A computational study and experiments to investigate the combustion and emission characteristics of a small naturally aspirated diesel engine through changes in combustion chamber geometry, injection parameters and EGR

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Abstract. Investigation of the combustion process in engines for improved fuel economy and emissions is best done by combining experiments and simulations. In the present work both experiments and simulations are conducted considering a naturally aspirated common-rail direct-injection (CRDI) diesel engine. The CFD model is developed based on experiments conducted at two operating points, representing a 0.9 l, two-cylinder, diesel engine. The developed CFD model is then used to study the effects of different in-cylinder strategies attempted at reducing emissions, without compromising on performance. Previous researches conducted on diesel engine CFD simulations are generally based on large-bore large-capacity single-cylinder engines, and mostly investigated a single operating point. The present study investigates the effects of combustion chamber geometry, injection timing, multiple injections as well as EGR, individually as well as in combination, on NOx and soot emissions, at two different operating points in a small naturally aspirated CRDI diesel engine.

1. Introduction
Internal combustion (IC) engines find application in automobiles, as well as in agricultural machines, industrial and domestic power generators, ships and many more. Battery electric vehicles, however, are yet to establish themselves as the chief transportation means for people, mainly due to the low range and the lack of infrastructure for charging the batteries, especially in a developing economy like India. Therefore, IC engine powered vehicles are expected to continue for at least another couple of decades. Legislations have been in place globally to control the amount of pollutants emitted by IC engines. From April 2020, India will move to the next emission legislation level, called Bharat Stage VI (BS VI) which would be equivalent to Euro 6b.

The main emissions from a diesel engine are nitrogen oxides (NOx), particulate matter (PM) including soot, carbon monoxide (CO) and unburned hydrocarbons (HC) [1]. One could reduce the emissions coming out from the combustion process itself, commonly known as in-cylinder emissions or engine-out emissions; alternatively, one could reduce the emissions using after-treatment systems. Indian market is very cost sensitive, and therefore, the engine should be cost effective as well as fuel efficient. The after-treatment systems required to control the emissions are quite expensive, bulky and
heavy, further affecting the fuel economy. Hence, considerable efforts are required to be put in to reduce the engine-out emissions using in-cylinder strategies to reduce the cost involved in the after-treatment systems.

Engine-out emissions from a diesel engine could be optimised through in-cylinder strategies like modifying the combustion chamber geometry, the fuel injection system parameters like injection pressure, injection timing, introducing multiple injections, thus optimising their interaction, and other techniques like EGR, i.e., exhaust gas recirculation. This, however, is a tedious process, as it takes multiple iterations trying out different combinations. To save on time, one could use computational fluid dynamics tools. A lot of research has been done in the past on optimising the piston bowl geometry and the fuel injection systems through experiments as well as CFD simulations, but most of them were on large-capacity and large-bore engines. Also, most of the previous studies investigated a single operating point. The engine used in this study is a small-bore small-capacity naturally aspirated two-cylinder diesel engine. The present study also discusses the effect of the combination of different in-cylinder strategies applied together, at two different operating points.

The objective of this study is to investigate the effects of different in-cylinder combustion optimisation techniques on the performance and emissions of a small naturally aspirated CRDI diesel engine through CFD simulations. The learnings from this study could further be used in optimizing each operating point. This engine is used in a commercial vehicle application, the specifications of which are given in Table 1. The work is carried out in two stages. First stage is the testing of the existing engine configuration where the in-cylinder pressure, air and fuel mass flow rates at two operating points are recorded. Second stage is the development of a CFD model of the base engine and its validation with the measured data, followed by various steps of modifications, starting with a new piston bowl geometry in line with the trends observed in the literature to reduce emissions. Studies are also done varying the fuel injection parameters like injection timing, introduction of pilot injection and adding EGR. The studies are done at two operating points - low load and high load at 1800 rpm. Figure 1 shows the layout of the valves and fuel injector. The spray angle is also given. As can be seen, the injector is vertical and is placed centrally in the bore.

Diesel combustion happens in different phases, starting with the start of injection (SOI), followed by the ignition delay, and then the pre-mixed combustion and the diffusion combustion phases. The time-period from the SOI to the start of combustion, which is marked by the instant at which the rate of heat release becomes positive [2], is called the ignition delay. It is affected by the temperature, pressure [3] and turbulence level of air at the time of injection, temperature of the wall [4], turbulence of the fuel jet which in turn is influenced by the injection pressure, and kinetic energy modification after the spray impingement, etc.

### Table 1. Engine specifications.

| Parameter                | Unit | Specification                  |
|--------------------------|------|--------------------------------|
| Engine type              | -    | Inline diesel, direct-injection|
| Number of cylinders      | -    | 2                              |
| Rated power              | kW   | 19 @ 3600 rpm                  |
| Maximum torque           | Nm   | rpm                            |
| Bore                     | mm   | 83                             |
| Stroke                   | mm   | 84                             |
| Compression ratio        | -    | 18.5:1                         |
| Connecting rod length    | mm   | 140.5                          |
| Wrist pin offset         | mm   | 0.5                            |
| Charging system          | -    | Naturally aspirated            |
| Swirl number             | -    | 2                              |
| Fuel injection system    | -    | Common-rail direct-injection   |
Combustion starts with pre-mixed combustion where combustion happens in local pockets of fuel-air mixture at near stoichiometric compositions, which increases the temperature and pressure of the surrounding mixture and initiates further rapid combustion resulting in very fast heat release and consequently fast pressure rise. A major proportion of NOx is formed during the pre-mixed combustion stage. Formation of NOx is triggered by the presence of oxygen at high temperature. NOx is composed of NO and NO₂, out of which typically 90% is NO. Figure 2 shows the relation between NOx formation rate, temperature and equivalence ratio [5]. Note that higher pre-mixed combustion results in higher temperature and pressure inside the engine cylinder, which creates more NOx [1].

