In automotive industry the new combustion processes focused on clean diesel combustion, decrease emissions such as particulate matter, NOx emission, unburned hydrocarbons (HC) and carbon monoxide (CO) emissions. At this point, prediction of in-cylinder combustion behavior, effects of turbulence levels, flow structures and emission modeling have an importance to design efficient engines. In this study, diesel engine combustion was modelled by a development combustion model Extended Coherent Flame Models 3 Zones (ECFM-3Z). During this modeling, a calculation was made about an engine configuration with compression, spray injection, combustion and emission of the diesel engine with direct injection. Effects of in-cylinder flow structures, fuel injection and design parameters were investigated for the engine performance and emission results. The results agree qualitatively with experimental and also zero dimensional computational studies.

Keywords: Diesel Engine; CFD; Heat Release; Combustion; Emission; Performance.
Computational Fluid Dynamics (CFD) modeling, and are used to develop the combustion chambers. This method is intensely helpful to get knowledge on the effect relationships, additively to the definition of the optimum set of values for the input parameters [5]. Choi et al. investigated the effect of the combustion chamber geometry and a double row nozzle with 12 holes on the emissions [6]. Atmanli et al. worked on a Response Surface Method to find the optimum diesel-n-butanol-cotton oil ternary blend ratios also to reduce emissions [7]. These studies have been widely applied also to the analysis and optimization of advanced combustion strategies. Genzale et al. tested how the emissions are affected by the combustion chamber geometry operating with the low temperature combustion (LTC) concept [8]. Benajes et al. studied the potential of the piston geometry to improve the results provided by the Reactivity Controlled Compression Ignition (RCCI) concept in terms of thermal efficiency and exhaust emissions [9]. In this study, it is aimed to find out the combustion characteristics of a single-cylinder, 1-L CI engine including detailed fuel injection and atomization process in order to investigate the engine performance and emissions. Also complete intake and compression stroke, fuel injection at the end of the compression stroke, combustion and emission simulated in 3D. Both naturally aspirated and turbo-charged modes of operations were studied. Real engine geometry of one-liter single-cylinder diesel engine was modelled including exhaust and inlet manifolds. In multi-dimensional modeling simulations were extended for both intake and exhaust ports to get proper boundary conditions at the valve lifts. Fine grids were tested with 1,500,000. Fine grid results are presented in the paper. Typical execution time for 408 °CA with fine meshes takes about 5 days on a workstation with 16 processors running in parallel processing.

As seen in literature, the most general methodology to solve fluid flow is based on modeling of the Navier-Stokes equations. This methodology includes that the continuity equation, Navier-Stokes equations of momentum and the energy equation are discretized to solve a specific fluid problem limited in space and divided in a large number of computational cells [12]. In time discretization, the entire sub-system was discreted into smaller volumes, where a flow split was represented by a single volume and pipes are divided into several volumes [13]. In methodology, if we put Y (t) in the current system state and Y (t +Δt) in the state at the later time (Δt is a small time step), then the explicit method is:

\[
\frac{\Delta t}{\Delta x} (u + c) \leq 0.8
\]

(1)

\(\Delta x\) where \(\Delta t\) is the time step, \(\Delta x\) the discretized length, u the fluid velocity and c the speed of sound. Using small time steps, the flow is reached by explicit time integration of the equations for continuity, momentum and energy [15]. Spray injection and mixture formation modeling using CFD in IC engines is a multi-component multiphase problem that contains liquid fuel and the various species that participate in mixture formation. Commonly,
the gas phase is treated in an Eulerian approach, which means that the property of a fluid $\varphi$ is computed in each cell, i.e. $\varphi(x,y,z,t)$. The liquid phase is treated in a Lagrangian approach, which means that an individual particle is traced and the property of this particle is calculated as it moves through the domain as a $\varphi(t)$. The interaction between the phases is accounted for by source terms in the Eulerian gas phase [15].

