CHAPTER 7

NUMERICAL SIMULATION OF COMBUSTION FOR VARIOUS BOWL GEOMETRIES

In this work, numerical investigations of flow and combustion in a direct injection (DI) diesel engine with different combustion chamber geometries have been carried out to optimize the combustion chamber design for experimental investigation. The modelling methodology, software and tools adopted are explained in this chapter. A three dimensional finite volume model of the baseline engine with standard piston-SP (Hemispherical Combustion Chamber) was created and validated against experimental data. The reacting flow simulation provided reasonably good agreement with experimental data. Further simulations are conducted for the reacting flow with modified pistons of MP1 (toroidal combustion chamber), MP2 (Swirl blade combustion chamber), and MP3 (shallow depth combustion chamber). The dimensions of the pistons are chosen so as to maintain the same piston bowl volume. The fuel injection quantity was maintained the same for all the piston geometries and it is chosen so as to represent the full load consumption.

7.1 INTRODUCTION

For a better performance of DI diesel engine the injected fuel has to evaporate, mix and distribute within the combustion chamber uniformly. This can be achieved by two methods: a) by employing a high pressure injector, b) by modification of the combustion chamber geometry with various bowl geometries to increase the swirl and hence turbulence. The first option requires additional electronics and additional parasitic losses. Moreover the mounting problems with the existing low speed mechanical injection system require extensive modification in the fuel circuit. Hence
a better option would be to enhance the turbulence by means of piston modification to generate better squish and swirl. Air motion inside the engine cylinder plays an important role, and they have a significant impact on the combustion quality [52]. Many researchers have investigated the effects of bowl geometry on the combustion. But the minute sub-physical processes like turbulence; fuel droplets penetration inside the combustion chamber and the evaporation of fuel can be best understood either by expensive non-intrusive methods like LDV or PIV. The computational fluid dynamic tool offers a clear theoretical understanding about the exact methods of emission formation and its mitigation. With the introduction of high pressure injection system the combustion efficiency has increased due to better mixing of fuel and air. With the introduction of modified piston like toroidal, re-entrant there is a possibility of impinging on the walls. Some researchers have suggested impinging sprays as giving improved results [53]. The turbulence levels can be changed by the bowl diffusivity. Some previous studies use multi zone [54] models to predict the spray-swirl interaction.

7.2 MATHEMATICAL MODEL DESCRIPTION

For the present investigation a commercially available CFD code STAR-CD is used, which is capable of solving complex three dimensional flows that also includes the effect of turbulent shear, wall effects, heat transfer and turbulent combustion. The flow and combustion process can be modelled by solving a complete set of Navier-Stokes equation, together with equation of state. The mathematical model incorporates the necessary initial and boundary condition for the initiation of the solution. The equations solved are continuity, momentum, energy and transport equations.
Continuity equation,
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad \text{-------------------------------------} \quad (1)
\]

Where, \(\rho\) is the density, \(\vec{u}\) is the fluid velocity vector.

The three dimensional fluid velocity is given by the vector,
\[
\vec{u} = u(x,z,t)\hat{i} + v(x,z,t)\hat{j} + w(x,z,t)\hat{k} \quad \text{--------} \quad (2)
\]

The momentum equation of the fluid mixture is given by,
\[
\frac{\partial}{\partial \rho} (\rho \vec{u}) + \nabla (\rho \vec{u} \vec{u}) = \frac{1}{a^2} \nabla A_0 + \left( \frac{2}{3} \rho k \right) + \nabla \sigma + \rho g + \vec{f}^s \quad \text{------} \quad (3)
\]

Where \(a\) is the dimensionless quantity characterized the type of flow, \(\rho\) is the fluid pressure, \(A_0\) is the value connected with the model of turbulence (\(A_0 = 1\) for turbulent flows and \(A_0 = 0\) for laminar flows), \(k\) is the turbulent kinetic energy, \(\sigma\) is the viscous stress tensor, \(g\) is the specific body force (assumed constant), \(\vec{f}^s\) is the rate of momentum gain per volume unit due to spray. The turbulent kinetic energy per unit volume is given by,
\[
k = \frac{1}{2} \rho \left( (\dot{v}_x)^2 + (\dot{v}_y)^2 + (\dot{v}_z)^2 \right) \quad \text{----------} \quad (4)
\]

Where \(V_x, V_y\) and \(V_z\) are the velocity fluctuations in \(x, y\) and \(z\) directions. \(P\) is the density of fluid.