The role played by the piston bowl geometry in determining the turbulence level of air near the top dead centre (TDC) location, or at the time of injection is extremely important, thereby directly affecting the quantity of fuel being prepared for combustion in the pre-mixed phase [6].

Typically, maximum in-cylinder pressure is achieved in the pre-mixed phase itself, and the combustion which occurs beyond the peak pressure is assumed to happen in diffusion burning. This phase is mainly mixing controlled combustion and depends on air motion and fuel jet turbulence. The rate of heat release is proportional to engine speed, as mixing rates scale up with engine speed. Approximately 80% of the heat release will be complete by the end of diffusion phase. Remaining 20% the heat release is said to happen in late heat release phase, typically into the expansion stroke [1]. Late combustion affects the soot emission, and to some extent the emission of unburned HC as well.

Delaying the SOI will reduce the maximum in-cylinder pressure and temperature; hence will reduce NOx as well. Introduction of pilot injection will help in reducing the ignition delay time which will also reduce NOx by up to 25% at light loads [7]. Another method to reduce NOx is to use EGR.
EGR reduces the concentration of oxygen in the intake charge and increases the heat capacity of the charge. This limits the formation of NOx. In the fuel jet, air entrainment is less at the spray tip, resulting in maximum soot formation in the locally rich mixture [8] – see Figure 3. Oxidation rates are high at the peripheral edges of the spray where air entrainment is very high. Soot concentration can be lowered by reducing the duration of diffusion burning, through better mixing. Higher temperature and oxygen concentration can promote the oxidation of soot [9, 10]. Soot level can also be reduced by impingement of fuel on piston bowl wall [11], probably due to better air-fuel mixing resulting in more pre-mixed phase of combustion.

From past studies done on formation and oxidation of soot in diesel engines [13], it is known that soot forms at local regions of higher equivalence ratios, typically more than 2, when remaining at high temperatures, typically above 1400 K. Higher temperatures till around 2200 K increases the soot
formation and oxidation rates. Figure 4 shows the combinations of temperature and equivalence ratio which promote the formation of NOx and soot.

Studies showed that for better oxygen utilization, the spray should target well within the bowl, neither towards the squish region, nor towards the floor, with smaller spray angles, allowing better mixing, as better air entrainment is possible with more oxygen above and below the spray [14]. The studies also suggested that with stepped bowl, it is possible to separate two injections to strike at two different regions – second below the first – so that the second injection fuel can utilize the unutilized oxygen from the first injection. In the case of conventional bowls, the fuel from the second injection is forced to mix with products of combustion of the first injection producing higher soot. The SOI of the second injection could also be adjusted to reduce NOx.

Narrow bowls produce more soot, too deep or too shallow bowls make more NOx, and longer lip region results in early spray impingement producing more NOx and less soot [15]. Higher bowl diameter for all arc radius gives low soot, fuel consumption, and high NOx [16]. The study also suggested that NOx was independent of arc radius. Another outcome of the study was that higher cone angle and advancement of SOI both give the same result individually, i.e. higher NOx, lower soot and BSFC. Higher the target point on bowl, higher the NOx, lower the fuel consumption and soot. Wider bowls are more tolerant to spray targeting variation, but might impact part load soot-NOx trade-off, low load HC, CO in low compression ratio applications.

Re-entrant bowls allow higher mixing rates which allow retarded injection with low NOx and soot, and similar fuel economy [17, 18]. Highly re-entrant bowl with less central projection generated high swirl and turbulence and was found to reduce NOx by 27% and soot by 85% through injection optimization [19]. Re-entrant bowl promotes swirl amplification, affects the squish flow strength, increases mixing inside the piston bowl by means of the higher turbulence created, thus allowing retarded SOI without affecting soot and BSFC [17, 18, 20, 21]. Re-entrant chambers trend seems to be toward becoming wider and shallower with every generation [22, 23, 24].

NOx is less sensitive to operating conditions and geometry, whereas soot is highly sensitive [25]. Narrow low throat radius, deep bowls with low pip height produce lower NOx, while larger throat radius and larger toroidal radius result in lower soot. Lip length does not have much effect on emissions. Soot and HC were found to be optimised by the same geometry. Wall wetting increases soot, early injection with smaller spray angle can avoid wall wetting and reduce soot [26].

Conditions favourable for reduction of NOx result in soot formation and vice versa. This makes the simultaneous reduction of both a challenging task. From the literature, it is evident that establishing an excellent trade-off between NOx and soot is quite difficult for all operating conditions. The general trend is to move towards a wider, shallower bowl, which will increase the air utilisation, and then optimize the fuel injection parameters to achieve the emission targets. For the present study, a similar approach has been followed.