2. Mathematical Modeling

\[ \frac{\partial}{\partial t} (\rho U_i) + \frac{\partial}{\partial x_j} (\rho U_j U_{ij}) = - \frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \mu \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right) \right) \]

(3)

\[ \frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x_j} (\rho E U_j) = \frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_j} (\sigma_{ij} U_j) + \frac{\lambda}{\partial x_j} \left( \frac{\partial T}{\partial x_j} \right) + \rho \bar{q}_g + \dot{Q}_s \]

(4)

Turbulent flow is present in most realistic flow situations. When turbulent flow is considered, it is advisable to express the instantaneous velocity by a mean and a fluctuating part. For instance, the velocity can then be expressed as follows:

\[ U_i = \langle U_i \rangle + u_i \]

(5)

The mean component $U_i$ can be calculated in three different ways: time average ($\bar{U}_i$), density average ($\bar{U}_i$) and ensemble average ($\bar{U}_i$) according to the following equations.

\[ \bar{U}_i = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau U_i(x_i,t) dt \]

(6)

\[ \rho \bar{U}_i = \lim_{\tau \to \infty} \frac{1}{\tau} \rho U_i(x_i,t) dt \]

(7)

\[ \bar{U}_i = \lim_{n_e \to \infty} \frac{1}{n_e} \sum_{i=1}^{n_e} U_i(x_i,t) \]

(8)

Two equation models are the most wide-spread models used in averaged Navies-Stokes simulation. By avoiding the problem inherent to the former models, namely requiring the specification of a flow-dependent length scale, they provide both a length and a time-scale by solving an additional equation. The simplest one is the standard $k-\varepsilon$ model, which is widely used in turbulence simulations because of its general applicability, robustness and simplicity. The equations of motion for the fluid phase can be solved turbulent flow for in-cylinder motion. The equation for conservation of species mass fraction $Y_\alpha$, momentum equation and energy equation are given in the following equations [12].

\[ \frac{\partial}{\partial t} (\rho Y_\alpha) + \frac{\partial}{\partial x_j} (\rho Y_\alpha U_j) = \frac{\partial}{\partial x_j} \left( \frac{\partial Y_\alpha}{\partial x_j} \right) + \rho \bar{q}_\alpha + \dot{Q}_s \]

(2)
the computational parcels are obtained from the Lagrangian conservation equations of mass, momentum, and energy in the normal way [18, 19]. In atomization model, Huh’s model was used as an atomization model in the simulations. This model is based on the premise that the two most important phenomenas in spray atomization are the gas inertia and the internal turbulence stresses generated in the nozzle [20]. The fuel particles may become unstable due to the interfacial forces acting on their surfaces during the relative motion according to the continuous phase. This problem was solved by using the break-up model of Reitz and Diwakar [21]. The collision model of O’Rourke was used for inter-droplet collisions in the computations. And also it was improved with a speed-up algorithm of Schmidt and Rutland [22, 23]. Moreover, this model includes a coalescence timescale highlighted by Aamir and Watkins [24].

Bai’s Spray impingement model was used in the simulations as a wall-interaction model for discrete phase. This model was formulated within the framework of the Lagrangian model, which is based on literature findings and mass, momentum and energy conservation constraints [25].

3. Combustion and Emission Modeling

Wiebe function for 1D approximation and Extended Coherent Flame Model (ECFM) for 3D CFD solution are used to carry out Combustion modelling. The Wiebe function can be expressed follows:

\[ x_b = 1 - \exp\left(-a\left(\frac{\theta - \theta_0}{\Delta \theta}\right)^{m+1}\right) \]  

(9)

Where \( x_b \) is the mass fraction burned, \( \theta \) is the crank angle, \( \theta_0 \), which fixes the timing is the crank angle at the start of combustion, \( a \) and \( \Delta \theta \) are adjustable constants that determine the combustion duration and \( m \) is an adjustable parameter that fixes the shape of the combustion progress curve.

The Extended Coherent Flame Model (ECFM) [26] and the 3-Zone ECFM (ECFM-3Z) broadly belong to the Coherent Flame Model (CFM) family, but are extended to non-homogeneous turbulent premixed and unpremixed (diffusion) combustion. In the ECFM3Z combustion model, the state of the gases mixture is defined in the 2D space. It is simultaneously described in terms of mixing and progress of reaction as schematically represented in Fig. 1 [27-28].

![Figure 1. Schematic of the ECFM-3Z model computational cell.](image)

The differential equations are formulated in a density-weighted ensemble-averaged frame to facilitate the use of mathematical models of the turbulent transport and combustion processes. Generally, ECFM-3Z can be used for all types of combustion regime whereas ECFM, being a subset of ECFM-3Z, is mostly suitable for non-homogeneous turbulent premixed combustion with spark ignition. As part of these models, two options are provided for modeling spark ignition:

A spark ignition model employing a correlation to account for the delay between spark and flame kernel appearance. A more complex model (AKTIM) where the physics of the spark are modeled in more detail. On the subject of auto ignition, two options are also provided, a simple model and a double-delay model for more accurate predictions, especially with engine simulations.

