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ORIGINAL ARTICLE

Numerical analysis of C.I engine to control emissions using exhaust gas recirculation and advanced start of injection

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Abstract As major limitation of diesel engines is the high soot and nitrogen oxide emissions which cannot be reduced totally with only conventional catalytic converters today, varying fuel characteristics became a focus of interest to meet the pollution emission legislations as they require very few or no changes in existing engine model. The present work deals with, numerical analysis of combined effect of Advanced Start of Injection (SOI) and Exhaust Gas Re-circulation (EGR) on performance and emissions which were studied, by performing numerical analysis on a Caterpillar 3401 single cylinder C.I engine model at constant speed using diesel as fuel via three dimensional computational fluid dynamics (CFD) procedures and validated with experimental data. The SOI is advanced from 11° Crank angle bTDC to 14.5° Crank angle bTDC and EGR as a fraction is increased from 0% to 10%. The modified conditions of these parameters resulted in simultaneous reduction of NO_x and Soot.

Abbreviations HCCI, homogeneous charge compression ignition; SI, spark ignition; CI, compression ignition; CR, compression ratio; SOI, Start of Injection; EGR, Exhaust Gas Recirculation; NO_x, nitrogen oxides; UHC, unburned hydrocarbons; CO, carbon monoxide; CO_2, carbon dioxide; CFD, computational fluid dynamics; bTDC, before top dead centre; aTDC, after top dead centre; CA, Crank angle; RPM, revolutions per minute

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1. Introduction

Over recent past years, strict emission norms have been imposed on NO_x, CO and particulate emissions emitted from automotive engines. Diesel engines are among the highest efficiency energy conversion devices and therefore heavily depend upon for many heavy vehicles, Industrial machinery, Marine engines and many construction equipment. Diesel engines are typically preferred due to low fuel consumption and very low CO emissions. However, the emissions from these engines are restricting their usage. Many researchers have done work on diminishing the emissions, yet the NO_x and Soot emissions from C.I engines still remain at high range. Hence, in order to meet the pollution norms, it is highly desirable to reduce the amount of NO_x and Soot in the exhaust gas. NO_x and Soot emissions emitted from diesel vehicles cause serious environmental problems. NO_x promote the formation of acid rain and also the formation of photochemical smog with the influence of sunlight. Acid rains damage buildings, vehicles and historical constructions. Soot particles can break into lungs and cause many serious health problems because of mutagenic hazardous hydrocarbons on their surfaces. Soot not only causes respiration problems but also plays role as carriers for carcinogenic compounds. As these pollutant emissions have unfavourable effects on the environment and human health, study is concentrated on reducing these emissions.

Advanced combustion practices such as homogeneous charge compression ignition (HCCI) and premixed charge compression ignition (PCCI) are established to be promising strategies for their capability in reduction of soot and NO_x emissions at the same time maintaining high level of thermal efficiency [1–4]. However, early-injection timing allows the spray to penetrate into a low surrounding temperature and density environment where vapourisation is low and spray liquid impingement upon the piston bowl and cylinder liner is likely to occur. As a result, low combustion efficiency, excessive unburned hydrocarbon (UHC) emissions and dilution of oil might happen [5]. Emissions after passing through treatment devices, however, may face some problems with cost and durability. Since emission after treatment systems such as Diesel Particulate Filters (DPF), Lean NO_x Trap (LNT) and Selective Catalytic Reduction (SCR) often increases fuel consumption, research is focused on in-cylinder technologies for emissions reduction. Also in order to maximise overall engine efficiency, an engine should curtail the need after treatment emission reduction. In order to reduce NO_x and Soot emissions in cylinder, as well as maintaining high thermal efficiency, many new diesel engine combustion strategies have been proposed.

Control of NO_x emissions from diesel engines remains to be a challenging problem for both academic research and practical application. In this paper, one to accomplish this is to reduce the in cylinder temperature. To achieve this Exhaust Gas Recirculation system (EGR) used.

External exhaust gas recirculation (EGR) is a strategy that is used in C.I engines to reduce combustion flame temperatures, which are mainly answerable for high NO_x formation. The effect of EGR utilisation is that most of the elemental nitrogen is emitted as non-toxic N_2 [6–11]. In addition, EGR also has a positive effect on engine noise as it limits the heat release rate (HRR) during premixed combustion. However, the use of the EGR can give rise to problems in terms of engine emissions and performance, such as particulate matter (PM), CO, unburned hydrocarbons (HC) and a deterioration in the brake specific fuel consumption (bsfc) [12–14]. In particular, high values of EGR negatively can be affected as they increase the soot emissions and induce a rise in the cycle-to-cycle changeability of combustion [15]. Nevertheless, the increase in soot generation for increasing EGR rates controls higher radiation and a resulting decrease in the flame temperatures can help to further diminish NO_x emissions [6]. Finally, EGR can adversely affect the quality of the lubricating oil and engine durability because of increased wear and tear between the piston rings and the cylinder liner [9,16–18]. In addition, EGR also has a positive effect on engine noise as it limits the heat release rate (HRR) during premixed combustion [19].

The present work explores the influence of EGR and SOI in reduction of NO_x and Soot in the exhaust emissions. In order to reduce the NO_x, EGR of 10% is introduced and to reduce soot in the exhaust, advancement of injection timing strategy is employed, which usually improves the indicated efficiency of the engine because the fuel mixture will get well mixed. The main effect of EGR is due to the CO_2 and H_2O species that are present in the exhaust gas and tend to separate during combustion, thus reducing the peak combustion temperature and paying to the reduction of NO_x formation [16]. And as the fuel is getting injected earlier it forms uniform mixture as compared to previous case, so the fuel mixture burns at uniform rate till the end of combustion process and due to this there are two possibilities for reduction of soot. (i) As the fuel is injected earlier, air–fuel mixture mixes effectively, and combustion happens completely. So there is less scope for soot formation. (ii) There is a chance for soot getting oxidised in the cylinder when temperature reaches above 1000 K (effective charge mix gives high combustion tendency and high temperatures). The injection timing of fuel is advanced by 3.5° (*i.e.* 11° CA bTDC to 14.5° CA bTDC). On the other hand advanced injection timing has a negative effect on peak pressure causing a serious increase of NO_x value. So, by making use of EGR and Advanced injection timing, both parameters compensate one's negative effects and result in reduction of significant NO_x and Soot. A published research paper [20] focused on "Effect of EGR on advanced injection", that focuses on the performance characteristics part of the engine and not on Emissions.

2. Numerical analysis

CAT 3401 (Caterpillar) engine is selected for the simulation analysis. The CFD simulation has been done for the baseline configuration using CONVERGE and the output results are analysed in the post processing software ENSIGHT. Here as the combustion process is mainly focused on the compression and expansion, the analysis of the model is made from −147° bTDC (i.e. Inlet valve closure) to 150° aTDC (i.e. Exhaust valve opening). This is because, as the analysis is focused on the emissions at the end of combustion, we need to carry on analysis till the exhaust valve opening.