The Newtonian stress tensor is given by,
\[
\sigma^{(i)} = \tau_{xx}^i + \tau_{yx}^j + \tau_{xz}^k \\
\sigma^{(j)} = \tau_{xy}^i + \tau_{yy}^j + \tau_{yz}^k \\
\sigma^{(k)} = \tau_{xz}^i + \tau_{yz}^j + \tau_{zz}^k \quad \text{---------------------} \quad (5)
\]
Here \( \tau_{xx}, \tau_{yy} \) and \( \tau_{zz} \) represent the x, y and z components of stress acting on the surface whose outward normal is oriented in the positive x direction. Thermal enthalpy is calculated by the equations

\[
\frac{\partial \rho h_i}{\partial t} + \frac{\partial}{\partial \alpha x_j} \left( \rho h_i u_j \right) + F_{h_{i,j}} = \frac{\partial p}{\partial t} + u_j \frac{\partial p}{\partial \alpha x_j} + \tau_{ij} \frac{\partial u_j}{\partial \alpha x_j} + S_h - \sum_m H_m S_{c,m}
\]

\[\text{------------------ (6)}\]

Here, \( h_i \) is the thermal enthalpy, defined by \( h_i = \overline{C_p} T - C^\omega_T T_o \) and \( F_{h_{i,j}} \) is the diffusional thermal energy flux in direction \( x_j \). \( S_{c,m} \) is the rate of production or consumption of species due to chemical reaction. Turbulence energy generation and destruction are calculated by the following expressions:

\[
\frac{\partial}{\partial t} \left( \rho \varepsilon \right) + \frac{\partial}{\partial \alpha x_j} \left[ \rho u_j \varepsilon - \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial \varepsilon}{\partial \alpha x_j} \right] = \mu_t (P + P_B) - \rho \varepsilon \left( \frac{2}{3} \left( \frac{\mu_t}{\sigma_k} \right) \frac{\partial u_i}{\partial \alpha x_j} \right) + \mu_t P_{NL}
\]

\[
\frac{\partial}{\partial t} \left( \rho \mu_t \right) + \frac{\partial}{\partial \alpha x_j} \left[ \rho u_j \mu_t - \left( \mu + \frac{\mu_t}{\sigma_e} \right) \frac{\partial \mu_t}{\partial \alpha x_j} \right] = C_{e1} \varepsilon \frac{\partial \varepsilon}{\partial \alpha x_j} \left( \mu_t P - \frac{2}{3} \left( \frac{\mu_t}{\sigma_e} + \rho k \right) \frac{\partial u_i}{\partial \alpha x_j} \right)
\]

\[
C_{e2} \varepsilon \frac{\partial \varepsilon}{\partial \alpha x_j} \mu_t P_B - C_{e3} \rho \varepsilon \left( \frac{2}{k} \frac{\partial u_i}{\partial \alpha x_j} \right) + C_{e4} \rho \varepsilon \left( \frac{2}{k} \frac{\partial u_i}{\partial \alpha x_j} \right) + C_{e1} \frac{\partial \varepsilon}{\partial \alpha x_j} \mu_t P_{NL}
\]

\[\text{------------------ (7)}\]

Where, \( P = S_j \frac{\partial u_i}{\partial \alpha x_j} \) and \( P_B = -\frac{g_{1j}}{\sigma_{h,1}} \frac{1}{\rho \sigma_k} \frac{\partial \rho}{\partial \alpha x_j} \)

\[\text{and} \quad P_{NL} = -\frac{1}{\mu_t} \frac{\partial u_i}{\partial \alpha x_j} \left( \frac{2}{3} \left( \frac{\mu_t}{\sigma_k} \right) \frac{\partial u_i}{\partial \alpha x_j} + \rho k \frac{\partial u_i}{\partial \alpha x_j} \right) \]

Where, \( P_{NL} = 0 \) for linear models and \( \sigma_k \) is the turbulent Prandtl number. The first term on the right hand side of equation 7 represents turbulent energy generation by shear and normal stresses and buoyancy forces, the second viscous dissipation, and the third amplification or attenuation due to compressibility effects. The last term accounts for the non-linear contributions.

