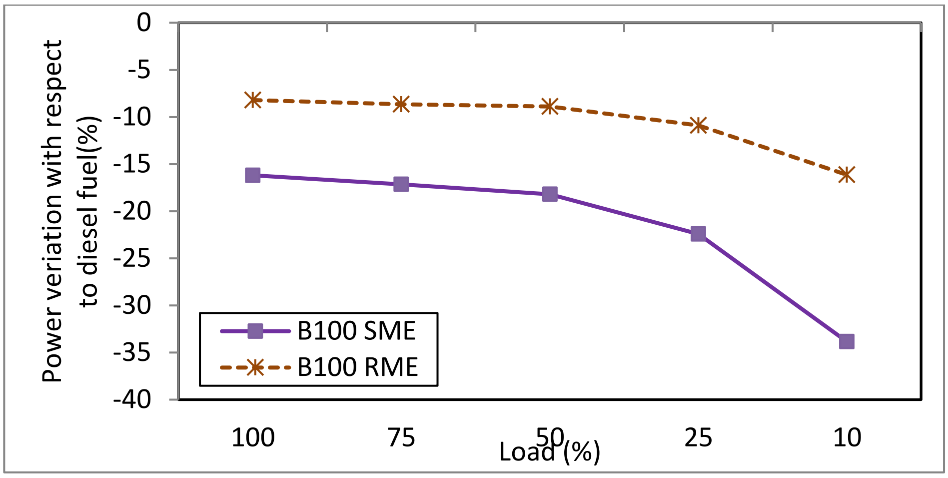

Fig. 7. Comparison diesel and biodiesels power output for same amount of fuel

Fig 8 shows that biodiesel produces less fuel than diesel engine for the same volume of fuel. High calorific value diesel and low heat of vaporization are the reason behind the same. As seen in Fig 8, the same amount of biofuel injected produces less amount of power than diesel. Hence, the sfc deteriorates at a reduced load on the engine. This impact is comparatively smaller with larger loads. Diesel-powered engines have the highest SFC at full load. As demonstrated in Fig 8, RME gives better performance than SME in terms of power output.

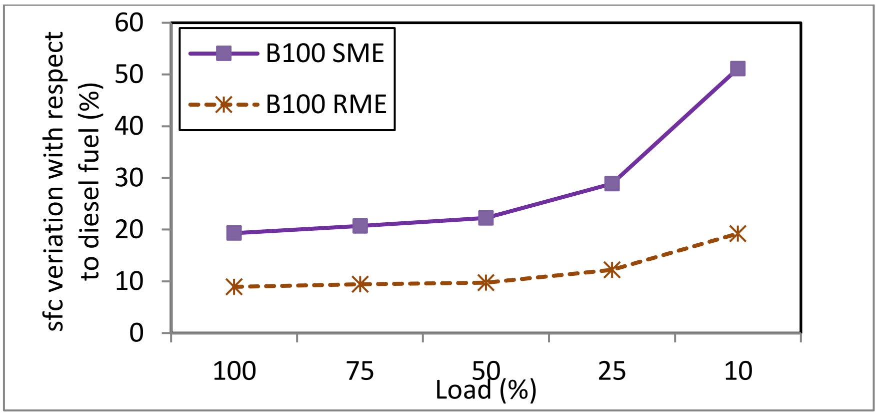

Fig 8. sfc comparison for diesel and biodiesels

The change in brake thermal efficiency is seen in Fig 9. Fuel efficiency is reduced when biofuels are used. This indicates that utilizing biofuel has a negative impact on engine efficiency. Fig 9 indicates that the decrease is significantly less at the rated load. However, it is 22.5% at 10% load while using B100 SME fuel.

