Premixed Charge Compression Ignition in a Direct Injection Diesel Engine using Computational Fluid Dynamics

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ABSTRACT

In this research work, numerical studies are carried out for different injection timings to arrive at premixed charge compression ignition in a direct injection Diesel engine. Various models and submodels accounting for turbulence, combustion and emission formation, droplet spray, wall impingement and collision are considered. The flame propagation phase is modeled by solving the transport equation for flame surface density equation in extended coherent flame model for 3 zones. A sector model of the engine cylinder is taken to avoid expensive computational resources. Standard k-ε model is used for modeling the turbulent flow in the cylinder. The species equation is discretised by monotone advection and reconstruction schemes. PISO algorithm is employed for solving the Navier-Stokes equations. The CFD code is validated against experimental data and further investigations are performed on various injection timings from 6 deg before TDC to 30 deg before TDC. From the studies, it is found that oxides of nitrogen increases and soot decreases as injection is advanced.

Key-words : 4-stroke constant speed diesel engine, Direct injection, Premixed Charge Compression Ignition (PCCI), Computational Fluid Dynamics (CFD), Extended Coherent Flame Model, Combustion, Emissions

1 INTRODUCTION

Premixed charge compression ignition (PCCI) combustion for diesel engines is receiving increasing attentions in recent years, because it is capable of providing both high efficiency and extremely low particulate emissions. Unlike conventional diesel combustion, PCCI combustion mode uses early in-cylinder fuel injection to avoid soot emissions . However, due to the low volatility and high ignitability of diesel fuel, several technical barriers, such as mixture preparation and control of combustion phasing, must be overcome before the commercialization of diesel PCCI engine [1].

In the PCCI combustion strategy, fuel can be introduced into the combustion chamber through port fuel injection, early direct injection, or late direct injection. Port fuel injection and early direct injection often suffer from incomplete fuel vaporization and fuel spray impingement on the cylinder walls, which causes high levels of hydrocarbon and carbon monoxide emissions as well as fuel/oil dilution [2]. Strategies to reduce fuel-wall impingement explored in the past include the use of narrow spray cone angle injectors. Late direct injection avoids fuel-wall impingement and provides good control over combustion phasing. Lechner et al. [3] evaluated the potential of using the injector nozzle with narrow spray cone angle for diesel PCCI combustion by varying the spray cone angle and advanced injection timing. It is found that carbon monoxide (CO) emission rises dramatically and combustion efficiency drops significantly as the fuel starts to miss the bowl. The Mie-scattering technique was used to investigate in-cylinder combustion and spray evolution processes by Fang et al. in a diesel PCCI engine with a 70-degree spray angle injector [4].

In PCCI combustion mode, since the fuel is injected well before top dead center (TDC), obtaining good mixing in the available time and preventing wall-wetting due to spray over-penetration can be challenging. A large number of injection strategies have been proposed for diesel PCCI combustion in recent years. The concept of narrow angle direct-injection (NADI) was suggested by Walter [5] and Gatellier [6] to keep the fuel target within the combustion bowl and avoid the interaction between the spray the cylinder liner at advanced injection timing. The results indicate that liquid fuel impingement on the bowl wall leads to fuel film combustion which is called “pool fire”. Because of rich air–fuel mixture and low temperature on the wall surface, the pool fire results in incomplete combustion and high soot formation for all early injection cases. Siewert [7] studied the effects of varying nozzle spray angle and rail pressure on emissions and thermal efficiency in a diesel PCCI engine with early injection timing. It is indicated that the amount of liquid spray that misses the piston bowl is directly linked to the increases in measured hydrocarbon (HC), CO and smoke emissions and reduction in thermal efficiency. It should be noted that injection timing does not provide an effective means of controlling ignition timing as in the conventional diesel engine, so that controlling the combustion phasing is still a critical issue for PCCI engine.

Nevin et al. [8] incorporated a hydraulically actuated variable IVC system into a single cylinder diesel engine to explore the potential of intake valve actuation on heavy-duty diesel engine. It is shown that late IVC results in a carbon mono-oxide and particulate emissions that could be dramatically reduced by nearly 70%. As one of the most promising strategies for controlling diesel PCCI combustion, variable valve actuation attracts increasing attentions recently because of its fast response time. By using late intake valve closing, the effective compression ratio is decreased and advanced combustion can be avoided, thus it is helpful for the increase of thermal efficiency. A more detailed study based on equivalence ratio - temperature map and three-dimensional computational fluid dynamics model was conducted by Murata et al. [9]. They found that the use of late IVC reduces soot emissions while maintaining the lower fuel consumption and performance, since local over-rich regions is avoided during the combustion processes. Genzale et al. [10] used a multi-dimensional computational fluid dynamics (CFD) model to explore the effectiveness of late IVC in controlling diesel PCCI combustion phasing over various loads, engine speeds and boost pressures.