This paper has been organized to flow as follows – first the details of the experiment set-up and the measurements are provided, followed by the details of the computation model with a brief description of the model and governing equations, sub-models, initial conditions and boundary conditions, grid independence study and validation of the model with experiment data. Then the paper discusses about the different iterations studied and the results are interpreted and discussed. Finally, the study is concluded with key observations and identifies a few areas for further study.

2. Experiment set-up and Numerical Framework

2.1. Experiment set-up

The experiment set-up is as shown in Figure 5. Table 2 lists out the two engine operating points which were tested and the corresponding measurements. The data recorded include in-cylinder pressure, air mass flow rate, fuel mass flow rate, pressure and temperature inside the intake and exhaust manifolds and timing of start and end of fuel injection. Gross IMEP and heat release rate are derived values from the in-cylinder pressure measurement. Even though the test set-up is capable of varying the EGR rate through a modulator, all test points considered are without EGR.
The engine has crank speed/position sensor and cam position sensor which work together to determine the top dead center location. In-cylinder pressure is recorded using a Kistler-make piezo-electric pressure transducer 6052C, mounted on cylinder one (from the front), through a machining adaptation. An average pressure trace based on hundred consecutive engine cycles is then calculated for each operating point. Kistler-make piezo-resistive pressure pick-ups 4007C and 4049B are used to measure the crank angle resolved pressures inside the intake manifold and exhaust manifold, respectively. Combustion data is recorded in KiBox.

Table 2. Engine operating points.

| Parameter                  | Unit | Case 1  | Case 2  |
|----------------------------|------|---------|---------|
| Speed                      | rpm  | 1800    | 1800    |
| Load                       | Nm   | 2       | 49.5    |
| Gross IMEP                 | bar  | 3.34    | 9.87    |
| Intake manifold pressure   | kPa  | 99.7    | 99.8    |
| Intake manifold temperature| °C   | 27      | 28      |
| Exhaust manifold pressure  | kPa  | 109.3   | 107.1   |
| Exhaust manifold temp.     | °C   | 120     | 334     |
| Fuel injection pressure    | bar  | 750     | 1300    |
| Mass flow rate of air      | kg/h | 52.14   | 50.63   |
| Mass flow rate of fuel     | g/h  | 729.18  | 2503.47 |
| EGR ratio                  | %    | 0       | 0       |
| EGR flow rate              | kg/h | 0       | 0       |
| Start of injection         | °aTDC| -6.6    | -6.6    |
| Injection duration         | µs   | 536     | 679     |
| Injection duration         | °CA  | 5.8     | 7.3     |
| Injection quantity         | mg/cycle | 6.75 | 23.18   |

Figure 5. Experimental set-up.
2.2. Computation model

The CFD software used in the present work is Converge. With the IC engine sub-models available in the package, the entire process from Intake Valve Closing (IVC) to Exhaust Valve Opening (EVO), including fuel injection is simulated. Despite being a symmetric combustion chamber, a full 360° combustion chamber simulation is performed rather than a sector simulation, to negate the effects of swirl-spray interaction errors (if any) in a sector simulation. The details of the model including the initial and boundary conditions, sub-models used, etc. are given in the following sections. Figure 6 shows the model 3D geometry at BDC and TDC locations.

![Figure 6. 3D model geometry at BDC and TDC.](image)

All conservation equations are solved in the finite volume method, with the surface values evenly interpolated, to get second order accurate spatial scheme. All governing equations are solved by successive over-relaxation (SOR) method, with some under-relaxation, calculated by Converge, to speed up convergence and ensure stability.

Compressible form of equations of mass and momentum are

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = S
\]

(1)

and

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + S_i
\]

(2)

where, the viscous stress tensor is given by

\[
\sigma_{ij} = \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \left( \mu' - \frac{\mu_t}{\kappa} \right) \left( \frac{\partial u_k}{\partial x_k} \delta_{ij} \right)
\]

(3)

where,

- \(u\) is the velocity,
- \(\rho\) is the density,
- \(S\) is the source term,
- \(P\) is the pressure,
- \(\mu_t\) is the turbulent viscosity,
- \(\mu'\) is the dilatational viscosity (set to zero), and
- \(\delta_{ij}\) is the Kronecker delta.

\[
\mu_t = \mu + C_{\mu} \rho \frac{k^2}{\varepsilon}
\]

(4)

where,
\( C_\mu \) is a turbulence model constant, \( k \) is the turbulent kinetic energy, and \( \varepsilon \) is the turbulent dissipation.

Gas flow is considered as compressible flow, and liquid flow is considered as incompressible flow. Redlich-Kwong equation of state, given below, is used.

\[
P = \frac{RT}{v - \beta_{rk} v_c} - \frac{(\alpha_{rk} \frac{p_c}{v_c})}{v^2 + \beta_{rk} v_c v}
\]

where, \( v_c = \frac{RT_c}{p_c} \), \( \alpha_{rk} = 0.42748 \), \( \beta_{rk} = 0.08664 \), \( v_c \) is the critical volume, \( T_c \) is the critical temperature, \( p_c \) is the critical pressure, \( \alpha_{rk} \) represents the attractive forces between molecules, and \( \beta_{rk} \) represents the volume of the molecules. Thermodynamic properties are considered functions of temperature. Critical temperature and pressure used are 133 K and 37.7 MPa, respectively.