For emission simulation, the 3-step Zeldovich model is available for NOx and three options are provided for soot [28]. The Mauss model based on a pre-computed soot source-term library and the PSDF model of moments, where the soot particle size distribution are transported. The moment source terms are calculated using the soot flamelet library. The soot formation reaction model uses an Arrhenius rate. The soot oxidation assumes two different reactive sites and the resulting oxidation rate is a function of soot properties (\( \rho_s \): density, \( D_s \): average diameter) and other kinetic parameters. The predicted soot emission is a result of the competition between formation and oxidation reactions.
Net soot mass = Soot mass formed – Soot mass oxidized

\[ \text{Net soot mass} = A_s^0.5 \exp \left( - \frac{E}{RT} \right) - \frac{6MW}{\rho D s \ M_R s_{\text{total}}} \]  \hspace{1cm} (10)

The NOx model uses the extended Zeldovich NO mechanism where, basically, there are no adjustable model constants. However, a scaling factor is provided for model calibration that accounts for differences in the computed NOx and measured NOx level based on different experimental techniques.

4. Computational Grid

The engine that is modelled is a single-cylinder 1lt light-duty diesel real engine. The geometrical specifications of the engine, as well as the engine's original valve timings are summarized before chapter. The computational grid and mesh dependency are shown in Fig. 2. It consists of about 800,000 cells at TDC. As it can be seen, the grid resolution is not adequate to capture the details of the boundary layer and the top-land crevice of the piston. This prevents the prediction of the low temperature regions in the cylinder, which can account for 5-10% of the total mass in the cylinder and are the main contributors to reduced combustion efficiency and increased unburned hydrocarbon emissions. This problem could be overcome by increasing the grid size; however this would increase dramatically the computational time. A finer grid could include the top-land crevice. In addition, a crevice model could be introduced in commercial CFD software, in order to simulate flow in the crevices and blow-by. Nevertheless, even though the low temperature regions are not captured well commercial CFD software, can still provide reasonable predictions for the bulk temperature in the cylinder and the overall temperature and composition distributions.

All the calculations were performed by means of the CFD code. The moving mesh (i.e. piston and intake valves regions) is provided be CFD code's tool designed to facilitate transient analyses of internal combustion engines. CFD solver pre-processor creates the fixed mesh (intake and exhaust ports). The computational grid is made up of cells of mainly hexahedral shape, whose number ranges from approximately 800,000 at TDC up to over 1,500,000 at BDC for fine mesh.

![Figure 2. Engine mesh structure view and mesh dependency.](image)

5. Boundary Conditions

In this study, single cylinder diesel engine combustion phenomenon was analyzed within a multi-dimensional framework under operating conditions given in Table 1 and Table 2. All the walls were treated with the turbulent law-of-the-wall. The heat fluxes to the walls are calculated assuming constant wall temperatures.

The prescribed boundary condition at the inlet of the intake port is that of "pressure inflow", while that at the outlet of the exhaust port is "pressure outflow".

<table>
<thead>
<tr>
<th>Table 1. Engine properties.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore / Stroke</td>
</tr>
<tr>
<td>Connecting Rod Length (mm)</td>
</tr>
<tr>
<td>Piston Pin Offset (mm)</td>
</tr>
<tr>
<td>Displacement/Cylinder (cc)</td>
</tr>
<tr>
<td>Total Displacement (liter)</td>
</tr>
<tr>
<td>Number of Cylinders</td>
</tr>
<tr>
<td>Compression Ratio</td>
</tr>
</tbody>
</table>
6. Engine Simulation

In cold flow study, moving mesh feature was used to analyse the flow structure inside the combustion chamber. Cold flow simulation in 3D was investigated as intake and compression strokes. Both intake and compression strokes were simulated including full geometry, intake port, exhaust port, intake valve, exhaust valve and combustion chamber in transient condition.

<table>
<thead>
<tr>
<th>Engine speed</th>
<th>2000 rpm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass of fuel injection</td>
<td>7 kg/h</td>
</tr>
<tr>
<td>Intake pressure</td>
<td>1.3 bar</td>
</tr>
<tr>
<td>Intake temperature</td>
<td>312 K</td>
</tr>
</tbody>
</table>

Table 2. Operating conditions.

![Velocity vectors in different views.](image)

Different flow structures can be easily distinguished inside the cylinder. The vector field shows less large structures and larger vortices can be seen in Fig. 3. As shown in Fig. 3, in a larger distance from the cylinder head, these vortices start to become small structure. During the intake stroke, air flow field under the valves has disordered structure. Smaller vortices and smaller vortex flow structures can be seen inside the combustion chamber in Fig. 3. Swirl flow structures can be also seen and the magnitude of the velocity vectors decreased compared to the previous vector fields. Moreover, at the bottom of the cylinder, higher velocity vectors can be seen in a clockwise swirl structure.