Simulation of combustion and emission requires improved computational techniques and efficient solver for influencing the application of computational fluid dynamic methods to reciprocating engine models. For the simulation study of the current work, the geometry of the engine is chosen from Payri et. al [11] and Jayashankara et. al [12]. These methods require movable domain boundaries and compressible/expandable meshes. The sub-models affecting physical processes such as fuel injection, spray formation, evaporation, mixing, ignition, combustion and pollutant formation need to be considered seriously. To accomplish all these challenges, a versatile computational fluid dynamics (CFD) package named as expert system on internal combustion engines (ES-ICE [13]) is used here for rapid in-cylinder diesel engine modeling. The Extended Coherent Flame Model (ECFM-3 zones) is developed to simulate combustion in premixed and diffusion modes. The ECFM model is based on a flame surface density equation which takes into account the wrinkling of the flame front surface by turbulent eddies and a conditioning averaging technique that allows precise reconstruction of local properties in fresh and burned gases even in the case of high levels of local fuel stratification. It is represented by three mixing zones (3Z): a pure fuel zone, a pure air plus possible residual gases zone and a mixed zone. A mixing model is presented to allow progressive mixing of the initially unmixed fuel and air. The ECFM-3Z combustion model has been validated in a comparative work between diesel engine experiments [14, 15]. The aim of the preset work is to study the combustion and emission characteristics in a DI diesel engine by advancing the injection timing in the engine cylinder using flame surface density equation in ECFM-3Z model. Comparison between the experimental data and CFD result is validated first and further studies are carried out to understand the combustion phenomena. The simulation is performed using ES-ICE & STAR-CD packages.

2 METHODOLOGY

2.1 NUMERICAL DETAILS

ES-ICE, a CFD software specially developed for in-cylinder simulations, is used in the present study to simulate the incylinder processes. It uses a cartesian coordinate system and a finite volume-based implicit discretization procedure. Unstructured meshing is utilized to mesh the complex intake manifold and cylinder geometry while taking valve motion into account. The PISO algorithm is used for pressure velocity coupling in the solution of the flow field. The two equation standard k–ε model has been implemented for estimating turbulence in terms of Turbulence Kinetic Energy (TKE). Spray break-up has been modeled by the Reitz-Diwakar break-up model. In this model, an infinitesimal axisymmetric surface displacement is imposed on the initially steady moving liquid surface which causes small axisymmetric fluctuations. It is assumed that drops are formed with a drop size proportional to the wavelength of fastest growing or most probable unstable surface wave. The maximum growth rate and its corresponding wavelength are related to pertinent properties of liquid and gas. The initial conditions required by the droplet model are calculated using the cylinder pressure, injection mass flow rate. The extended coherent flame model in three zones (ECFM-3Z) is used to simulate the auto-ignition of diesel fuel. This model assumes that the chemical reactions usually have time scales that are very short compared to the characteristic times of the turbulent transport processes. Thus, the rate of combustion is determined by the rate of intermixing on a molecular scale of eddies containing reactants and hot products. The Zeldovich mechanism which is based on equilibrium assumptions has been used for predictions of NOX. Soot emission is predicted using Mauss model.

2.2 PROBLEM FORMULATION

Re-entrant piston bowl is obtained by trimming the 30 degree 3-D sector geometry. Radial, axial and piston top cells are selected appropriately and sector mesh is shown in Fig.1 for both TDC and BDC. Table 1. shows the engine in-cylinder data and fuel injection details. Initial and boundary conditions are set up in ES-ICE tool and the computations are carried out by STAR-CD solver. The time accurate computations are performed in a Intel Xeon CPU (3.30 GHz, 3.24 GB RAM). The total elapsed CPU time is nearly 20 hours for a total of 4400 timesteps which leads to total time period of 20 milliseconds of 120^o engine crank angle (from 680^{o}CA to 800 ^{o}CA). Fuel injection starts as 714^o CA and stops at 722^o CA. Auto-ignition in the cells takes place nearly at 719 ^{o} CA corresponding to time-step around 1200.

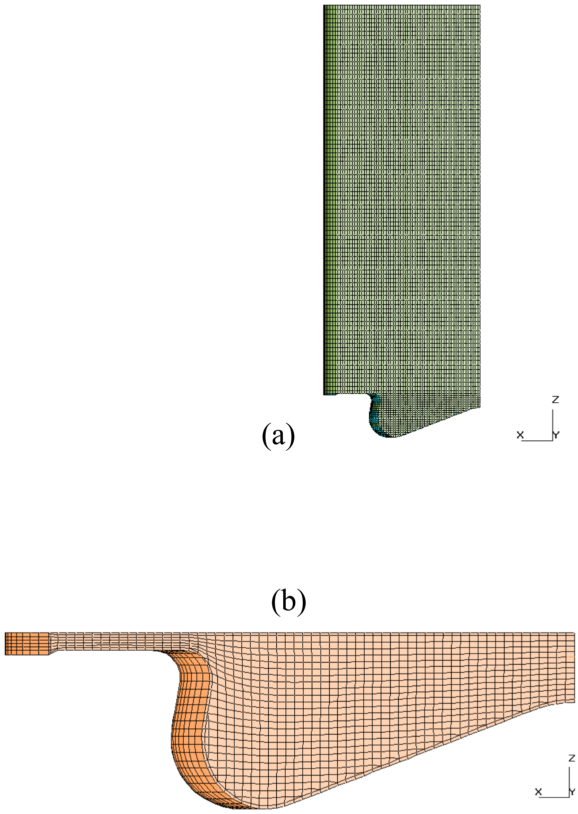
STAR-CD (Simulation of Turbulent flow in Arbitrary Regions – Computational Dynamics) has been used to solve the discretized Navier–Stokes equations. The standard k–ε model with standard wall function has been employed for physical modeling. The program is based on the pressure-correction method and uses the algorithm formulated for Pressure Implicit Splitting of Operators (PISO). The first order upwind differencing (UD) scheme is used for the spatial discretisation of momentum, energy and turbulence equations with implicit temporal discretization. ECFM-3Z combustion model is used to characterize ignition and combustion. The Reitz–Diwaker model is used to characterize droplet break-up, with rebound boundary condition at the walls. Monotone Advection and Reconstruction Scheme (MARS) is used to discretise species scalars. NOx emission is modelled by using extended Zeldovich mechanism. The soot emission model written in the Arrhenius single step form which considers the rate of change of soot mass is used to model soot emissions. The initial values of pressure and temperature are considered as homogeneous in the whole domain. The initial turbulent intensity is set at 10 % of the mean flow, and the integral length scale is set at 0.1 m. Temperatures at the cylinder head, the cylinder wall and the piston bowl that form the walls of the combustion chamber are specified as given in Table 2. Fuel injection is accomplished using lagrangian multiphase droplets. Vertex data is used for interpolation method and under-relaxation factor of lagrangian sources is set at 0.5. The droplet trajectory maximum file size is kept at 400 Mb, where maximum number of parcels are 500000. Turbulent dispersion, collision model and gravity effects for the droplets are taken into account. For droplet breakup, Reitz model is considered and to account for droplet wall interaction, Bai spray impingement model is accounted. Wall heat transfer, thermal break-up and boiling effects are also considered when the droplets encounters the hot environment. $C_{14}H_{30}$ (N-Tetradecane) is selected as fuel from the National institute of standards and technology (NIST) table since it incorporates correct liquid fuel density. Huh atomization model is used. The injector nozzle L/D is chosen to be 6 and its coefficient of discharge is 0.7. Injection temperature is set at 310 K. The injector hole diameter is 0.4 mm and a separate lookup table is given to specify the injection timings with fuel injection quantity.