The selected reference/base model [21] is analysed and post processed, and its performance is further improved by modifying such parameters (Advancing the Start of Injection 3.5° &

Table 1 Engine specifications and conditions of Caterpillar Engine.

Engine Specifications	
Cylinder bore × stroke (mm)	137.6 × 165.1
Connecting rod length (mm)	261.62
Displacement volume (L)	2.44
Compression ratio	15.1
Number of nozzle orifice × diameter (mm)	6 × 0.259
Number of cylinders	1 (Single)
Spray angle (from cylinder head)	27.5°
Combustion chamber	Quiescent
Piston crown	Mexican Hat
Intake valve closure	−147° CA aTDC
Swirl ratio (nominal)	1.0
Inlet air temperature (°K)	310
Inlet air pressure (KPa)	184
Engine speed (rpm)	1600 rpm
Fuel	Diesel
Injection system	Common rail
Injection pressure (MPa)	90
Fuel injected (g/cycle)	0.1622
Overall equivalence ratio	0.46
Injection duration	21.5 Crank angle degrees
Start of Injection	−11° (baseline), −14.5° aTDC

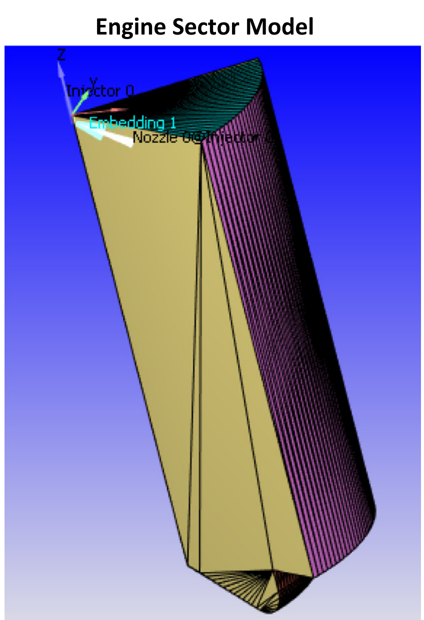


Figure 1 An engine cylinder sector geometry created automatically by the make surface utility, as viewed in CONVERGE Studio.

introducing EGR up to 10%). The specifications of engine are shown in Table 1.

An engine sector produced with the *make surface* utility (Fig. 1) is free of surface defects, appropriately boundary-flagged, and the periodic faces will match perfectly. This utility is an alternative to using CONVERGE Studio to prepare the surface. As the in-cylinder nozzle has six uniform holes, a 60° sector model (Fig. 2) is prepared for analysis, in the view of less analysis time. CONVERGE also uses Adaptive Mesh Refinement (AMR) a cutting edge technology which automatically refines the grid, based on fluctuating and moving conditions.

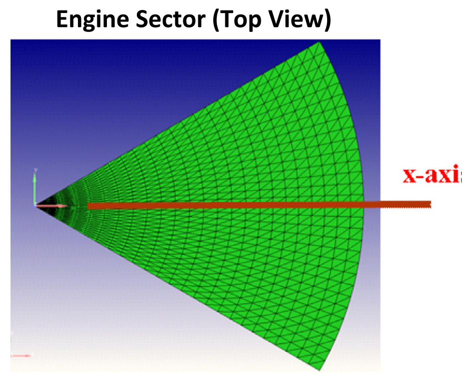


Figure 2 A sector model geometry with the periodic boundaries appropriately symmetric about the XZ plane.

360/60 = 6 (so, 6 equal sector models can be created, and each sector model is considered to have one nozzle hole).

2.1. Boundary conditions & Initial conditions

Inlet air pressure	1.97 bar
Overall equivalence ratio	0.46
Inlet air temperature	310 K
Cylinder wall temperature	433 K
Piston wall temperature	553 K
Head temperature	523 K
Initial gas temperature	365 K
Spray temperature	341 K

2.2. Combustion model

SAGE combustion model is used in the analysis. This is one of the detailed chemistry solvers for CONVERGE, which calculates the reaction rates for each elementary reaction based on Arrhenius type correlation, while the CFD code solves the transport equations.

With an accurate reaction mechanism, SAGE can be applied for modelling any combustion regime such as ignition, premixed and mixing-controlled in gasoline and diesel combustion scenarios. It is to be noted that the SAGE is commonly used with a multi-zone solver, which solves the cells with similar thermodynamic conditions in groups and saves run-time.

2.3. Validation of simulation results

Validation of the simulation results has been done using experimental data from Curtis et al. [21]. Data were available for several Start-of-Injection (SOI) timings for the Caterpillar 3401 engine, and are used to verify the simulation results.

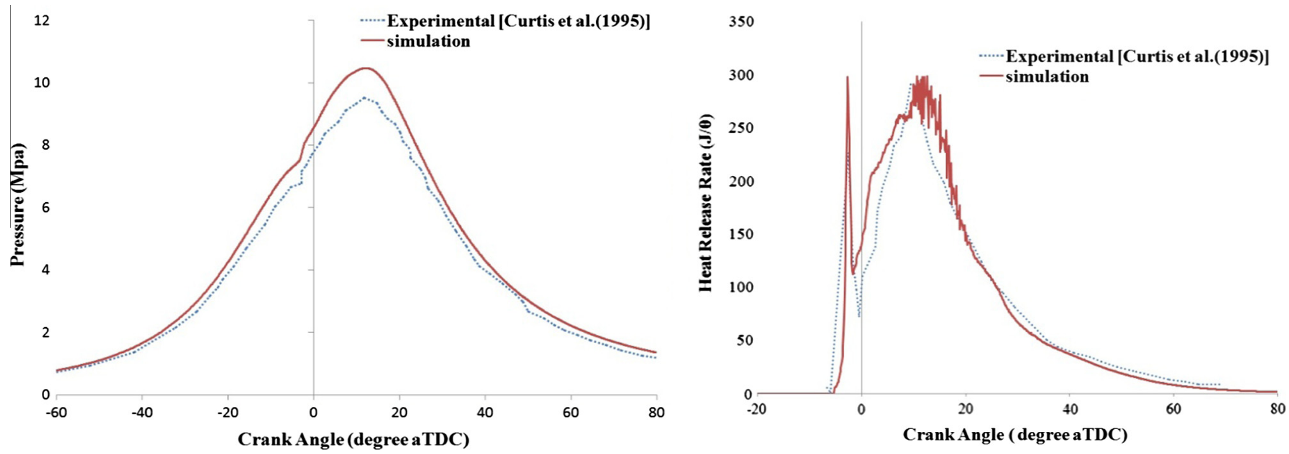


Figure 3 Validation of "Pressure vs Crank angle" and 'Heat release rate vs Crank angle" of experimental data and simulation data of baseline case.