Energy equation with convection and diffusion terms, given below, is solved for specific internal energy conservation.

\[
\frac{\partial \rho e}{\partial t} + \frac{\partial \rho u_j e}{\partial x_j} = -P \frac{\partial u_j}{\partial x_j} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left( K_{\partial \rho e} \frac{\partial e}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \rho D \sum_m \frac{\partial Y_m}{\partial x_j} \right) + S
\]

where, \( \rho \) is the density, \( Y_m \) is the mass fraction of species \( m \), \( D \) is the mass diffusion coefficient, \( S \) is the source term, \( P \) is the pressure, \( e \) is the specific internal energy, \( K_{\partial \rho e} \) is the turbulent conductivity, \( h_m \) is the species enthalpy, \( \sigma_{ij} \) is the stress tensor, and \( T \) is the temperature.

\[
K_{\partial \rho e} = K + c_p \mu_t K_t
\]

where, \( c_p \mu_t \) is the turbulent Prandtl number, \( c_p \) is the specific heat at constant pressure, \( \mu_t \) is the turbulent viscosity, \( K \) is the thermal conductivity, and \( K_t \) is the turbulent conductivity.

The source term accounts for turbulent dissipation. Compression and expansion are accounted for by the pressure work term \(-P \frac{\partial u_j}{\partial x_j}\). Kinetic energy dissipates into heat through viscous dissipation and is accounted for by the viscous dissipation term. Energy transport due to species diffusion is accounted for by the species diffusion term \( \frac{\partial}{\partial x_j} \left( \rho D \sum_m \frac{\partial Y_m}{\partial x_j} \right) \).

Mass fraction of each species, in a cell is calculated as:

\[
Y_m = \frac{M_m}{M_{tot}} = \frac{\rho_m}{\rho_{tot}}
\]

where, \( M_m \) is the mass of species \( m \), \( \rho_m \) are the density of species \( m \), \( M_{tot} \) is the total mass of the cell, and \( \rho_{tot} \) is the total density of the cell.

Species conservation equation, given below, is solved:

\[
\frac{\partial \rho_m}{\partial t} + \frac{\partial \rho_m u_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D_t \frac{\partial Y_m}{\partial x_j} \right) + S_m
\]

where, \( \rho_m = Y_m \rho \), \( u \) is the velocity, and \( D_t \) is the turbulent mass diffusion coefficient given by:
where, \( S_C_t \) is the turbulent Schmidt number.

Evaporation, combustion chemical reactions and other sub-models are taken into account by the source term \( S_m \). The diffusion coefficients are calculated independently of the species.

A modified pressure implicit with splitting of operators (PISO) is used for pressure velocity coupling. The algorithm starts with solving the momentum equation implicitly (or semi-implicitly), through a predictor step, followed by deriving and solving the pressure equation, which forms the corrector step, and this is continued till the desired accuracy is achieved. From these two, the pressure-velocity relation is established. Pressure is solved through conservation of mass, with relation between density and pressure taken from the equation of state. The solved pressure value is used to calculate the velocity, and the process is iterated till convergence.

A variable time-step method is used in the model, with the initial time-step as \( 1 \times 10^{-7} \) s. The model will try to achieve convergence with the biggest time step possible, satisfying all conditions including conditions, if any, from sub-models. Lower order scheme is used for convective flux spatial discretization for momentum, turbulence and other transport equations, with first order upwind scheme for turbulence equation, and second order central difference method for momentum and other transport equations.

For closed cycle simulation, only wall temperature boundary conditions are applicable. The temperatures are controlled by law of wall, where the turbulent viscous sub-layer is not resolved. Neumann boundary condition of zero normal gradient is given for turbulent kinetic energy for all boundaries, and Dirichlet boundary conditions for the turbulent dissipation calculated at the center of the cell near the wall by the wall model

\[
e = \frac{\varepsilon_k^{0.75} k^{1.5}}{k_y}
\]

(11)

where, \( \varepsilon \) is the turbulent dissipation, \( k \) is the turbulent kinetic energy, \( y \) is the distance from the wall to the middle of the cell, \( C_\mu \) is a turbulence model constant, and \( \kappa \) is von Karman’s constant equal to 0.4187.

Piston motion is governed by the equation

\[
z = 2a - l \left[ 1 - \cos \left( \frac{a \sin \theta + x}{l} \right) \right] - a (1 - \cos \theta)
\]

(12)

where, \( z \) is the position of piston along piston motion direction, \( a \) is half stroke, \( l \) is the connecting rod length, \( x \) is the wrist pin offset, and \( \theta \) is the crank angle.

Grid refinement is done only at relevant regions and/or times, to minimize the computation effort. Adaptive mesh refinement and fixed embedding features of Converge are used for this. Adaptive mesh refinement is based on the variation in temperature and/or velocity in a cell. Figure 7 shows the grids at the start of computation (at IVC), at TDC, and at the end of computation (at EVO). It is evident that at the start of computation, the grid size is uniform across the computational region, and grid refinement happens as the simulation progresses, with critical regions such as boundary walls and fuel spray have a fine grid size. Similar levels of refinement could be seen at the end of simulation as well.

RANS RNG \( k-\varepsilon \) model has been used to model turbulence, which has been proven to be very accurate in previous studies. Liquid diesel has been modeled with a library fuel available in Converge called DIESEL2, while the vapour phase is modeled as \( n \)-heptane \((C_7H_{16})\). SAGE detailed chemical kinetics solver has been used for solving the 168 reactions possible through the 42 participating species, to evaluate the mass of each species formed at a cell at every instant and the cell temperature, by solving the governing equations of the cell.
Figure 7. Grid size at (a) IVC, (b) TDC and (c) EVO.