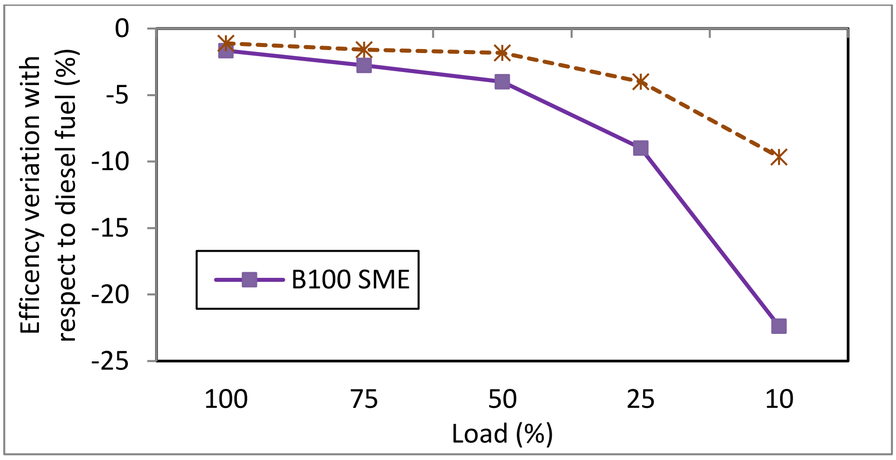

Fig 9. Efficiency comparison for diesel and biodiesels

Table 4 gives the details of the maximum cylinder pressures formed inside the combustion chamber. As indicated the temperature with SME fuels is lower than the RME and both these produce lower temperature than diesel fuel. To give a better comparison, Table 5 assesses the comparative differences between Diesel, SME and RME fuels. The higher loads show significantly lower temperatures in biofuels than in diesel. However, the variation is reduced at lower loads and the temperatures are somewhat higher in biofuels than in diesel.

Table 4. Peak temperature of combustion

Mode	Speed	Load	Peak combustion temperature (ºK)		
	RPM	%	Diesel	SME	RME
1	1500	100	1822	1677	1736
2	1500	75	1752	1600	1659
3	1500	50	1618	1494	1545
4	1500	25	1297	1269	1303
5	1500	10	1141	1158	1149

3.2. *Simulation results – Emission comparison*

Fig 10 shows the variance of NOx at various loads. B100 SME reduces/improves NOx performance at higher and medium loads, while a slight increase is observed at 10% load. Nevertheless, the use of B100 SME produces reduced NOx. However, the B100 RME shows higher NOx at loads of 25% and 10% where the PCCI combustion is applied. NOx has been generated due to the elevated temperature of the combustion chamber. This can be easily visualized in Fig 10 and Table 5. The value of the temperature of biofuels is higher at 10% load for both SME and RME fuels along with 25% load for RME. These are the same points where the NOX values are higher than diesel in Fig 10.

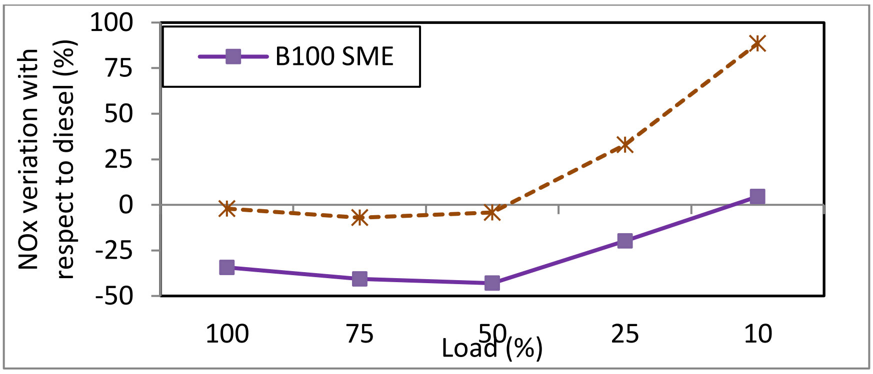

Fig 10. Comparison of diesel and biodiesels for NOx emissions

Table 5. Peak combustion temperature in comparison to diesel

Mode	Speed	Load	% Variation	
			B100 SME	B100 RME
1	1500	100	-8.0	-4.7
2	1500	75	-8.6	-5.3
3	1500	50	-7.7	-4.5
4	1500	25	-2.2	0.4
5	1500	10	1.8	4.3

The most serious drawback of DI combustion is particle pollution. It is the outcome of incomplete combustion caused due to non-homogenous mixture formation due to fuel injection. Fig 11 shows the trend of PM at different loads. Fig 11 shows that utilizing biodiesel resulted in considerable PM reductions at all loads. This can be attributed to oxygenated biofuel. The PM reduction is to the tune of 85% for both SME and RME biofuels.