Engine modelling is done with the same geometrical specifications of Table 1 and the simulation run has been taken by imposing the same initial and boundary conditions (Fig. 3).

The input parameters such as Boundary conditions, Spray modelling parameters, Turbulence modelling parameters, material, and grid select of the cylinder and engine have been given to CONVERGE.

3. Results and discussion

Here in this chapter, a clear impact of EGR and advanced SOI on engine performance and exhaust has been shown clearly. CFD analysis is done on both reference model and improved model. The results below proved that reduction of NO_x and Soot is possible with simultaneously introducing the new parameters (introducing both EGR of 10% and Advancing SOI by 3.5°). And the in-cylinder combustion pictures are shown at CAD 21 aTDC and at the end of combustion.

3.1. Individual effect of EGR and advanced SOI

But, before analysing the combined effect of the SOI and EGR, the individual effects of each should be studied.

(1) Advanced SOI: SOI -14.5° CAD aTDC, EGR 0%.
(2) EGR: SOI -11° CAD aTDC, EGR 10%.

The modified parameters of the model are analysed in CONVERGE and Graphs are plotted w.r.t baseline case.

(i) NO_x vs Crank angle (°).
(ii) Soot vs Crank angle (°).
(iii) Pressure vs Volume (m^3).
(iv) Temperature vs Crank angle (°).

The above plots are shown for both Individual effect of "SOI" and "EGR".

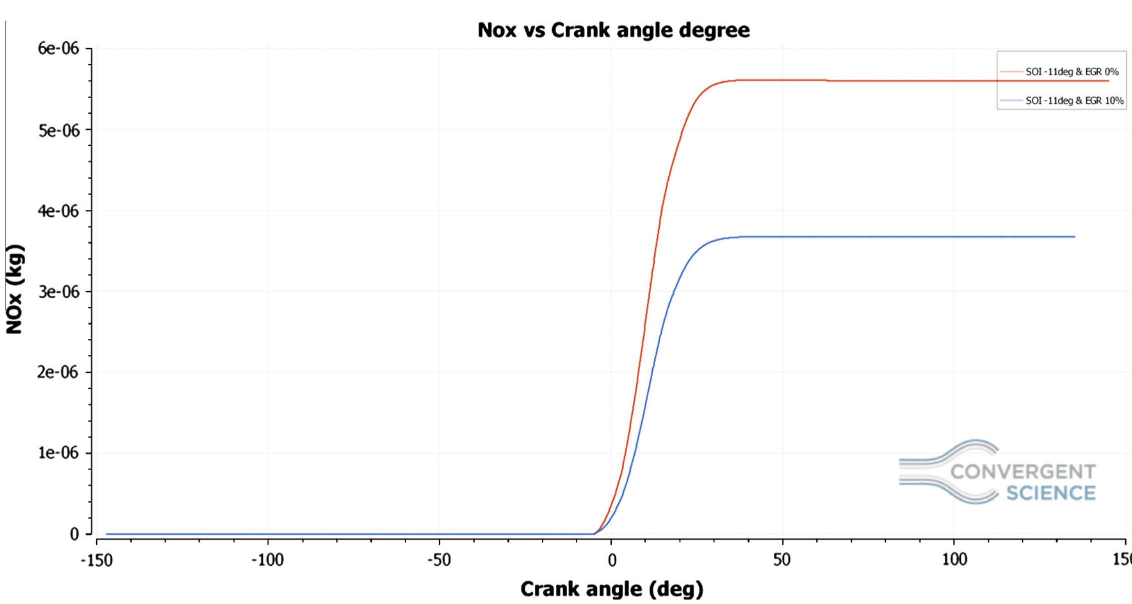


Figure 4 Variation of NO_x with Crank angle in both baseline (red) and improved strategy (blue). NO_x has been decreased by 34.41%.

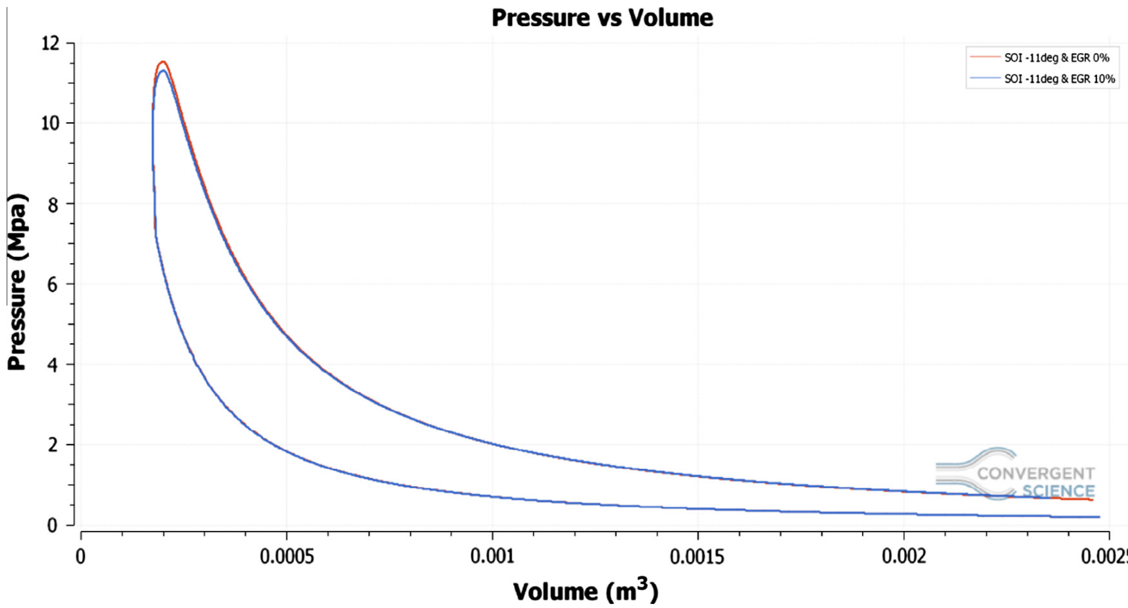


Figure 5 Variation of in-cylinder pressure with Volume in both baseline (red) and improved strategy (blue). The in-cylinder peak pressure has decreased by 0.30 MPa.

3.1.1. Plots of "introducing EGR"

From the graph (Fig. 4), it clearly indicates that NO_x has reduced in improved case (Start of Injection- SOI 11°CA bTDC and EGR 10%). The NO_x content in the exhaust has been reduced by 34.41%, as the EGR used absorbed some amount of the heat released in the cylinder. So, use of EGR suppressed the NO_x content in the Exhaust.

Rate of NO_x formation is the ratio of 'Amount of NO_x released at exhaust (g)' and 'Amount of fuel sprayed into cylinder (kg)'. At the end of combustion in baseline case, the NO_x released at exhaust is $5.59 * 10^{-3}$ (g) and in the modified case it is $3.669 * 10^{-3}$ (g). From Table 1, fuel injected into cylinder is $162 * 10^{-6}$ (kg). So, Rate of NO_x formation in baseline case is 34.46 (g/kg of fuel) and in modified case the rate of formation is 22.66 (g/kg of fuel).