Table 1: Engine Specifications

Bore, Stroke	130 mm, 150 mm
Connecting Rod Length	275 mm
Compression Ratio	15.5
Engine Speed (N)	2000 RPM
Crank Angle Start	680 deg
Crank Angle Stop	800 deg
Fuel	n-Dodecane
Fuel injection quantity	207 mg/cycle
Fuel Injection Duration	8 deg
Start of Fuel Injection	6 deg bTDC to 30 deg bTDC

Table 2: Initialization and Boundary conditions

Cetane number	50
Swirl Ratio	4.1
Turbulence intensity	10 %
Equivalence ratio	0.8
Exhaust Gas Recirculation (EGR)	10 %
Combustion dome temperature	450 K
Piston crown temperature	450 K
Cylinder wall temperature	400 K
Pressure @ 680 ^{o}CA	9.5 bar
Temperature @ 680 ^{o}CA	550 K



(a)

(b)

Figure 1: Computational domain of engine cylinder at (a) 720 ^{o}CA and (b) 800 ^{o}CA

3 VALIDATION

Fig. 2 shows the comparison of simulated and experimental [14] in cylinder pressures and heat release rate for the direct injection diesel engine. The computed in-cylinder pressure and heat release rates are in good agreement with the measured data. In particular, the simulation data matches exactly the time of auto-ignition and the peak pressures from this study with the experimental data. This very good agreement in peak pressure is achieved by time step independent tests (Fig. 3) and computational grid independency tests (Fig. 4). Crank angle step interval of 0.025^{o}CA (i.e. 2.0835 x 10^{-6} seconds) and mesh with 45000 cells at TDC position are selected as suitable values for further studies. Table 3. shows the data of the engine [15] to be validated with the CFD packages in this work.

Table 3: Engine Specifications for the validation study

Bore	0.085 m
Stroke	0.088 m
Compression ratio	18
Connecting rod length	0.0145 m
Injector hole diameter	148×10^{-6} m
Spray Angle	152 deg
Speed	1640 rpm
Start of injection (deg bTDC)	6
Injection duration (deg)	8.03
Injected mass (g)	0.0144
F/A equivalence ratio	0.67
EGR rate (%)	31
Swirl ratio	2.8

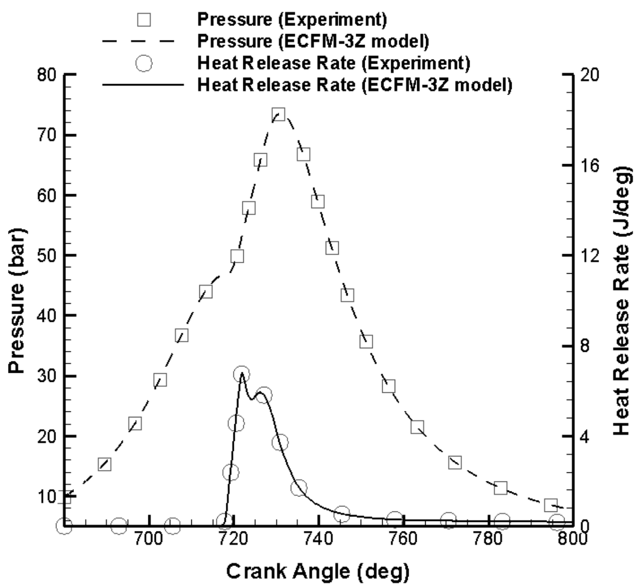


Figure 2: Validation of pressure and heat release rates [17]