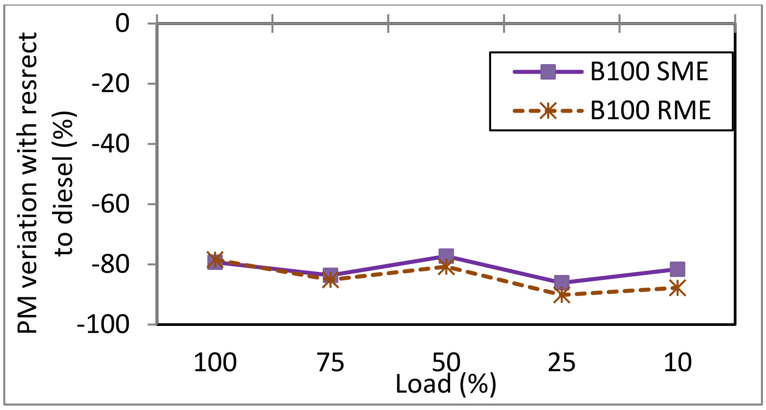

Fig 11. Comparison of diesel and biodiesels for PM emissions

3.3. *Simulation results –In-cylinder Combustion parameters*

The graphical visualization gives better understanding. The outcome of the simulation is visually illustrated in the diagrams below. This will provide better parameter visualization at varying crank angles. The variance at 100% load is only compared in the following section.

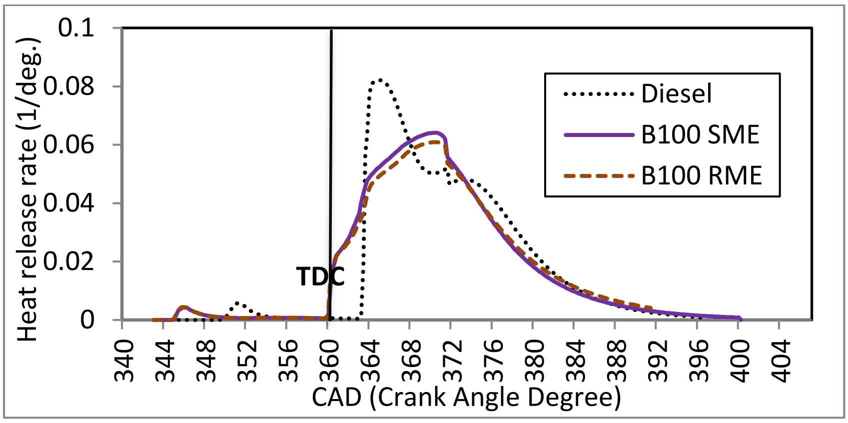

Fig 12. Rate of heat release

The heat release rate per crank angle is shown in Fig 12. This is significant to the burning taking place inside the combustion chamber. The higher rate of combustion (heat release per crank angle) produces higher temperatures and pressures inside the combustion chamber which are explained in the upcoming sections.