So, the NO_x has decreased by 34.41%, as compared to the baseline case.

In Fig. 5, the in-cylinder peak pressure has decreased by 0.30 MPa. This is because, the introduction of EGR makes mixture become homogenous and combustion happens smoothly, which in turn reduces the peak pressure.

As EGR is sent into the pre-combustion mixture, the oxygen concentration is reduced. When the oxygen quantity gets diluted, the oxygen is not available for perfect combustion. As the combustion is not happening properly, this results in formation of excess soot.

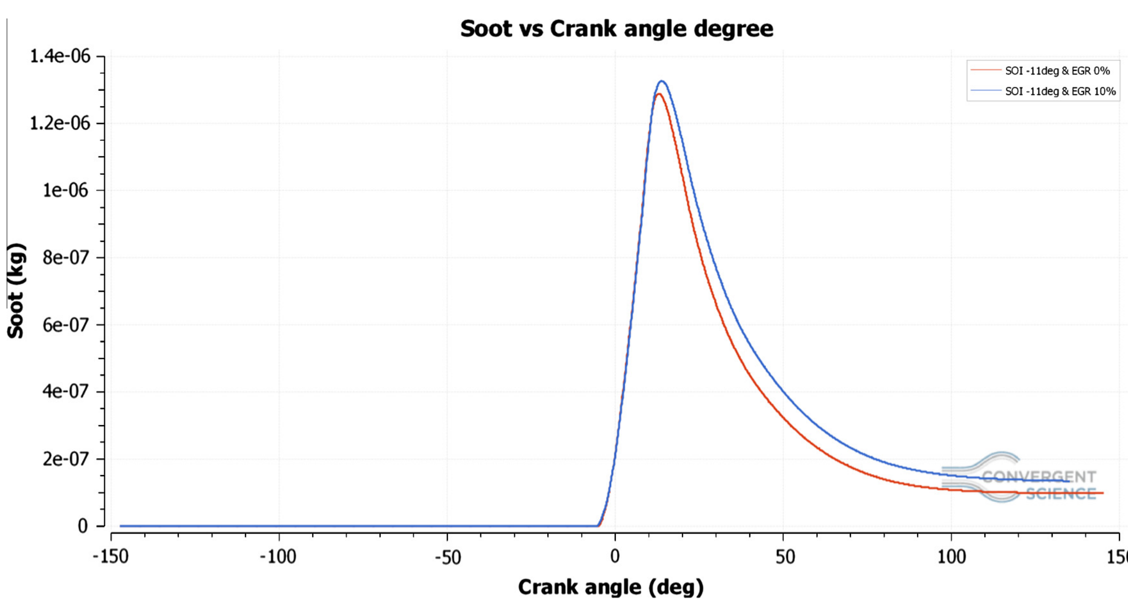


Figure 6 Variation of Soot with Crank angle in both baseline (red) and improved strategy (blue). The soot at the end of combustion has been increased by 37.2% compared to baseline case.

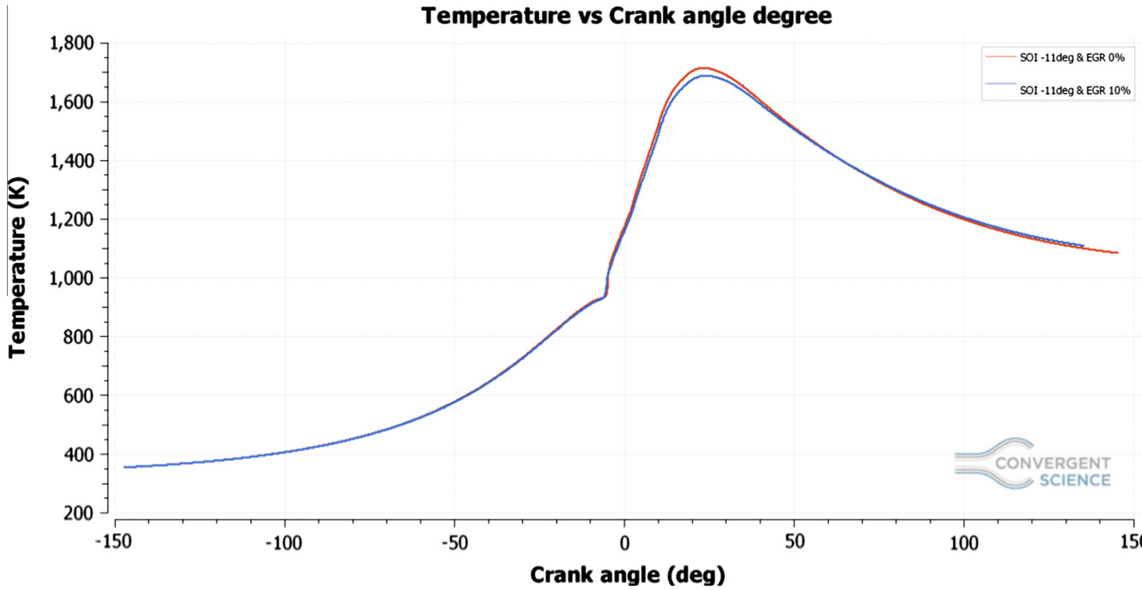


Figure 7 Variation of in-cylinder temperature with Crank angle in both baseline (red) and improved strategy (blue). The peak temperature has been reduced due to high specific heat of CO_2 present in the EGR.

Rate of Soot formation is the ratio of 'Amount of Soot released at exhaust (g)' and 'Amount of fuel sprayed into cylinder (kg)'. At the end of combustion in baseline case, the soot released at exhaust is $9.77 * 10^{-5}$ (g) and in the modified case it is $1.34 * 10^{-4}$ (g). From Table 1 fuel injected into cylinder is $162 * 10^{-6}$ (kg). So, Rate of Soot formation in baseline case is 0.602 (g/kg of fuel) and in modified case the rate of formation is 0.8261 (g/kg of fuel).

So, Soot has increased by 37.2%, as compared to the baseline case, which can be clearly observed in Fig. 6.

When the EGR is introduced into the cylinder, the CO_2 present in it has high specific heat compared to the other gases. So, this nature makes CO_2 to absorb the in-cylinder temperatures. So this makes to reduce the peak temperatures (Fig. 7).

3.1.2. Plots of advancing "SOI"

From the graph (Fig. 8), it clearly indicates that NO_x has increased in improved case (Start of Injection- SOI 14.5°CA bTDC and EGR 0%). The NO_x content in the exhaust has been increased by 7.4%, as the SOI is advanced by 3.5°. The effect of advanced start of injection improves the homogeneity of mixture as it gets long time to mix properly. And as a result the in-cylinder temperature on an average rises, which in turn gives opportunity for high formation of NO_x.