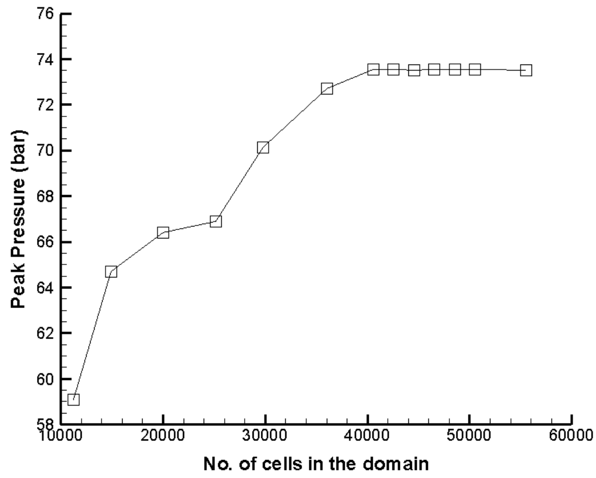


Figure 3: Grid independent study

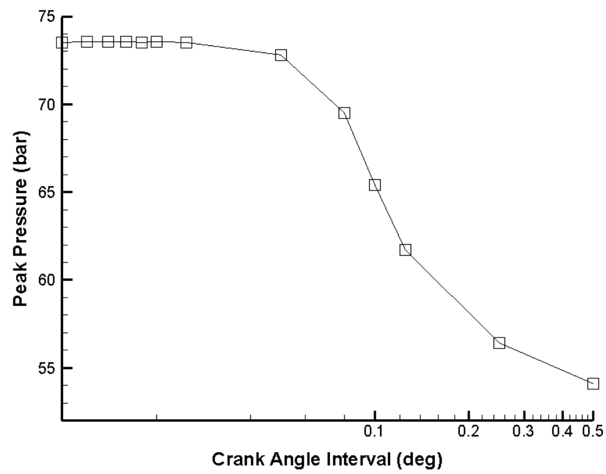


Figure 4: Time independent study

4 RESULTS AND DISCUSSIONS

Once the boundary and initial conditions in the solver are supplied, the time accurate computations are allowed until the residual reaches below the specified values. The convergence values for the residue momentum (for all the three coordinates) and temperature, pressure, turbulence kinetic energy and turbulence dissipation are set as 1×10^{-3}, 1×10^{-4}

as $1x10^{-3}$ respectively. The monitor output frequency is set after every 5 timesteps and the backup frequency for writing all combustion and emission data in a file occurs after every 400 timesteps. Fig. 5 shows the residual history of mass, momentum, enthalpy and turbulent kinetic energy. Fig. 6 shows the spray in a mexican hat piston bowl at TDC 720°CA from top of the combustion chamber towards the bowl. The sequence of injection is advanced to obtain 13 deg bTDC, 20 deg bTDC and 30 deg bTDC. The residual values and the corresponding information of incylinder data is separately written into the history file for understanding about the details regarding the fuel parcels undergoing collision, evaporation, boiling and mixing with the air. The place of autoignition is also recorded for every timestep, thus understanding the incylinder details clearly with the ES-ICE & STAR-CD CFD packages.

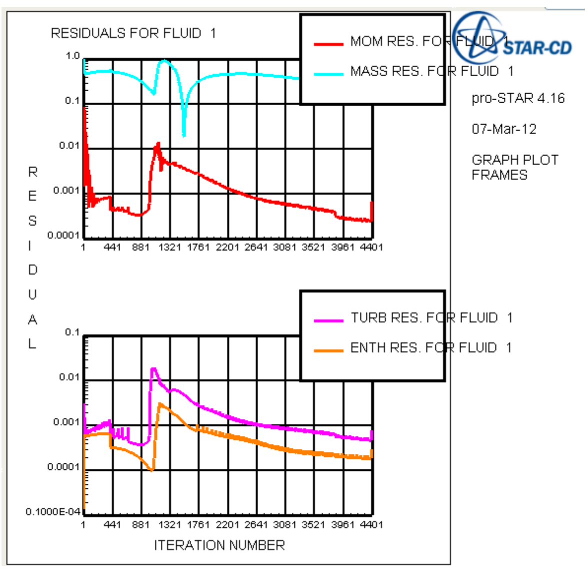


Figure 5: Residual history

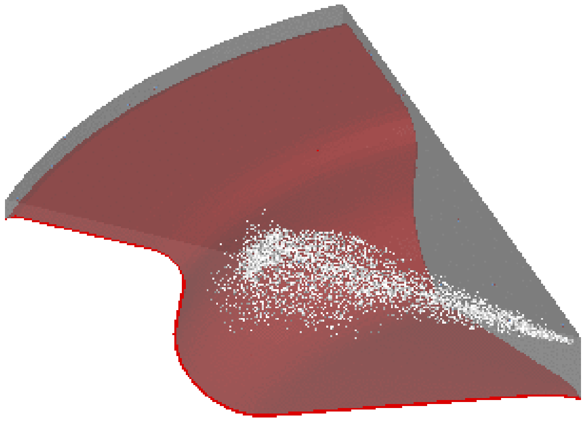


Figure 6: Fuel spray at TDC (720 deg CA)