\( \sigma_k \) is the turbulent Prandtl number and \( C_1, C_2, C_3 \) and \( C_4 \) are coefficients whose values are 1.44, 1.92, 1.44 and -0.33 respectively. The continuity equation for species I,
\[
\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \vec{u}) = \nabla \cdot \left[ \rho \nabla \left( \frac{\rho_i}{\rho} \right) \right] + \dot{\rho}_i + \dot{\rho}_i \delta_i, \quad \text{--------- (8)}
\]

Where \( \dot{\rho}_i \) is source term due to chemistry, \( \delta_i \) is Dirac delta function. Combustion is modelled by ECFM – 3Z compression model. This model is suitable for non-homogeneous premixed combustion and employs the conditional average technique. This model is capable of simulating the complex mechanisms of turbulent mixing, flame propagation diffusion and pollutant emission that characterize modern internal combustion engines. The '3Z' stands for the zones of mixing, namely the unmixed fuel zone, mixed gases zone and unmixed air plus EGR zone. The three zones are too small to be resolved by the mesh and are therefore modelled as sub-grid quantities. The mixed zone is the result of turbulent + molecular mixing between gases in the other two zones and is where the combustion takes place. The mass fractions of species in the mixed zone can be defined as the fractions conditional averages:

\[
Y_i^m \mid Y_i \mid_{z=m} = \int \ldots \delta(Z(x',t) - Z_m) dV' \quad \text{--------- (9)}
\]

7.3 INITIAL AND BOUNDARY CONDITIONS

Numerical simulations were also conducted on the same engine, for the same engine and piston configurations and validated against the experimental data. Three more piston configurations, MP1, MP2 and MP3 were designed in such a way that the piston bowl volumes of these modified bowls are exactly the same with that of the original engine. This will ensure a similar compression ratio between models. In the design of MP2, a small baffle plate is welded in the piston as shown in the figure 7.1. The swirl inducing blade has six holes of 2.5mm diameter were drilled. This setup
was chosen to investigate, how the distribution of vortices inside the bowl enhances combustion. The four piston configurations are shown below in figure 7.1.

All dimensions are in “mm”

Figure 7.1 Dimensions of four different piston bowl geometry

Due to same clearance, compression ratio is maintained a constant, and the effect of compression ratio change is ruled out between the cases. The geometrical modelling was done in an open source CAD modeller Salome-Mecca and exported to pro-surf for surface preparation. The prepared surface mesh is exported to es-ice for the generation of mesh, mesh movement algorithm and application of combustion models. Pressure boundary conditions were applied at the intake and exhaust boundaries. The computational model was initialized with 5% residual gas. Computations were started at $20^0$ before TDC (340ºCA in star CD) and ended at the
end of power stroke. The turbulence is initialized at 5% of the mean flow at the beginning of computation. Table 7.1 gives the details of fuel injection and input condition for the computational model.

(a) P-θ

(b) Heat Release Rate

Figure 7.2 Comparison of pressure and heat release rate for the hemispherical bowl
Table 7.1 Input conditions for fuel injector

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>N-dodecane</td>
</tr>
<tr>
<td>Fuel injection</td>
<td>23° bTDC</td>
</tr>
<tr>
<td>Injection duration</td>
<td>28°</td>
</tr>
<tr>
<td>Injection pressure</td>
<td>210 bar</td>
</tr>
<tr>
<td>Fuel injection quantity at Full load</td>
<td>31.1 mg/cycle</td>
</tr>
<tr>
<td>Number of injector holes</td>
<td>3</td>
</tr>
<tr>
<td>Hole diameter</td>
<td>0.17 mm</td>
</tr>
</tbody>
</table>

The computational results for the base engine geometry like pressure and heat release rate are validated against experimental data (Hemispherical Combustion Chamber- HCC) was validated against the experimental data like pressure and heat release rate. Figure 7.2 shows the validation of temporal variation of pressure and heat release rate for a cycle. From the plots it can be concluded that the CFD results validates reasonably well with experimental data. The peak pressure predicted by CFD simulation is same as experimental value at 68 bars. But this peak occurs at 8° later. This may be due to the cetane number value specified for actual fuel and simulation.

Based on the confidence obtained through the validation three more bowl geometries with dimensions as shown in figure 7.1 are designed and simulations conducted for the same boundary and initial condition. The sectional view of the bowl and combustion geometry is shown in figure 7.3. The simulations were conducted for a single cycle. The boundary conditions applied were appropriate to the experimental
conditions. The next section shows the results of the computational study conducted with the modified pistons.