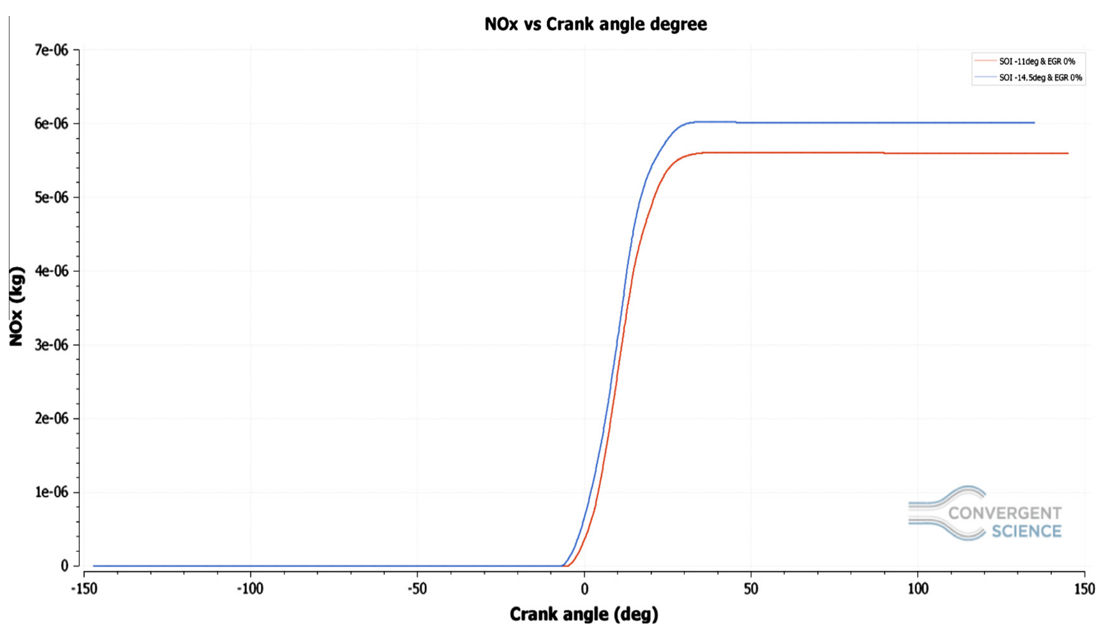


Figure 8 From the graph (Fig. 8), it clearly indicates that NO_x has increased in improved case (Start of Injection- SOI 14.5°CA bTDC and EGR 0%). The NO_x content in the exhaust has been increased by 7.4%, as the SOI is advanced by 3.5°.

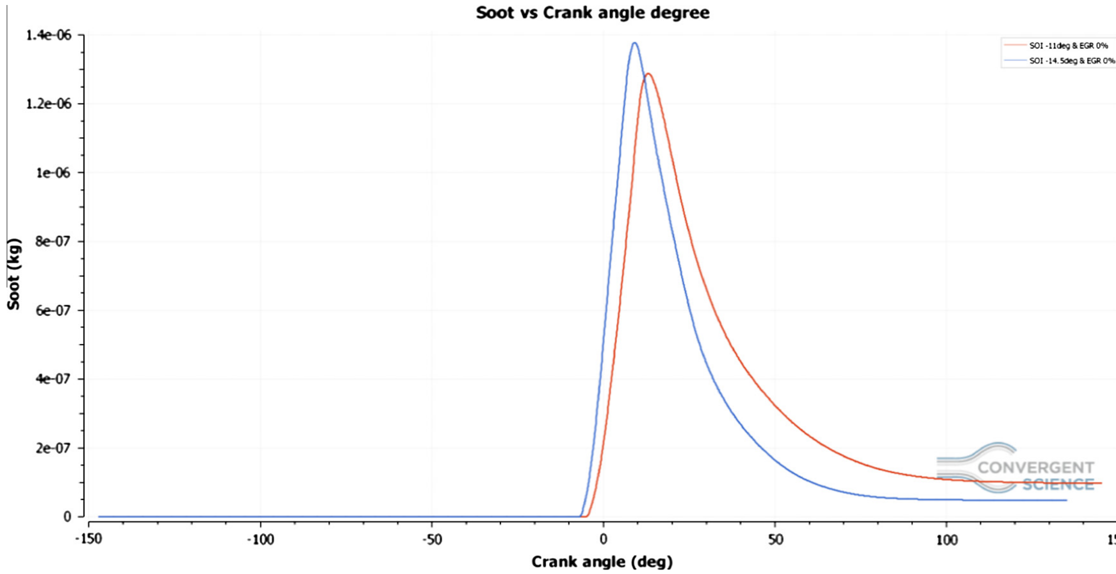


Figure 9 Soot has decreased by 51.96%, as compared to the baseline case, at the end of the combustion. This is because early injection gives high temperatures during expansion stroke, which tends to oxidise soot particles quickly.

Rate of NO_x formation is the ratio of 'Amount of NO_x released at exhaust (g)' and 'Amount of fuel sprayed into cylinder (kg)'. At the end of combustion in baseline case, the NO_x released at exhaust is $5.59 * 10^{-3}$ (g) and in the modified case it is $6.008 * 10^{-3}$ (g). From Table 1, fuel injected into cylinder is $162 * 10^{-6}$ (kg). So, rate of NO_x formation in baseline case is 34.46 (g/kg of fuel) and in modified case the rate of formation is 37.04 (g/kg of fuel).

So, the NO_x has increased by 7.4%, as compared to the baseline case.

The earlier injection leads to higher temperatures during the expansion stroke, and more time in which oxidation of soot particles occurs and homogenous mixture leads to less soot formation.

Rate of Soot formation is the ratio of 'Amount of Soot released at exhaust (g)' and 'Amount of fuel sprayed into cylinder (kg)'. At the end of combustion in baseline case, the Soot released at exhaust is $9.77 * 10^{-5}$ (g) and in the modified case it is $4.69 * 10^{-5}$ (g). From Table 1 fuel injected into cylinder is $162 * 10^{-6}$ (kg). So, Rate of Soot formation in baseline case is 0.602 (g/kg of fuel) and in modified case the rate of formation is 0.289 (g/kg of fuel).

So, soot has decreased by 51.96%, as compared to the baseline case, which can be clearly observed in Fig. 9 (see Fig. 10).