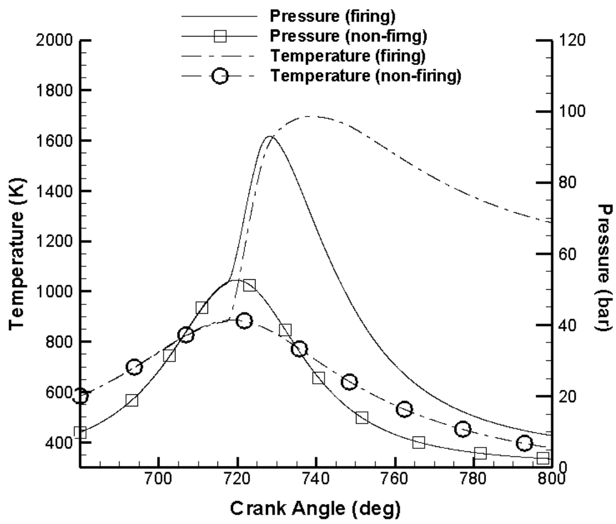


Figure 7: Cylinder averaged pressure, temperature

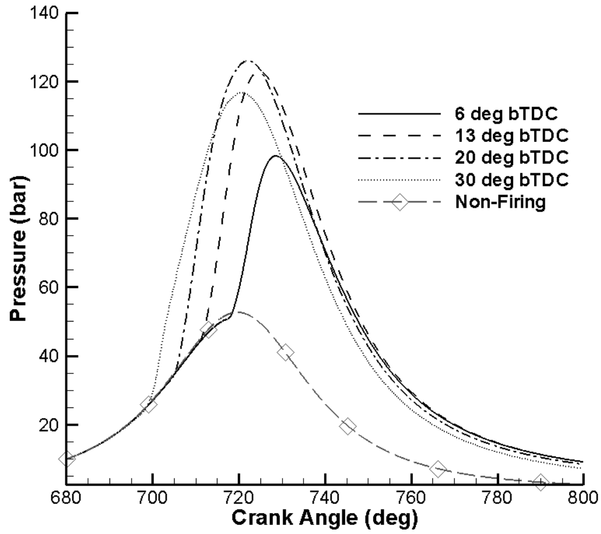


Figure 8: Cylinder averaged pressure for firing and non-firing conditions at different start of injection

Fig.7 shows the in-cylinder pressure, temperature with non-firing or motoring conditions at 6 deg bTDC whereas the Fig. 8 shows the cylinder averaged pressure data at different injection timings.. As injection timing is advanced, in-cylinder pressure is increased till the start of injection SOI =.20 deg bTDC, thereafter it decreases. Advancing the injection timing increases the ignition delay as the fuel is injected in a less favorable air environment. This results in a higher percentage of fuel burned in premixed combustion, producing higher peak cylinder pressures and temperatures. In contrast, retarding injection has, in general, the opposite effects with the lower level of pressures and temperatures reducing the amount of NOx emissions but adversely affecting engine startability, smoke emissions and power output. Deviation from the optimum timing in either direction affects negatively engine efficiency. The choice of the optimum injection timing as a function of engine speed and load. The optimum injection timing from the CFD study is 20 deg bTDC.