Fuel spray breakup has been modeled using modified Kelvin-Helmholtz Rayleigh-Taylor model. NTC collision model and dynamic drop drag model have been used. Spray-wall interaction has been modeled using the rebound/slide model. O’Rourke film splash model has been used. Blob injection model has been considered, therefore the injected droplets have the same diameter as the nozzle.

NOx emission has been modeled using the extended Zel’dovich mechanism, defined by the three reactions:

\[
\begin{align*}
O + N_2 & \rightleftharpoons NO + N \\
N + O_2 & \rightleftharpoons NO + O \\
N + OH & \rightleftharpoons NO + H
\end{align*}
\]

NOx is estimated from the calculated NO using a factor of 1.533, which is the ratio of molecular weights of NO\(_2\) to NO [27].

Hiroyasu-NSC model has been used to estimate soot emission. This model calculates the rate of formation of soot as the difference between the rate of production of soot and the rate of oxidation of soot. Soot oxidation is modeled using NSC oxidation model. Both formation and oxidation are strong functions of temperature. This model does not take into consideration the agglomeration of soot particles and the condensation of hydrocarbons on the soot surface.

2.2.1. Model validation. It is very important to utilise the minimum amount of resources to get the output at the desired level of accuracy. To ensure this, a grid independence study is conducted. Three base grid sizes are used – starting with coarse grid of 8 mm, medium grid of 4 mm and fine grid of 2 mm. These three sizes are tried at one operating point. Fixed embedding and adaptive mesh refinement features are also used.

Figure 8 shows the pressure curves for the three grid sizes around TDC. Table 3 lists out the minimum number of cells and the maximum number of cells during the entire simulation period.
Figure 8. A comparison of cylinder pressure traces with base grid size of 8 mm, 4 mm and 2 mm.

Table 3. Details of grid independence study.

| Base grid size | Minimum cells | Maximum cells |
|----------------|---------------|---------------|
| 8              | 4666          | 226792        |
| 4              | 32300         | 1016153       |
| 2              | 63450         | 2035423       |

From the pressure traces, it is clear that there is not much difference between the traces with base grid size of 4 mm and 2 mm, however, the number of cells for the case with grid size of 2 mm is almost double than that of the 4 mm case, indicating the requirement of higher computation effort. Converge also recommends using the base grid size of 4 mm, and therefore, the present model is prepared with 4 mm base grid size. Once the base grid size is fixed, the next step is to validate the model.

Validation is done on one operating point (i.e. Case 2). In-cylinder pressure trace and heat release rate are the two parameters considered for the validation purpose. A decent match is obtained for both the parameters. To prepare the model, numerous input parameters are given, which include some parameters which are measured on the test bed and some which are not. The parameters which are not measured are varied within a reasonable range to achieve a satisfactory level of match between model and experimental results. It is to be noted that start of fuel injection and end of fuel injection values from the experiment represent to the electrical signal from the ECU, however, actual start and end of fuel injection would be different due to reasons such as hydraulic lag, inertia, hysteresis and the fuel trapped in the injector sac volume. Logical changes are made on the start of fuel injection and injection duration as well. Other parameters which are varied are initial in-cylinder temperature at IVC, the species concentrations which will have some residuals from previous cycle, boundary wall temperature, start of injection, injection duration and injection rate profile. No change is made on parameters which were measured and known with good level of accuracy which include air quantity, fuel quantity, fuel injection pressure and in-cylinder pressure at IVC. Figure 9 shows the valve timing and the simulation period.

As the model considers only the closed cycle period, i.e. from IVC to EVO, the initial conditions required are the composition of the charge mass inside the cylinder at IVC, its pressure, temperature, turbulent kinetic energy and turbulent dissipation rate. The initial values used are summarized in Table 4.
Valve timing and simulation period.

Table 4. Initial conditions used in the model.

| Parameter                                | Unit      | Initial value |
|------------------------------------------|-----------|---------------|
| Pressure                                 | Pa        | 124340.23     |
| Temperature                              | K         | 375.42        |
| Turbulent kinetic energy                 | m$^2$/s   | 62.0271       |
| Turbulent kinetic energy dissipation rate | m$^3$/s   | 17183.4       |
| Turbulent kinetic energy specific rate of dissipation | 1/s | 17183.4 |

The initial temperature inside the cylinder was calculated to match the trapped mass based on air mass flow rate. 7% residual gases, modeled as CO$_2$, from previous cycle is considered in the calculation, to match the motoring pressure curve.

Since the computation is done from IVC to EVO, there are no in-flow and out-flow boundary conditions. The only boundary conditions used are the temperature boundary conditions for the liner, cylinder head and piston walls. Constant temperature boundary conditions are used for all the three boundaries. The temperatures used are in-line with the temperatures used in the literature, as well as comparing with the estimated temperatures in real engine operating conditions. Same temperatures are used for all operating conditions, even though in reality the temperature would vary based on the speed and load conditions. However, the variation will not be drastic and its effect is minimal on the simulation results. The wall temperatures used in the model are given in Table 5.