In Fig. 11, as the start of Injection is advanced by 3.5°, it makes clear that the fuel gets more time to get mixed and become more homogeneous. This makes clear that,

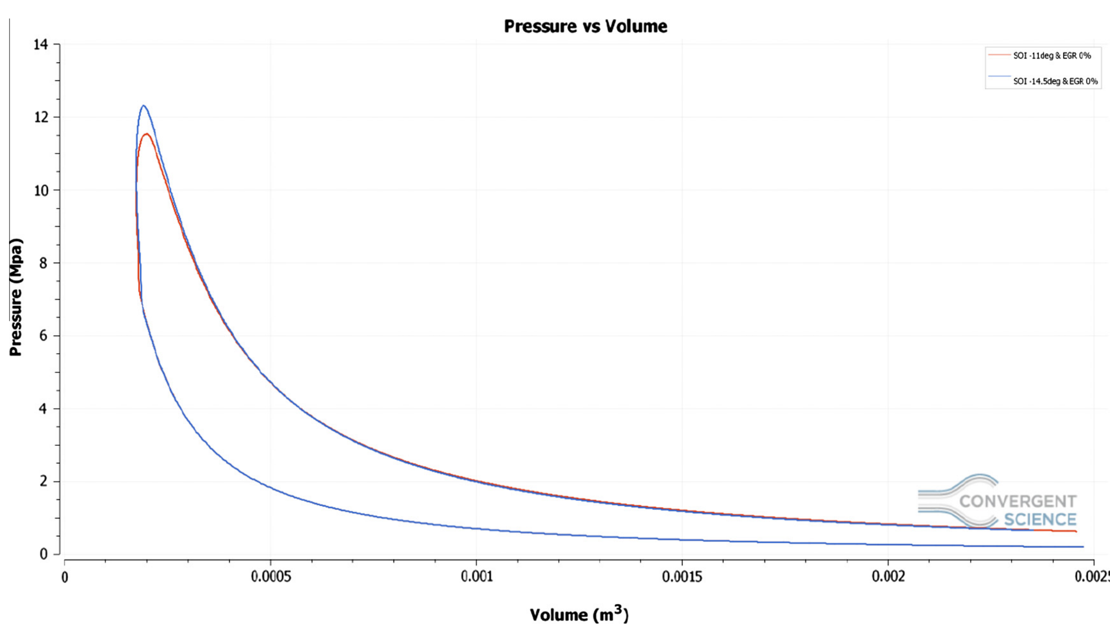


Figure 10 Shows the variation of pressure w.r.t volume, where the peak pressure is higher for the baseline case.

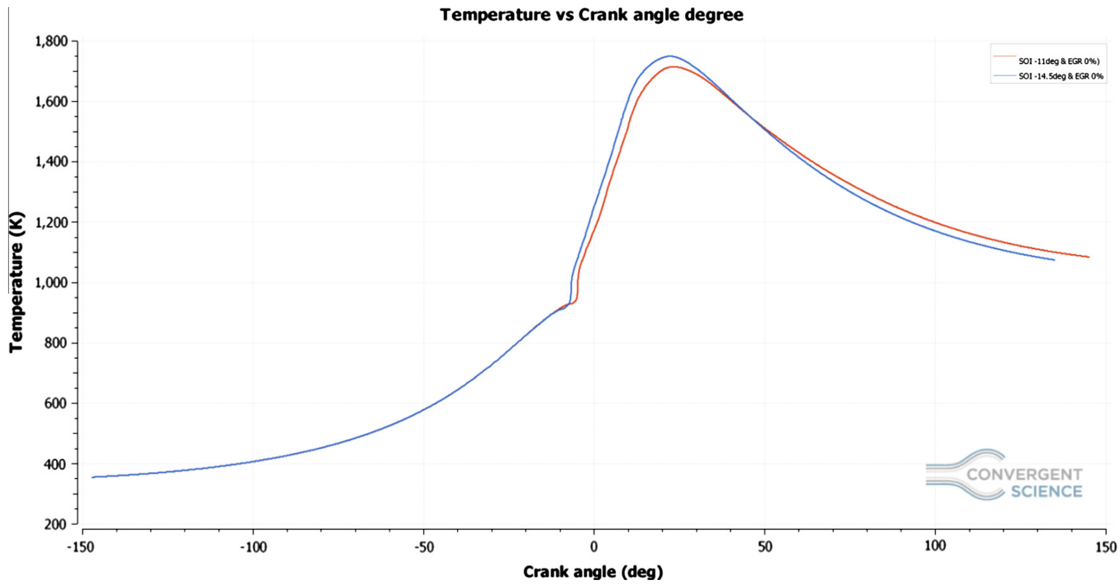


Figure 11 In Fig 13: As the start of Injection is advanced by 3.5°, it makes clear that the fuel gets more time to get mixed and become more homogeneous, and hence the combustion peak temperature is higher.

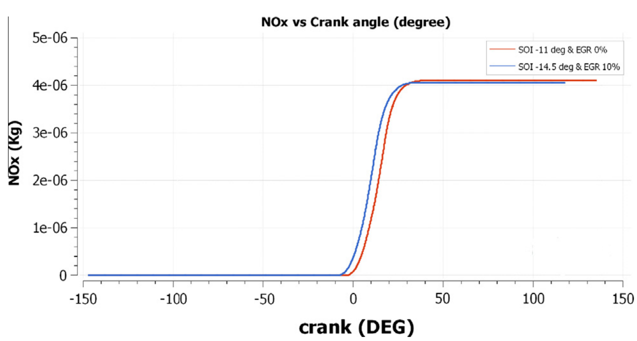


Figure 12 Variation of NO_x with Crank angle in both base-line (red) and improved strategy (blue). The plot clearly indicates that NO_x at the end of combustion has decreased by 1.2% compared to baseline case.

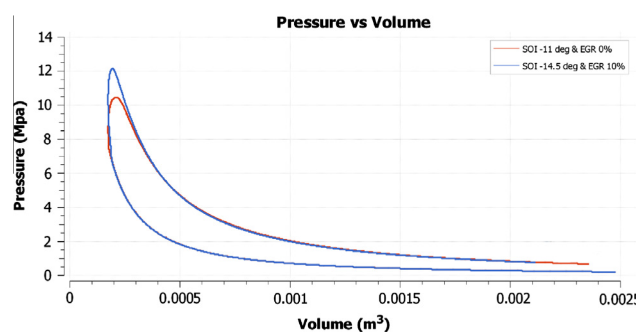


Figure 13 Variation of in-cylinder pressure- with Volume in both baseline (red) and improved strategy (blue). In the plot, it shows that peak pressure in the second case has been increased by 0.8 MPa (which in result increases the work done).

combustion happens more efficiently than the baseline case. So this makes an increase in peak temperatures.

3.2. Combined effect of SOI and advanced EGR

The new parameters of the model are analysed in CONVERGE and Graphs are plotted.

(i) NO_x vs Crank angle (°) (Fig. 12).
(ii) Soot vs Crank angle (°) (Fig 14).
(iii) Pressure vs Volume (m^3) (Fig. 13).
(iv) Temperature vs Crank angle (°) (Fig. 15).

From the graph (Fig. 12), it clearly indicates that NO_x has reduced in improved case (Start of Injection- SOI 14.5° CA bTDC and EGR 10%). The NO_x content in the exhaust has been reduced by 1.2%, as the EGR used absorbs the heat released in the cylinder. So, use of EGR Suppressed the NO_x content in the Exhaust. Though the flame temperatures are higher, the NO_x is reduced because of lesser oxygen concentration due to the EGR fraction.