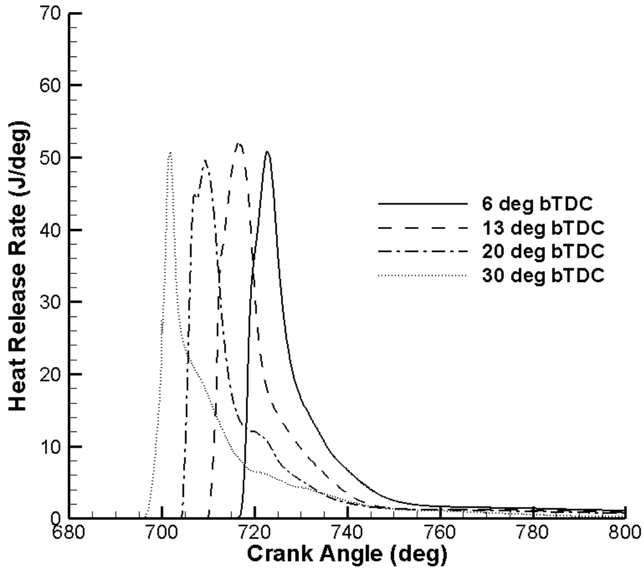


Figure 9: Cylinder averaged heat release rate at different injection timing

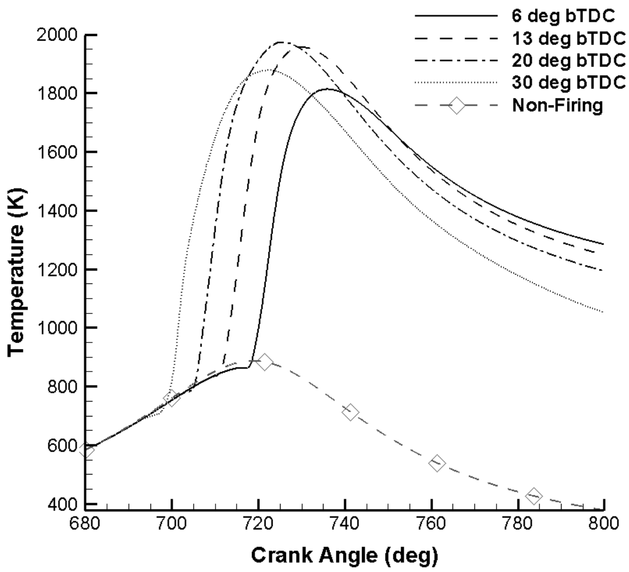


Figure 10: Cylinder averaged temperature for various start of injection

The heat release rates and in-cylinder averaged temperature are shown in figures 9 and 10 respectively. The temperature increases till 20 deg bTDC thereafter decreases. Fig. 13 show the contours of in-cylinder temperature at TDC. For retarded conditions, a single heat release peak is observed, indicating that premixed combustion dominated the combustion process with a slight diffusion-controlled portion. With the moderately advanced injection timing, a two-stage heat release pattern was observed: the first stage was associated with low temperature reactions, and the second stage was associated with high-temperature reactions. Figures 11 and 15 show the reaction variable for different injection timings. When fuel evaporates into burnt gases (i.e. the progress variable becomes 1) or when there is insufficient oxygen to even burn the existing fuel partially into CO, an additional fuel species is created. However, the fuel wil not burn in premix mode but behind the flame (diffusion-mode combustion).

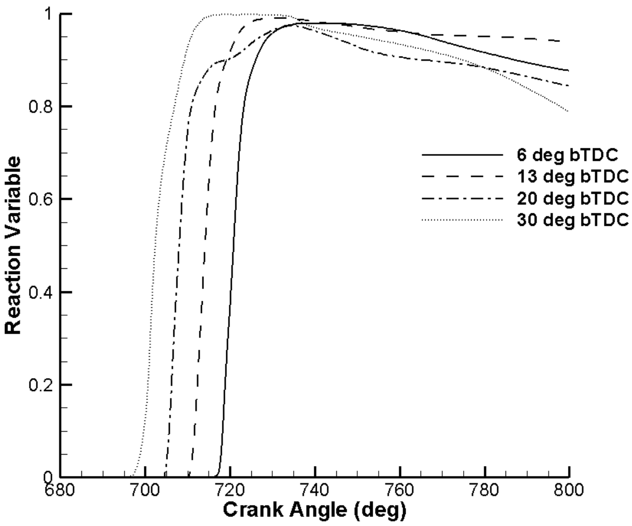


Figure 11: Reaction variable for different injection timing

Fig. 12 show the variation of flame surface density increasing with the advance of injection timing. This is evident from the contours of flame surface density from Fig. 14. The reactions start when the fuel is injected as early inside the cylinder thereby increasing the flame surface density. Flame area is higher at advanced injection timing since the progress reaction variable (Fig. 11) indicates that reactions are nearly complete at an injection timing of 30 deg bTDC. This leads to the increase in flame surface density for early injection towards premixed charge compression ignition.