![Figure 7.3 Sectional view of the combustion chamber at top dead centre (720 °CA)](image)

7.4 RESULTS AND DISCUSSION

7.4.1 Flow field characteristics

The main purpose of provision of bowl in a piston is to conserve the momentum during the end stages of compression stroke. While the tumbling and swirling vortices are destroyed in a flat piston engine the momentum is conserved in bowl and piston arrangement. Swirl is the predominant air motion prevailing in a DI diesel engine. Depending on the geometrical configurations of the bowl the swirl motion is conserved in the engine. In order to understand the crank angle rotation used, the beginning of induction stroke is specified at 360° and end of compression is specified as 720 °CA. Figure 7.4 compares the swirl values of the four bowl configurations. The swirl motion can be divided into three stages. The first stage is the swirl generation due to the induction process. The swirl increases until the peak valve lift around a crank angle of 480° aTDC (120° during suction). The second stage is the swirl decay period, which starts around 480° aTDC and continues up to approximately
the middle of compression process (670°aTDC). After this period, the swirl is mainly affected by upward moving piston. Due to the movement of air mass into the bowl, called squish motion, the swirl is also enhanced. The swirl enhancement during the final stage of compression ends near TDC and decays rapidly afterwards.

The Z-swirl calculates the swirl ratio about the cylinder axis. Amongst the four bowl configurations MP1 shows a significantly higher swirl at the time of fuel injection. The MP1 has approximately 33% more swirl than the SP. The swirl sustained by MP2 is slightly lower during the suction process. The modified geometries MP1 and MP3 also shows similar trend during the starting stage. As the piston moves near TDC, the swirl sustained by MP2 is in between SP and MP3 with MP1 showing a highest swirl value near TDC. As the fuel is injected, the swirl motion will certainly enhance the droplet dispersion and its evaporation. Amongst the three bowl configurations the MP1 has the highest swirl followed by MP2, compared to other configurations. Figure 7.5 shows the kinetic energy generated inside the engine cylinder.
Figure 7.4 Comparison of swirl for the four piston geometries

(a) Kinetic energy
(b) Kinetic energy during fuel injection

Figure 7.5 Comparison of turbulent kinetic energy for the four piston geometries

Figure 7.6 Temporal evolution of fuel vapour for the four piston bowl geometries
It is observed that the energy generated is same for the four cases. A closer look at the kinetic energy trends near the fuel injection period (697° to 727° aTDC) reveals that while SP and MP3 shows a higher kinetic energy due to injected fuel, the MP1 has a slightly lower rise in energy level. But the MP2 shows the highest amongst the piston geometries investigated. This is due to the quicker destruction of vortices by the baffle plate, to result in higher turbulent kinetic energy. Also due to the positioning of the plate, there is more possibility of droplet-wall interaction which significantly affects the evaporation quality. While a same fuel injector is used in all the four cases there is a variation in the injection generated turbulence. This may be due to the piston shape. The SP and MP3 pistons allows the droplets to penetrate deep into the chamber before hitting the piston surface thus allowing itself more time by the droplets to interact with the air inside. In case of the toroidal combustion chamber due to its projection in the piston at the centre, the droplets have less time before they hit the piston surface at the middle. This is an indirect indication of the droplets interaction with wall. A plot about the temporal evolution will provide more insight about other aspects of combustion. Figure 7.6 shows the plot of fuel vaporisation against crank angle. This plot also shows the fuel injected quantity.

Fuel injection starts at 23° bTDC (697° aTDC). By the time the piston reaches 704° the evaporation patterns are similar for all four bowl. Beginning from 704° the MP1 has more evaporation than the other three bowls. From 720° aTDC (20° from TDC) the evaporation from MP3 has a higher value. Hence MP1 may have a higher in-cylinder pressure due to rapid vaporisation. This higher vaporisation is possible only due to wall evaporation in MP2 piston, because other physical, initial and boundary conditions are similar for the other cases.
Figure 7.7 Comparison of velocity vector on a sectional plane passing through the centre of bowl at top dead centre (720 °CA)

Figure 7.7 compares the velocity vector plots on a plane perpendicular to cylinder axis passing through the middle of the bowl. It is observed that the flow field is vigorous in MP1 and MP3. Here a clear indication of flow field being affected by the injected droplets can be seen, with three distinct regions of higher velocity field aligned along the spray direction. For the SP there is a spray affected region between the intake and exhaust valve. Figure 7.7 (c) shows the flow field vectors for MP2. It can be observed that the flow field is not vigorously organised and it is obstructed by the plate provided at the bowl. Due to this there is a less intense rotary motion and it is an indication that the swirl velocity is being destroyed near TDC, which helps in higher turbulence. This is cross verified with respect to figure 7.5 (b).
7.4.2 Combustion and emission characteristics

In the previous sections the flow field variation due to piston geometry and the effect of fuel injection on flow field has been studied and it was found that the MP2 bowl gives a better evaporation and higher TKE. This should result in higher heat release rate and higher in-cylinder temperature. Figure 7.8 shows the comparison of pressure histories of the engine fitted with the four piston configurations.