Table 5. Boundary conditions used in the model.

| Surface     | Temperature (K) |
|-------------|-----------------|
| Liner       | 473.15          |
| Cylinder head | 473.15        |
| Piston      | 573.15          |
The model prepared for Case 2 is extended to the other operating point as well. Practically, there would be some changes happening on the boundary wall temperatures, but as the present study is focusing on a comparative discussion, the impact of this would be quite small. However, the variable parameters like air quantity, fuel quantity, fuel injection duration, fuel injection pressure and in-cylinder pressure and temperature at IVC are varied.

Figure 10 shows the plots of in-cylinder pressure and heat release rate for both cases, overlapped with corresponding data calculated from the experiments. The level of match is deemed satisfactory for the present study.

![Figure 10](image_url)

**Figure 10.** A comparison of simulation and experiment results of in-cylinder pressure and heat release rate – case 1 and 2.

### 3. Results and Discussion

With the validation, the baseline case is also ready. The baseline emission levels are estimated at the two operating points. In the next step, the effect of various parameters on emissions and performance is studied. A step-by-step approach is followed, and each step is being considered as an iteration. In iteration 1, only the piston bowl geometry is changed. In iteration 2, with the new geometry, the main injection timing is also retarded by 1.1° CAD. In iteration 3, pilot injection with 10% of total fuel quantity is introduced to iteration 2. The main injection fuel quantity and duration are adjusted to keep the total fuel quantity and injection pressure the same. In iteration 4, EGR is added to iteration 3. EGR is simulated by adding CO₂ to the air mixture at the start of simulation. Therefore, in iteration 4, the effects of all changes together are studied, i.e., retarded main injection with pilot injection and EGR along with the new geometry piston bowl. Once again, for the comparison purpose, the fuel quantity and fuel injection pressure are kept same as the baseline cases. These four iterations are carried out at both the operating points. Table 6 lists out the details of each iteration. In the below sections, each iteration is reviewed in detail.
Table 6. Details of changes in parameters between iterations.

| Parameter       | Baseline | Iteration 1 | Iteration 2 | Iteration 3 | Iteration 4 |
|-----------------|----------|-------------|-------------|-------------|-------------|
| Piston bowl     | Base     | Modified    | Iteration 1 | Iteration 1 | Iteration 1 |
| Start of injection (°aTDC) | -1.6 | -1.6 | -0.5 | -0.5 | -0.5 |
| Injection duration | Base | Base | Base | 0.9 x Base | 0.9 x Base |
| Start of injection (°aTDC) | - | - | - | -10.5 | -10.5 |
| Injection duration | - | - | - | 0.1 x Base | 0.1 x Base |
| EGR             | -        | -           | -           | -           | 15%         |

3.1. Iteration 1 – Modified piston bowl geometry
In this iteration, the bowl geometry is changed. The changes applied are in line with the recent trends in industrial applications and academic research studies. The baseline piston bowl is a slightly re-entrant bowl with a well-defined lip and pip regions and a fairly big toroidal radius. Figure 11 shows the important parameters of a piston bowl. The bowl geometry shown is the baseline bowl. It is to be noted that $D_{\text{max}}$ is the bowl diameter, $D_t$ is the throat diameter, $h$ is the bowl depth, $p$ is the pip height, $l$ is the lip height, $R$ is the toroidal arc radius and $\alpha$ is the pip cone angle. Table 7 compares these parameters between the baseline design and the modified design. The percent change of each parameter can also be seen here. Figure 12 shows the differences between the two bowl designs.

![Figure 11. Geometrical parameters of piston bowl.](image)

![Figure 12. Comparison of new bowl with baseline bowl.](image)

Table 7. Parametric comparison of new bowl with baseline bowl.

| Parameter | Unit | Baseline | Iteration 1 | % change |
|-----------|------|----------|-------------|----------|
| $D_{\text{max}}$ | mm | 46.5 | 48 | 3.23 |
| $D_t$ | mm | 41.5 | 43 | 3.61 |
| $h$ | mm | 14.65 | 13.332 | -8.99 |
| $p$ | mm | 5.5 | 5.5 | - |
| $l$ | mm | 1.655 | 0.3 | -81.87 |
| $R$ | mm | 5.2 | 5.2 | - |
The new bowl is wider, i.e., $D_{\text{max}}$ is more, throat diameter $D_t$ is also higher, and the depth $h$ is reduced to keep the compression ratio same. Toroidal radius is kept same, which has resulted in reduced lip height. Pip height and cone angle are also kept same as the old bowl. The new geometry has been arrived at through extensive literature review, and it was observed that wider bowls tend to result in less soot and are more tolerant to variation in spray targeting. Wider bowls must be shallower to retain the same compression ratio. Too shallow bowls result in higher NOx too. Generally, conditions favourable for reducing soot result in higher NOx. In the present study, the intention of the geometry change is to reduce soot, and then use other strategies to reduce NOx if found higher.

In-cylinder pressure trace and heat release rate trace are plotted for this iteration for the two operating points. Figures 13 and 14 show how these parameters compare with the baseline curves. Only the region around TDC is shown here, so that the difference could be identified with ease.

![Figure 13](image1.png)

**Figure 13.** Case 1 iteration 1 simulation compared with baseline simulation in-cylinder pressure and heat release rate.

![Figure 14](image2.png)

**Figure 14.** Case 2 iteration 1 simulation compared with baseline simulation in-cylinder pressure and heat release rate.