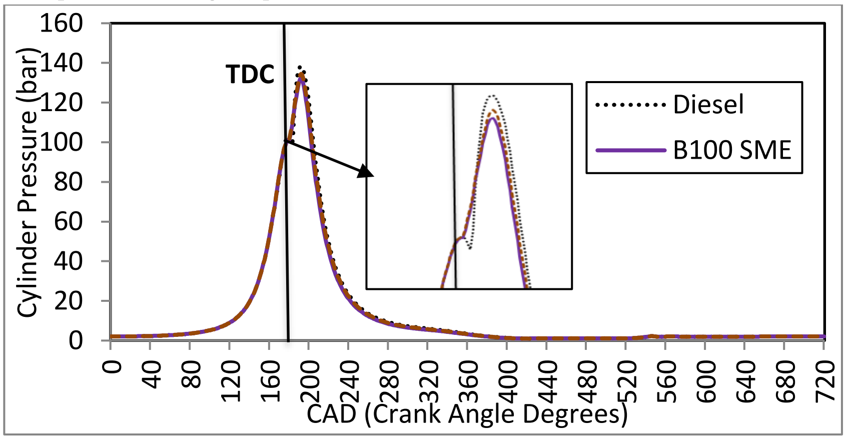

Fig 13. Graph of combustion pressure during a combustion cycle

Table 6. Peak cyl. pressure

Mode	Speed	Load	Peak cylinder pressure (Bar)		
	RPM	%	Diesel	SME	RME
1	1500	100	138.2	132.4	134.5
2	1500	75	119.9	113.7	115.9
3	1500	50	92.0	91.4	93.2
4	1500	25	79.9	82.9	83.8
5	1500	10	66.5	68.3	69.5

Fig 13 gives P-theta diagram for the three fuels under consideration. The analysis shows that the pressure is in a similar range for all three fuel types. This is depicted in Table 6 as well. This suggests that changing the fuel has minimal impact on peak pressures.

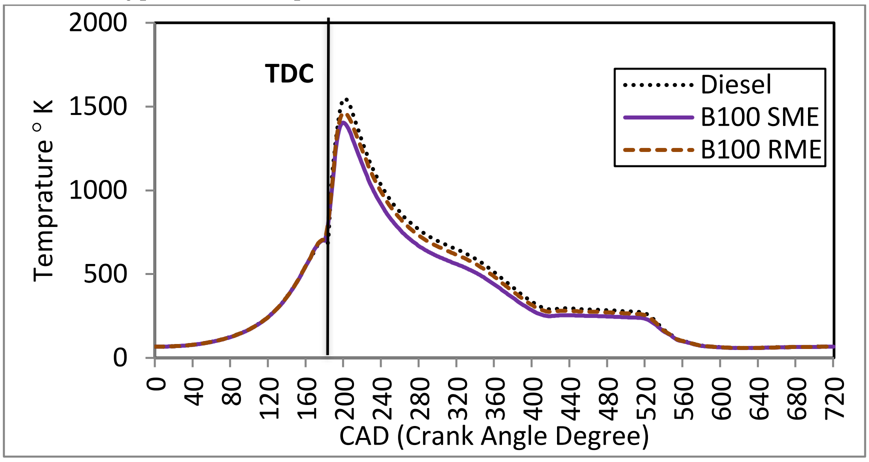

Fig 14. Graph of gas temperature against crank angle

Fig 14 shows a comparison of PCCI and DI modes cylinder temperatures. Fig 13 illustrates a pattern of Table 4 shows the peak cylinder temperature change pressure that contrasts with the trend of temperature. defined in values.

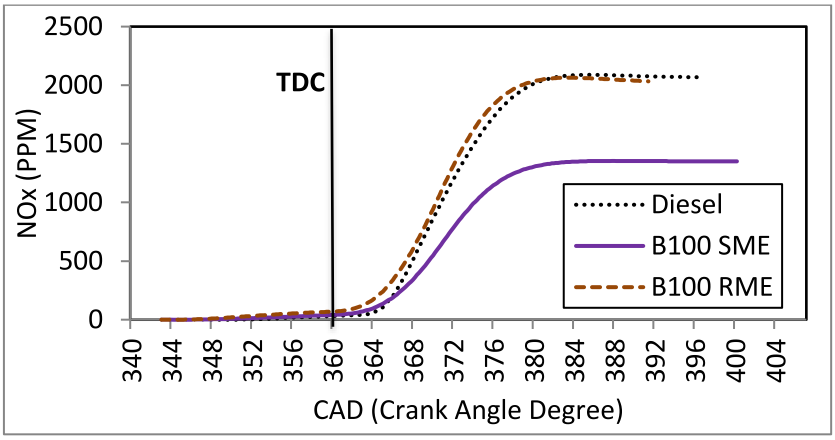

Fig 15. NOx formation with change in crank angle

Combustion chamber NOx generation is analyzed in Fig 15. lowest NOx is given by B100 SME than RMS and diesel. Lower cylinder temperature inside the combustion chamber is the reason for this reduced NOx. This can be seen in Fig 14.