The induction stroke of the previous section was followed by the compression stroke. In case of compression stroke, not only the velocity fields but also the kinetic energy fields were evaluated. The kinetic energy is directly depended on turbulence phenomenon and air fuel mixture will be occurred just after the end of the compression stroke. Through the compression stroke vector fields have more homogeneous structure when compared to the intake stroke. As shown in figures there are some vortices which have less intensity. At the beginning of the compression stroke large clockwise swirl structures exist. When piston goes from BDC to TDC, magnitude of the swirl structure decreases during the compression stroke. The velocity magnitude during the compression stroke decreases due to friction causes less intensity on the flow structure. Velocity vectors were evaluated in all direction. The maximum air flow velocity was obtained around the maximum valve lift. After maximum valve lift, velocity vectors gradually decrease during the intake stroke and compression stroke. Turbulence and air velocities generated purely during the compression stroke are much smaller than those generated during the intake stroke and can therefore be neglected [29]. During the compression stroke velocity vectors start to decrease due to the friction as shown in figures. During the compression stroke, turbulence dissipates due to the decrease of kinematic viscosity and increase of temperature and pressure. At the beginning of the compression stroke, higher velocity levels are necessary to have high turbulence intensity for a good air fuel mixture at the end of the compression stroke.

Contours of the z-velocity were depicted in Fig. 4 to analyses parallel flow to the cylinder axis. Air flow was still influenced by the flow features of the induction stroke at 586 °CA. Air flow is largely driven by the piston movement half of the compression stroke because of there is no extra energy entrance by the compression and z-velocity contours were flattened. Turbulence level is very effective on the combustion process turbulence and thus inextricably connected to the turbulent kinetic energy. The kinetic energy is directly related to the velocity magnitudes. It is therefore not
it surprising that the kinetic energy, as well as the velocity, decreases with increase of crank angle. This decrease of kinetic energy starts rapidly. At TDC in Fig. 4 (a) when looked at to velocity magnitudes about half of the maximum kinetic energy is increased compared to the BDC. Velocity magnitude inside the cylinder was shown in Fig. 4 (b). This also will provide high kinetic energy levels.

Several calculations for the flow in the engine cylinders have been previously carried out and established on the literature. Zur Loye et al. (1989) and Kono et al. (1999) performed calculations of the compression stroke. In particular, Kono et al. presented the analysis of the swirl intensity effects on spray formation and obtained reasonable agreement with experimental data. However, since the intake process was not included in Kono’s calculation, the initial swirl was entered as a parameter. In this study, intake and exhaust strokes were added in the calculation and swirl intensity effects on spray formation in simulation at different crank angles [30-48]. In this study, AVL FIRE CFD code was used as software. In meshing geometry, hexahedral cells which are proper for moving mesh were used in edge size of 0.8mm. RNG k-e model as turbulence, Reitz-Diwakar model was used to model spray, Wiebe function for 1D combustion and ECFM-3Z were used for 3D combustion, Mauss model for soot, 3-step Zeldovich mechanism for NOx emission were used. In injector geometry, four holes were defined with 171µm diameter. Nozzle size was selected from software library and injection pressures were calculated by mass flow rate.

6.1. Spray Modeling

Diesel fuel injector was defined at the center of cylinder. As seen in Fig. 5 the fuel is injected directly to the combustion chamber. If the fuel spray velocity is high enough, fuel air mixture generates an additional flow vortex in the fuel spray direction and therefore some fresh air is driven to the piston bowl dome, replacing the fuel/air mixture, allowing the second and more injection to take place in a ‘fresh’ air area and hence leading to improved bulk air utilization [17].

In addition, the combustion process in true spray injection process allows better control of maximum heat release leading to less combustion noise and NOx emissions. Also, early injection timing occurs at the pre-heat release by low temperature oxygen reactions before combustion. Several injection strategies were introduced as a concept of ignition-enhancing to solve the problem in wall wetting [39]. According to literature review, injection strategies are very effective on exact combustion and exhaust emission. In 1D and 3D spray simulation, real engine injector data were...
used. Injection strategy was modeled by injecting of fuel near TDC; diesel fuel was injected at 12° bTDC. 1D, 3D and real engine experimental results were obtained and good agreement each other. In CFD calculation, injector which has four holes was defined using cylindrical coordinate system. Start of injection, spray duration defined using CAD, cone angle and hole diameter were defined in millimeter. Diesel fuel injector nozzle was defined with spray cone angle to get exact combustion inside the combustion chamber. As can be seen from Fig. 6, spray and combustion simulation were performed by choosing proper parameters for fuel operations.