![Figure 7.8 Temporal variation of pressure](image)

From the plot it is evident that MP1 provides a higher pressure which is nearly 6% more than that of the SP. This may be due to higher burning rate of fuel in the case of MP1. Comparing the pressure characteristics of MP2 it can be observed that it is almost exhibiting a similar trend as that of MP1. In order to understand that whether this assumption is correct or not, a plot of the heat release rate is shown in Figure 7.9.
Figure 7.9 Comparison of heat release rate for four piston bowl geometries

The comparison from Figure 7.9 reveals that the heat release rate is the highest for MP1, followed very closely by MP2, MP3 and standard piston respectively. The higher heat release rate is possible due to a rapid premixed combustion in MP1 as compared to SP and MP3. Also due to better evaporation and turbulence of MP2, the heat released is better than SP. The second phase of combustion which is a diffusion combustion is not as fast as the premixed combustion. But they are important in a sense that they are the main precursors of NO\textsubscript{x} and soot generation.
Figure 7.10 Comparison of NO\textsubscript{x} and soot for the four piston bowl shapes

(a) NO\textsubscript{x}

(b) Soot production

Figure 7.10 Comparison of NO\textsubscript{x} and soot for the four piston bowl shapes
Figure 7.10(b) shows the plot of soot generated inside the engine with respect to time (crank angle). It is evident that the soot generation during the initial stages of combustion (710° to 730 °aTDC) is the highest for MP2. It is followed by MP3, SP and MP1. Beginning from 730° the soot generation starts declining. Because at this point the fuel injection has already stopped, and the soot generation is now entirely controlled by the interaction of fuel droplets and high temperature zones inside the combustion chamber. By this time the exhaust value opens the MP3 bowl show highest soot followed by MP2. This may be due to higher wall wetting in MP3 and MP2 bowls.

Figure 7.11 Comparison of equivalence ratio plots at top dead centre (720 °CA after top dead centre) for the four bowl geometries

(a) SP (b) MP1 (c) MP2 (d) MP3
A three dimensional plot of the equivalence ratio inside the combustion chamber will provide more light into the exact mechanism with which the pollutants are formed. Figure 7.11 shows a comparison of fuel equivalence ratio inside the combustion chamber for the four cases at the crank angle of 710°, through a plane passing between the intake and exhaust valves. It can be seen that the spray travels more distance in the case of SP and MP3 compared to MP1 and MP2. In the MP1 and MP2, the droplets encounters the piston top and piston baffle plate respectively. The effect of this may lead to two situations, either it may enhance evaporation due to wall heating, or it may hinder evaporation due to piston film formation. While it is true that wall heating of droplets evaporation may also result in droplet decomposition near the wall region to form soot. Since the MP2 geometry is more susceptible to for droplet-wall interaction, a higher vapour mass of fuel is seen near the central region of the bowl (figure 7.11(b) and 7.11(d)). This can be verified with figure 7.10 (b) where the MP2 produces higher soot. In figure 7.10(b) it is observed that MP3 piston shows a higher soot formation. This can be better explained with figure 7.11(c) and 7.6 where MP3 shows a higher vapour formation. But it can be seen in figure 7.11 (c) the droplets have lesser distance to travel before hitting the bowl. Since the bowl surface is little far away compared to the MP2 there is both film formation and higher evaporation. The same scenario can be observed for MP2 piston. Since the blade is near the combustion region, it will lead to rapid droplet decomposition resulting in more soot.

Figure 7.12 compares the temperature contours of burning fuel inside the combustion chamber at TDC. It can be seen from figures 7.12(b) MP1 and 7.12(d) MP2 there is combustion near the central region compared to other two piston
geometries. This is in conformity with earlier turbulence and evaporation data which shows the order of performance from MP1 as having best followed by MP2.

![Comparison of temperature contour inside the combustion chamber at top dead centre](image)

**Figure 7.12 Comparison of temperature contour inside the combustion chamber at top dead centre**

### 7.5 CLOSURE

A three dimensional CFD analysis of four different bowl geometries were done. Some of the important conclusions inferred are;

- Performance Characteristics (pressure, temperature) of MP1 configuration shows better characteristics compared to other configurations.

- The MP2 configuration shows a slightly lower pressure and temperature characteristics curves, but higher than MP3 and SP.
- The NO\textsubscript{x} emission from MP1 shows higher value when compared to that of MP2 configuration.

- While the soot emission for MP2 is higher when compared to that of MP1 configuration.

Hence it can be concluded that with respect to performance and emission point of view MP1 and MP2 can be chosen with slight trade-off between performance and emission.