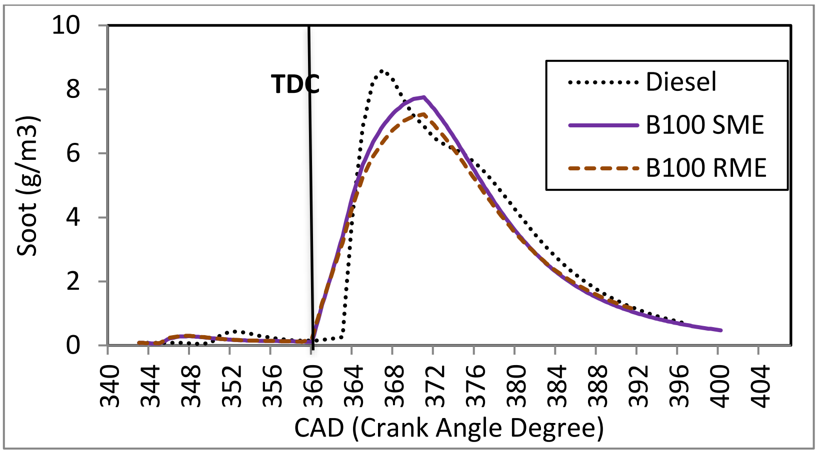

Fig 16. Soot formation with change in crank angle

Fig 16 shows the soot production in a combustion cycle. The diesel combustion is sharp and this reflects in soot formation. The combustion is sluggish in biodiesel as seen in Fig 16. Both the effects are visible in heat release rate diagram (Fig 12).

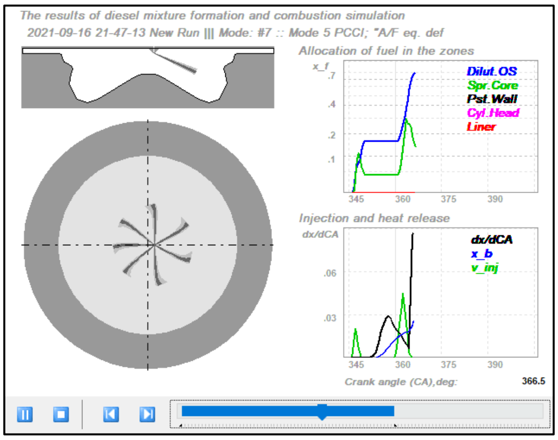

Fig 17. Combustion visualization in diesel-RK software

Simulation software shows the actual fuel flow and combustion process. Fig 17 is one such representation. This is a graphical representation of combustion to help you understand it better. Actual numerical values are always saved in data files for further examination.

4. Conclusion And Way Forward

The summary of inferences drawn is as follows.

- For the same quantity of diesel injected, the diesel has the lowest sfc compared to biodiesels. This is due to the lower calorific values of the biodiesels over pure diesel.
- The sfc comparison between the SME and RME indicates the poor performance of SME biofuel over RME biofuel.
- The heat release rate is rapid for the diesel while lesser for SME and further less for the RME. This has an impact on the peak cylinder pressure and temperature generation.
- However, the peak pressure for RME is slightly less than SME as the pressure is also impacted by the cylinder volume based on the crank angle.
- A proportional correlation is observed between the cylinder pressure and temperature for all fuels.
- The NOx emissions for the SME are lesser in all loads except at 10% where it is slightly higher than diesel. This makes the SME a preferred fuel for NOx reduction.
- NOx is significantly higher at 25% and 10% loads for RME bio-fuels while lesser at higher loads.
- The particulate emissions are significantly lower for biofuels, the reduction is in the range of 85% over diesel fuel.

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