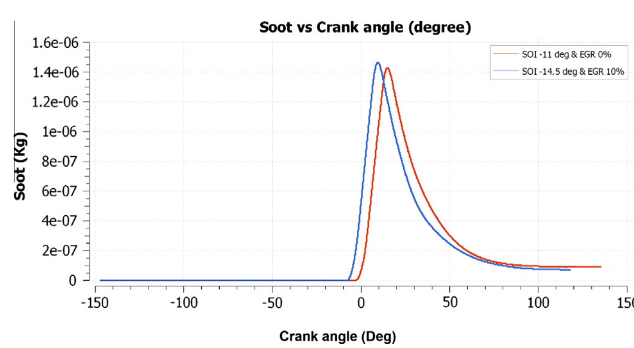


Figure 14 Variation of soot with Crank angle in both baseline (red) and improved strategy (blue). In the above plot, it is clear that soot at the exhaust has been decreased by 21.3% compared to base-line case.

Rate of NO_x formation is the ratio of '*Amount of NO_x released at exhaust* (*g*)' and '*Amount of fuel sprayed into cylinder* (*kg*)'. At the end of combustion in baseline case, the NO_x

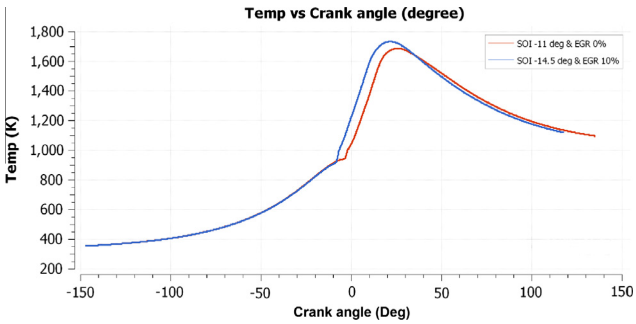


Figure 15 Variation of in-cylinder Temperature- with Crank angle in both baseline (red) and improved strategy (blue).

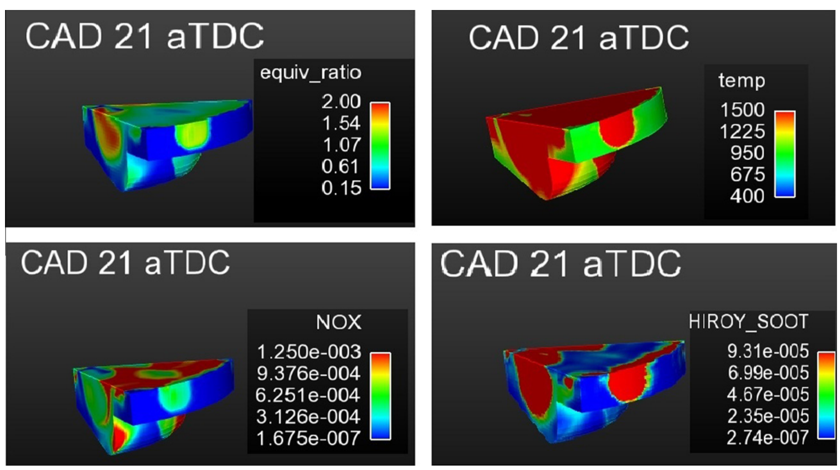
released at exhaust is $4.098 * 10^{-3}$ (g) and in the modified case it is $4.049 * 10^{-3}$ (g). From Table 1, fuel injected into cylinder is $162 * 10^{-6}$ (kg). So, rate of NO_x formation in baseline case is 25.296 (g/kg of fuel) and in modified case the rate of formation is 24.99 (g/kg of fuel).

So, the NO_x has decreased by 1.2%, as compared to the baseline case, and it can be observed in the graph NO_x vs Crank Angle (Fig. 12).

In Fig. 13, the in-cylinder pressure has increased by 0.8 MPa. This is because of advanced SOI, and the mixture becomes homogenous. So the Work Done/IMEP by the engine increased. And finally efficiency of the engine is also increased.

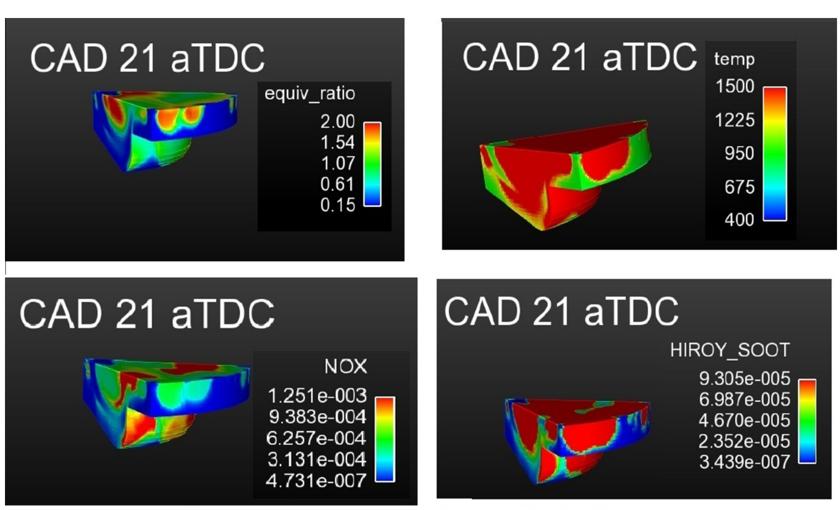
The earlier injection leads to higher temperatures during the expansion stroke, and more time in which oxidation of soot particles occurs and homogenous mixture leads to less soot formation.

Rate of Soot formation is the ratio of '*Amount of Soot released at exhaust* (*g*)' and '*Amount of fuel sprayed into cylinder* (*kg*)'. At the end of combustion in baseline case, the Soot released at exhaust is $9.09 * 10^{-5}$ (g) and in the modified case it is $7.19 * 10^{-5}$ (g). From Table 1 fuel injected into cylinder is $162 * 10^{-6}$ (kg). So, Rate of Soot formation in baseline case is 0.561 (g/kg of fuel) and in modified case the rate of formation is 0.44 (g/kg of fuel).



SOI (14.5 deg bTDC) & EGR 10%

Figure 16 Modified strategy [Equivalence Ratio, NO_x, Soot formation, Temperature in cylinder at 21° CA aTDC.



Base line: (Curtis et al) SOI (11 deg bTDC) & EGR 0%

Figure 17 Baseline case [Equivalence Ratio, NO_x, Soot formation, Temperature in cylinder at 21° CA aTDC aTDC.