Figure 15 shows the comparison of gross IMEP, NOx and soot between baseline simulation and iteration 1 with the modified geometry of the combustion chamber.
As expected, soot emission has come down with the geometry change for the higher load case. Gross IMEP has increased for both the operating points. This indicates better air utilization, hence also raised the peak cylinder pressure and combustion temperature for the cases with modified geometry, and therefore, resulted in an increase in NOx for both cases. In the low load case, the soot emission has marginally increased over the baseline case, and the increase in NOx is also lesser compared to the higher load case. Soot formation starts around 5 CAD and freezes by 50 CAD. Soot formation rate and oxidation rate in case 1 are found to be similar for both baseline and iteration 1. A look at the equivalence ratio distribution within the cylinder shows that the mixing level in iteration 1 is quite similar to the mixing level in the baseline case. This is evident from the comparison of mass fraction of various equivalence ratios from 0 – 2 in steps of 0.1, as shown in Figure 17 for the crank angles 5, 25 and 40 CAD aTDC. The mixing level is found better in case 2, where there is a reduction in mass fraction of richer equivalence ratios. In the higher load case, there are less regions with very lean or very rich equivalence ratios, which indicates better mixing and better combustion, and this has resulted in raising the cylinder pressure and temperature compared to the baseline case, producing more NOx. This is in line with the observation from the pressure curve and heat release rate curve of both the cases, that in case 1, the curves almost overlap the baseline, while in case 2, there is a marked differentiation with higher peak cylinder pressure and slightly higher rates of heat release till around 20 CAD. In the soot history too, in the higher load case, the peak soot formed itself is lower than the baseline case.
Figure 17. Equivalence ratio distribution in terms of mass fraction at 5 CAD, 25 CAD and 40 CAD, for Case 1.

3.2. Iteration 2 – Modified piston bowl geometry with retarded main injection

It has been known from previous studies that retarding the main injection timing will reduce the ignition delay, thereby reducing the amount of fuel and air undergoing premixed combustion. This is the reason behind lower NOx and higher soot. Retarding the main injection timing will typically reduce the peak firing pressure and hence NOx and gross IMEP. Since the new bowl geometry has resulted in an increase in IMEP, there is an opportunity to retard the main injection timing. Therefore, the new bowl geometry is taken, and the main injection timing is retarded by 1.1°, the new SOI at -0.5° aTDC, which is within reasonable limits of late main injection.

In-cylinder pressure trace and heat release rate trace are plotted for this iteration for both operating points. Figures 18 and 19 show how these parameters compare with the iteration 1 curves.

Figure 18. Case 1 iteration 2 simulation compared with iteration 1 simulation in-cylinder pressure and heat release rate.
It can be seen from Figures 18 and 19 that the values of peak cylinder pressure are lower than iteration 1, and the start of pressure rise and heat release have been shifted. Soot formation history (Figure 21) for the two cases show that the peak soot formed is lower in case 1, but the oxidation is also less, compared to baseline. This is probably due to the lower cylinder temperatures prevailing during the combustion as less heat release is happening during the initial stages of combustion. In case 2, however, the peak soot formed is slightly higher than baseline, but the oxidation rates are also higher, which is probably due to the higher temperatures in the later stages of combustion after 30 CAD. Peak temperature is also lower than that of iteration 1 in both cases and occurs at one to two CAD later than that of iteration 1, as shown in Figure 22. The entire heat release rate curve is offset, thereby increasing the burn rate in the later phase. This is evident from the cumulative heat release curve (Figure 23) as well. In both the cases, the cumulative heat release is lower than baseline till around 25 CAD, after which it is almost equal to baseline in case 1, and slightly higher in case 2. This higher heat release in case 2 after around 30 CAD has resulted in higher average cylinder temperature compared to baseline, after around 30 CAD.
3.3. **Iteration 3 – Modified piston bowl geometry with retarded main injection (90% of total fuel mass) along with pilot injection (10% of total fuel mass):**

Iteration 2 is extended by introducing the pilot injection, i.e. pilot injection with retarded main injection. Injection pressure and total fuel quantities are kept same, hence the durations are taken as...
10% and 90% of the original duration for pilot and main injections, respectively. It has been an established fact that a small quantity of pilot injection helps in reducing the amount of premixed combustion that will happen, by reducing the ignition delay period of the main injection. Reduction of premixed combustion helps in reducing NOx, with an associated increase in soot emission. In-cylinder pressure trace and heat release rate trace are plotted for this iteration for both operating points. Figures 24 and 25 show how these parameters compare with the iteration 2 curves.

**Figure 24.** Case 1 iteration 3 simulation compared with iteration 2 simulation in-cylinder pressure and heat release rate.

**Figure 25.** Case 2 iteration 3 simulation compared with iteration 2 simulation in-cylinder pressure and heat release rate.