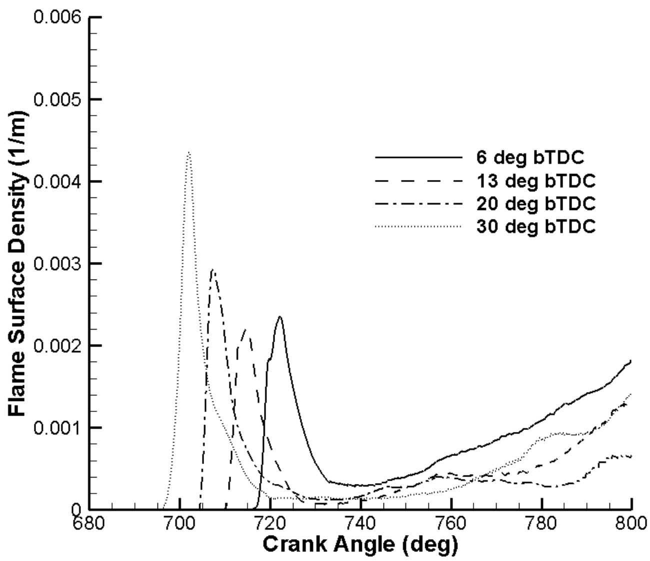


Figure 12: Flame surface density at different injection timings

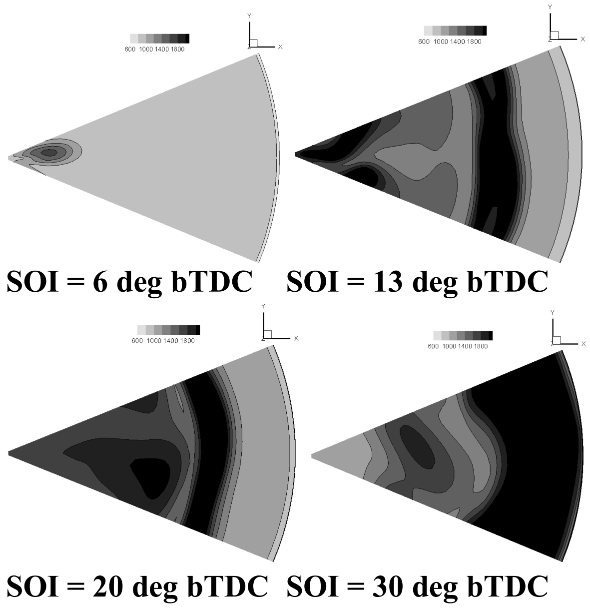


Figure 13: Contours of temperature (K) for different injection timing

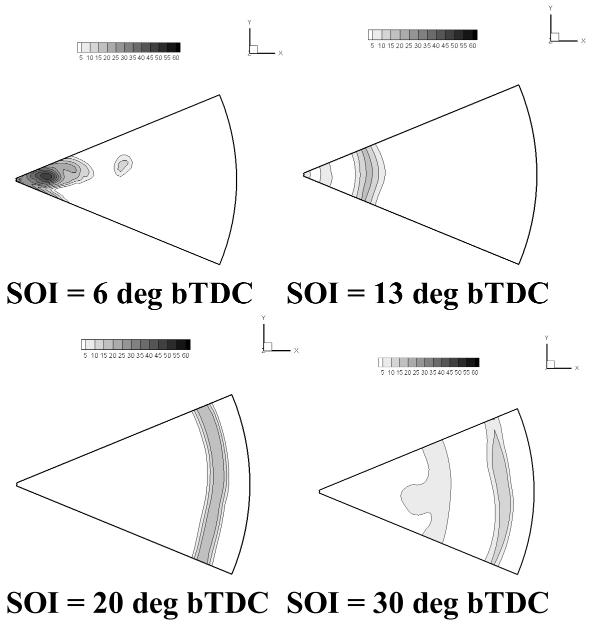


Figure 14: Contours of flame surface density (1/m) for different injection timing

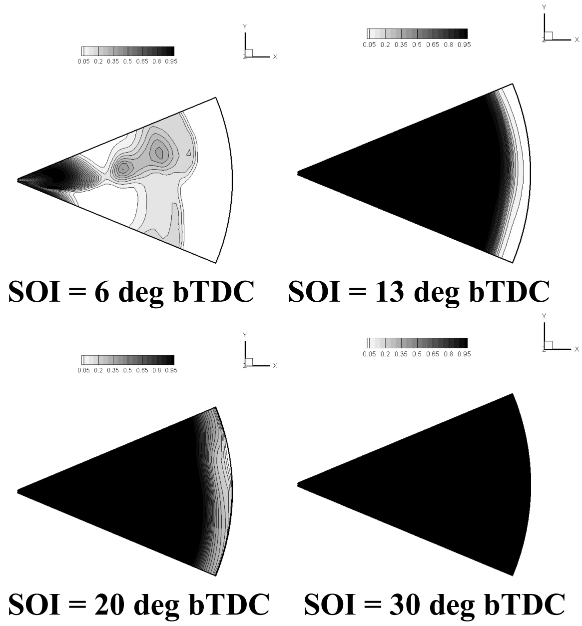


Figure 15: Contours of progress reaction variable for different injection timing

Fig. 16 show the soot decreasing with the advancement of injection timing. As the injection timing is advanced, fuel penetration is enhanced, leading to fuel impingement on the surface of the piston, providing a source of fuel-rich zones that burned with soot. The soot of conventional diesel combustion are lower than those in the PCCI regime. PCCI combustion is not meant to completely eliminate soot emissions but rather reduce them to acceptable levels. A retarded injection timing has a lower maximum in-cylinder temperature, while advancing the injection timing led to a gradual rise in the in-cylinder temperature until 20 deg bTDC, which drastically reduces in-cylinder temperature for PCCI combustion at 30 deg bTDC. This is due to the reason that NOx increases with advanced injection timing (Fig. 17). Figures 18 and 19 show the distribution of soot and NOx in the cylinder at TDC. Table 4. lists the cylinder variables at peak condition for different injection timing. The incylinder pressure and temperature increases till SOI=20 deg bTDC and then decreases. This is due to the dilution of the mixture in the combustion chamber by burnt products of combustion. It is found that ignition delay increases with the advancement of injection timing (Table 5). Soot and NOx emissions are shown in Figures 16,17 and the corresponding contours are shown in Fig. 18 and Fig. 19.

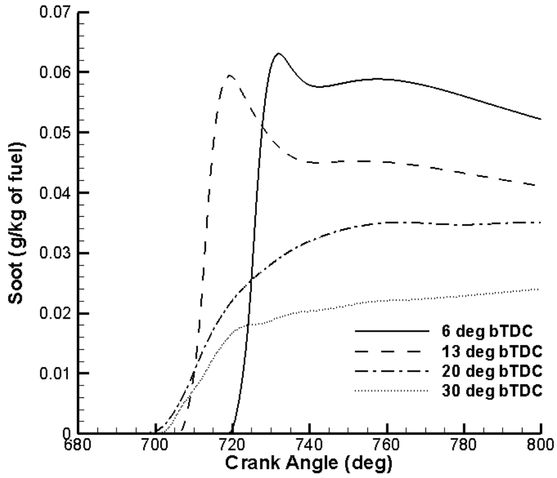


Figure 16: Soot distribution at different injection timing

Table 4: Variation of peak quantities with start of injection

SOI (bTDC)	Peak Pressure (bar)	Peak Temperature (K)
6	98.2	1810.5
13	122.7	1955.7
20	125.8	1971.9
30	116.4	1877.5