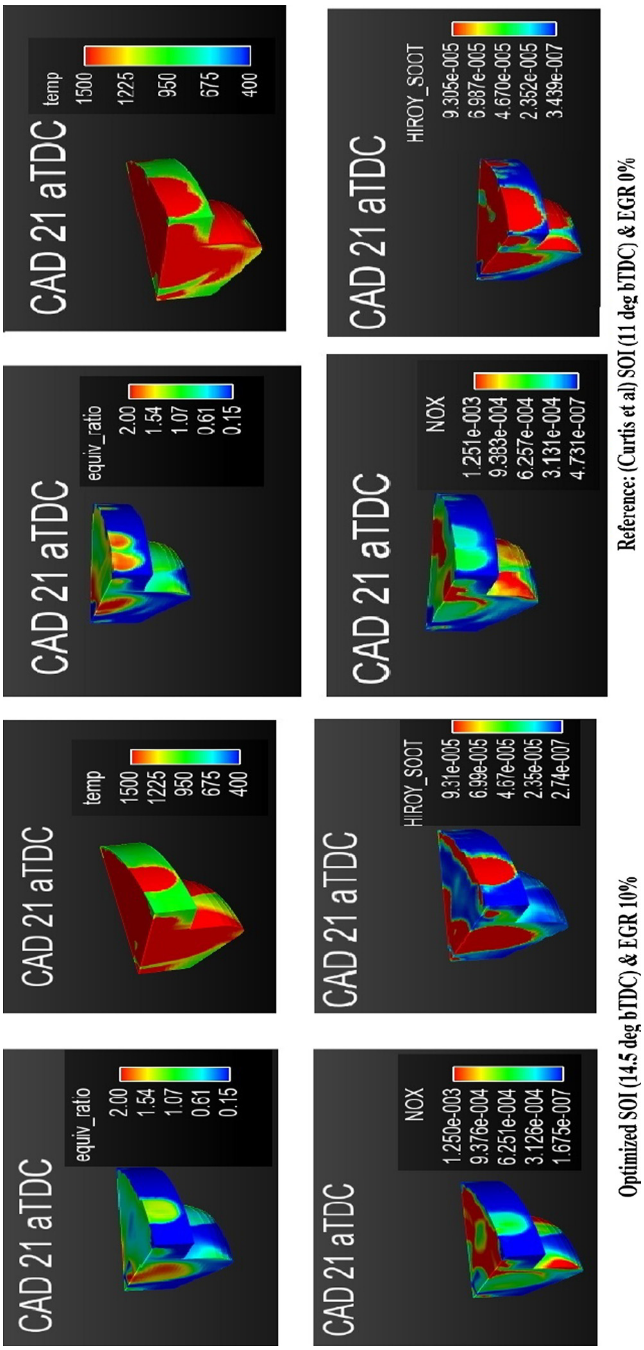


Figure 18 Comparison of NO_x and Soot released between modified strategy and baseline/reference strategy. Visual images clearly show that NO_x and Soot decreased with the combined effect of SOI and EGR.

So, Soot has decreased by 21.3%, as compared to the baseline case, which can be clearly observed in Fig. 14.

As the combustion takes place earlier than the baseline case, the temperature in the cylinder increases due to homogenised mixture. Although EGR tries to absorb the in cylinder temperature, the advanced SOI increases it (Fig. 15).

Images of the in-cylinder combustion mechanism of mixture are collected at 21° aTDC. It can be clearly inferred from

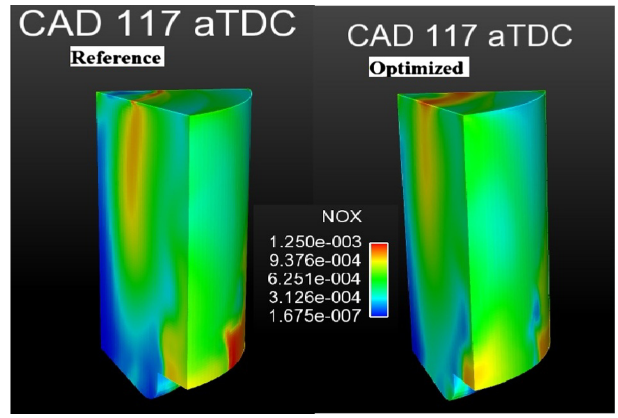


Figure 19 NO_x content at the end of combustion in the cylinder. NO_x has been decreased by 1.2% only compared with the baseline case.

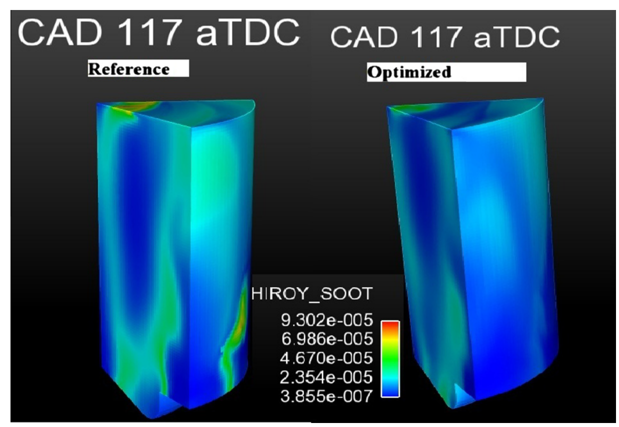


Figure 20 Soot content at the end of combustion in the cylinder. Soot has been decreased significantly by 21.3%.

the images that Soot and NO_x have decreased in Fig. 16 than in Fig. 17 which is Baseline case. It is observed that, at higher temperatures and low Equivalence ratios the NO_x content increases. And at higher temperatures and higher equivalence ratios the soot concentration increases. In Fig. 18, emissions can be compared clearly between the modified and approved cases at 21° CA aTDC.

The NO_x and Soot are also decreased at the end of the combustion compared to baseline in Fig. 19. The higher cylinder mean temperature (> 1000 K) helps soot to get oxidised and homogenous mixture will be responsible for complete combustion, which reduces the soot (Fig. 20). Thus, high cylinder temperatures and proper mix of fuel and air favour soot reduction.

4. Summary and conclusion

The baseline model is analysed and results are found; it is further got improved exhaust emissions and performance as well, by varying the following:

(i) Advancing Start of Injection by 3.5°.
(ii) Recirculating the Exhaust gas by 10%.

This model with improved parameters is again post processed and positive results are found.

- The soot in exhaust has been reduced by 21% and NO_x by 1.2%, by the use of "advanced SOI by 3.5° and 10% of EGR.
- Making use of varied EGR and SOI at a same time will compensate each other's negative effect.
- Increasing the EGR decreased the NO_x and increased the soot content as EGR actually contains some soot content, but use of "advanced SOI" controls it. At the same time use of advanced SOI, increased NO_x and decreased the soot. The increased NO_x is controlled by EGR. Hence the combined effect has proved that NO_x and Soot can be reduced in exhaust.
- The area under the P–V curve has increased in the modified strategy, which results in increase of work done/IMEP. And the Efficiency is also increased.

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