Figures 26 shows the comparison of gross IMEP, NOx and soot between iteration 2 and iteration 3.
From the pressure and heat release rate traces, it is clear that the ignition delay for the main injection has been reduced, as the combustion process due to pilot injection had already begun and was almost completing by the time main injection happens. The main injection fuel is injected into hotter gas and the evaporation is also faster, reducing the ignition delay. Thus, the combustion due to main injection also happens much slower, as can be seen from the gradual rise of pressure and lower heat release rates. Gross IMEP has also increased for both cases. Peak pressure is slightly higher and happens around 1 CAD earlier for the higher load case. NOx has decreased for the lower load case, as expected, while it has increased for the higher load case, which is surprising. This could be because the injection timing of both pilot and main are not optimised for the operating point, and once an optimum timing could be established, it would be possible to observe reduction of NOx in line with previous results. Previous studies [28] had established that there exists an optimum spacing between pilot injection and main injection, as well as an optimum quantity split for the split injection strategy. Their study noted that as the SOI of pilot injection is advanced, initially the NOx increases and then decreases. So, by advancing the pilot injection in case 2, one could expect that NOx will come down. With this not so optimum injection timing, the pilot injection combustion products get compressed further to higher temperatures and with the main injection starting, there are local pockets conducive to NOx formation, resulting in higher NOx than expected. Soot formation history is in line with the expectation of higher soot formation due to more diffusion combustion, as main injection fuel is being injected onto the hot gases from pilot injection, giving little time for mixing. However, higher oxidation is observed in the higher load case. Soot oxidation is promoted by the presence of oxygen at high temperature, with temperature playing the more dominant role. Higher NOx in case 2 is a clear indicator of higher local temperatures. Case 2 also has higher average cylinder temperatures till around 50 CAD, where soot oxidation is also almost frozen. This higher temperature has resulted in higher oxidation of soot in case 2.

3.4. Iteration 4 – Modified piston bowl geometry with retarded main injection (90% of total fuel mass) along with pilot injection (10% of total fuel mass) and EGR

Iteration 3 is extended by adding the EGR. In addition to 10% pilot injection and 1.1° retardation of the main injection timing with respect to the baseline case, a total of 15% EGR (7% residuals as internal EGR and an additional 8% external EGR) is considered. Total trapped mass is kept same as the baseline case. In-cylinder pressure trace and heat release rate trace are plotted for this iteration for both operating points. Figures 27 and 28 show how these parameters compare with the baseline curves.
Figure 27. Case 1 iteration 4 simulation compared with baseline simulation in-cylinder pressure and heat release rate.

Figure 28. Case 2 iteration 4 simulation compared with baseline simulation in-cylinder pressure and heat release rate.

Figures 29 shows the comparison of gross IMEP, NOx and soot between baseline and iteration 4.

Figure 29. Comparison of gross IMEP, NOx and soot between baseline and iteration 4.

Compared to the baseline simulation, the changes done in iteration 4 has resulted in a marginally lower gross IMEP at both operating points. NOx is significantly lower, while soot is more in both
cases. The effect of EGR is quite evident in lowering the overall temperature and oxygen availability. Both these things have resulted in lower peak cylinder pressures and lower peak of heat release rates. Start of combustion is earlier than baseline due to pilot injection, allowing for an overall slower combustion, as can be seen from the slow rate of change of pressure and heat release from the pressure and heat release rate curves, respectively. Soot formation history shows higher soot formed in both cases, with less oxidation in iteration 4. Lack of oxygen and pilot injection has resulted in higher local equivalence ratios and has resulted in higher soot formation in both cases. The lack of oxygen and overall lower temperatures inside the cylinder has resulted in slower rates of oxidation.

4. Conclusion
Summarised below are the important conclusions from the study, where each change is being discussed one by one:

1. New geometry
   a. Wider, shallower re-entrant bowl has resulted in higher NOx in both operating points, and lower soot in the higher load case
   b. The new geometry did not have a significant effect on the lower load case in terms of changing the mixing levels, which has resulted in relatively less change of NOx and soot with respect to the baseline case

2. New geometry with retarded SOI of main injection
   a. Retarding main injection timing has resulted in reduction of NOx in both cases
   b. Engine out soot has increased in the lower load case, while it decreased in the higher load case. Peak soot formed has in fact increased in the higher load case, but final soot is less as higher oxidation is seen in the higher load case, attributed to higher heat release in later combustion resulting higher temperature, promoting more soot oxidation

3. New geometry, retarded SOI of main injection with pilot injection
   a. Pilot injection has reduced NOx and increased soot in the low load case
   b. It increased NOx and reduced soot in the high load case
   c. There is immense scope in optimizing the timing and quantity of both pilot and main injection, to achieve lower NOx in both cases

4. New geometry, retarded main injection, pilot injection with EGR
   a. Addition of EGR has significantly reduced NOx and increased soot in both cases, in line with previous studies
   b. 15% EGR could be more than necessary, especially for the higher load case and there is scope to optimise the EGR quantity

The effect of each change on gross IMEP is not quite high, seen varying within ± 2%, which cannot be considered significant. It is to be noted that the changes done in both operating points are the same, meaning the same percentage of pilot injection, the same amount of retardation and the same amount of EGR has been applied across the operating points. Also, the baseline injection timings are also far from optimum, and were selected from purely a comparison perspective, and not from an optimisation perspective. Further optimization potential is available, by varying the parameters independently based on operating point. For example, EGR could be reduced for the higher load case, thereby increasing the IMEP, without compromising much on NOx. This should result in lower soot as well, as a higher oxidation rate would be expected with lesser EGR. Similarly, there is immense scope to tune both operating points to the best performing state with the lowest emission levels, in terms of pilot injection and main injection timing and pilot injection quantity. Another parameter which has been kept constant in these simulations is the fuel injection pressure. With improved fuel injection hardware, higher injection pressures can be achieved which would result in lower soot at all operating points.
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