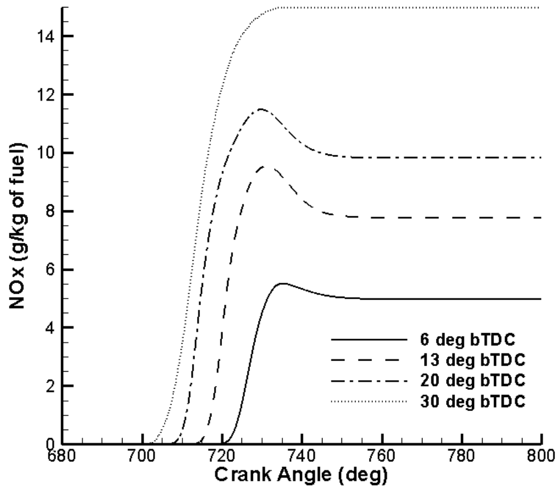


Figure 17: Nitrogen oxides at different injection timing

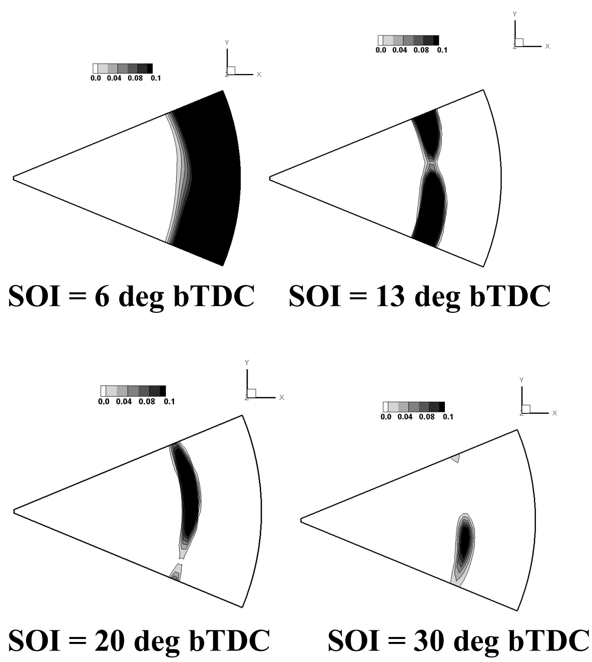


Figure 18: Contours of soot emissions (g/ kg of fuel) for different injection timing at TDC

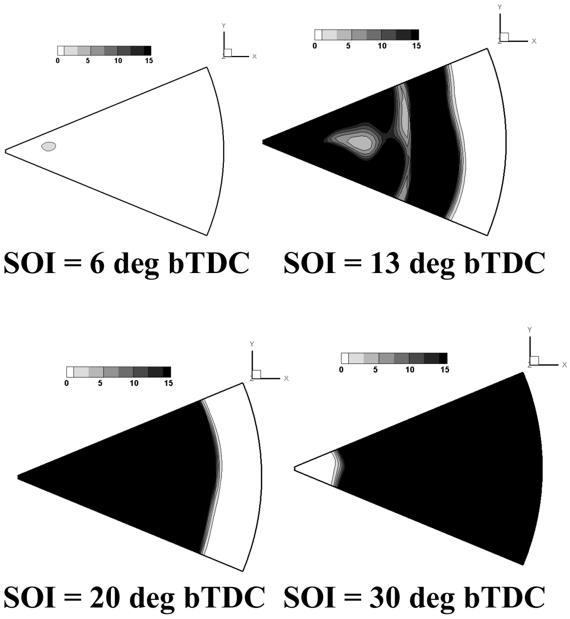


Figure 19: Contours of NOx emissions (g/ kg of fuel) for different injection timing

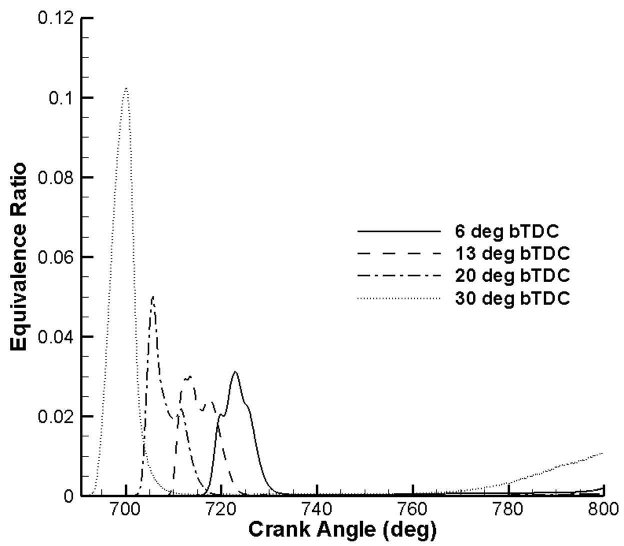


Figure 20: Variation of equivalence ratio in the pioston bowl at different Crank Angle

Equivalence ratio increases and decreases after the injection as shown in Fig. 20. This is due to the incylinder combustion happening after the fuel spray penetrates into bowl and evaporates. Once the fuel is burnt with the surrounding air, the equivalence ratio drops.

Table 5: Variation of ignition delay with start of injection

SOI (bTDC)	Ignition Delay (deg)
6	4.0
13	4.7
20	5.6
30	9.5

5 CONCLUSIONS

In the present work, ECFM-3Z model is used to model the combustion and emission in direct injection diesel engine. CFD and experimental results are in close match together. By advancing the injection timing from 6 deg bTDC to 20 deg bTDC, it is found that

- The peak in-cylinder pressure rises by 21.9 %.
- The peak in-cylinder rises by 8.2 %.
- The ignition delay increases by 1.6 degrees.

From the study of PCCI combustion, the soot levels fall down by 66.7 % and NOx increases nearly twice the levels when the injection angle varies from 6 deg bTDC to 30 deg bTDC. It is recommended to admit EGR of nearly 40 % to control NOx emissions for SOI=30 deg bTDC case.

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