6.2. Combustion and Emission Results

1D engine code was used to simulate engine performance and exhaust emissions such as CO and NOx gases. The combustion pressure and in-cylinder temperature were evaluated under engine geometry conditions in order to verify 3D and experimental results. Wiebe function for 1D approximation and Extended Coherent Flame Model (ECFM) for 3D CFD solution were used to carry out combustion modeling. 3D engine code was used to find out flow structure in-cylinder and behavior of the mixture combustion. Results reported in this section the engine operating conditions of 2000 rpm and diesel fuel injection with 7 kg/hr. The detailed operating conditions are listed in Table 2. The 3D results at the level of TDC were shown in Fig. 7 with a section that passes through the cylinder center.

Fig. 6 shows the result of spray simulation in real engine geometry with four injection points on the injector. Fuel particles follow mainly the bowl shape and recirculation motion generated inside the bowl as can be seen in these figures. On the other hand, Fig. 6 shows that the horizontal cross-section spray simulation was affected from the flow structure. In addition, fuel consumption of diesel fuel was decreased especially in specified engine conditions.

Because of the shifting of combustion event to earlier side, this causes the increase of negative operating conditions for a conventional diesel engine. These trends are regarded as typical problems of injection strategies and injection rates that lower the thermal efficiency and
increase the incomplete combustion products such as the HC and CO emissions [40, 41].

1D engine code was employed to validate 3D results as shown in Figure 9. ECFM and the 3-Zone ECFM (ECFM-3Z) broadly belong to the Coherent Flame Model (CFM) family, but are extended to non-homogeneous turbulent premixed and unpremixed (diffusion) combustion. In the ECFM-3Z combustion model, the state of the gases mixture was defined in the 3D space. In-cylinder 1D pressure value is slightly bigger than 3D engine simulation and experimental results as shown in Figure 9. 1D, 3D pressure value reached maximum value near 4° CA aTDC however, experimental analysis reached a few degree crank angle later than engine codes, (near 6° CA aTDC, Figure 9). At the same time, 3D temperature results reached maximum value near 3° CA aTDC and 1D analysis yields a maximum about 20° CA aTDC (Figure 9). It is shown that a few difference between 1D, 3D CFD and experimental results possibly due to the injection parameters used in CFD calculation (i.e. maximum droplet and parcel number). In figure10, NOx and CO emissions were compared for 1D and 3D analyses.

7. Conclusions
In this study, development combustion model ECFM-3Z has been employed successfully to get more information about the in-cylinder combustion and emission events. Effect of in-cylinder design parameters on cold flow
structure and performance in a diesel engine were investigated and reported. Pressure and temperature distributions were also in the expected ranges according to validation results. In cold flow part, turbulence models were tested includes k-ε/Standard, k-ω, k-ε/RNG, Chen’s k-ε and k-ε/Speziale to find the optimum model and selected proper models. 1D and 3D analyses results illustrated that turbulence is driven by combustion effect. 1D and 3D results have little difference due to dimensional differences. Swirl and tumble which are a result of intake port also squish flow motion inside the combustion chamber were also affected 3D results. Also, fuel injection at high inlet pressure was another main parameter on turbulence level and 3D results. During intake stroke results, as the intake valve opens an impingement to the cylinder wall occurs from above the valve which creates levels of turbulence kinetic energy as high as 130 m²/s² at 80 °CA aTDC. Also, different effects of injection parameters on the emission of diesel engine were presented.

Acknowledgement
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Abbreviations
aBDC : after bottom dead center
aTDC : after top dead center
BDC : Bottom Dead Center
BMEP : Brake Mean Effective Pressure
Bscf : Brake specific fuel consumption (g/kWh)
CO : Carbon monoxide
CR : Compression Ratio
HCCI : Homogeneous Charge Compression Ignition
NOx : oxides of nitrogen
PCCI : Premixed Charge Compression Ignition
PM : Particulate Matter
PPCI : Partially Premixed-Charge Compression Ignition
ROHR : Rate of Heat Release
SIMPLE : Semi-Implicit Method for Pressure-Linked Equations
SOC : Start of Combustion
SOI : Start of Injection
TDC : Top Dead Center
UHC : total Unburned Hydro Carbon

8. References
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