A Theoretical Investigation on the Effects of Combustion Chamber Geometry and Engine Speed on Soot and NOx Emissions

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ABSTRACT

The objective of the present investigation is to assess the influence of the combustion chambers geometry and engine speed on the velocity flow fields, temperature distribution and NOx and soot emissions mechanism of formation. The investigation has been carried out both experimentally and by numerical simulations. A modified version of the computational fluid dynamics (CFD) Code KIVA-3V has been used for modeling combustion process and engine emission. In particular five different combustion chamber geometries were investigated, using as basic shape a mexican-hat piston bowl, and introducing later changes to the piston cavity and to the fitting radius to the piston crown.

Key-words: Diesel Engine, Combustion Chamber Geometry, Emissions.

INTRODUCTION

Engine manufacturers, facing the more and more stringent emission standards concerning environmental regulations, are producing their efforts to reduce both soot and nitrogen oxides (NOx) emissions.

One of the feasible emission control strategies consists in reducing the engine out pollutant concentration by optimizing engine combustion both with an improved combustion chamber design and an adequate injection strategy.

Unfortunately, previous studies have shown that NOx and soot emissions are related, thus strategies developed to reduce particulate tend to produce an increase of the amount of released NOx. The development of a procedure able to control simultaneously both these pollutants requires the knowledge of where NOx and soot are formed as well as of their mechanisms of formation. Many studies have been carried out to clarify the effect of exhaust gas recirculation, injection pressure and strategy (multiple injection), combustion chamber geometry on NOx and soot mechanisms of formation. In particular, in [1] has been shown that the extended Zel'dovich mechanism was able to well model the NOx production in diesel engines. In the same study was also found that soot mechanism of formation could be appropriately modeled by a single-step competition between the soot mass formation rate, as predicted by Hiroyasu's model, and oxidation rate predicted with Nagle and Strickland-Constable model.

In the present study experimental results and three dimensional simulations are used to asses the effect of the combustion chamber geometry on the velocity flow fields and high temperature domains, which are decisive factors in the formation and the evolution of NOx and particulate. Simulations were carried out by using a modified version of KIVA-3V code.

NUMERICAL MODELS

The numerical models are based on the KIVA-3V code [2, 3]. The modified RNG $\kappa$–$\varepsilon$ turbulence model proposed by Han and Reitz [4] was adopted in the present investigation. This model differs from the standard RNG $\kappa$–$\varepsilon$ for the presence of an extra term in the dissipation equation, in order to account for the compressibility of the flow. The modified RNG $\kappa$–$\varepsilon$ model has been shown [4] to reproduce the large-scale flame structures in a more realistic way improving the prediction of the high temperature domains and, in concert, the accuracy on the prediction of NOx and soot emissions. Injection was modeled by using the “Blob” injection model, described in [5] and the TAB breakup model [6]. The multistep Shell ignition model [7], was used in conjunction with the laminar and turbulent characteristic time combustion model [8] to describe the entire process. A temperature threshold of 1000 K to switch from ignition chemistry (T<1000 K) to combustion chemistry (T>1000K) was chosen. The soot emission model adopted in this study is the Hiroyasu formation model [9] and the Nagle and Strickland-Constable oxidation model [10]. Soot concentration is predicted by a single step equation which considers the temporal rate of change of the soot mass due to the rates of formation and of oxidation:

$$\frac{dM_{\text{soot}}}{dt} = \frac{dM_{\text{form}}}{dt} - \frac{dM_{\text{oxid}}}{dt}$$

(1)

Where the rate of formation has the following expression:
\[
\frac{dM_{\text{soot}}}{dt} = A_{\text{soot}} \frac{M_{\text{fuel}}^{\text{exp}}}{P} \exp\left(-\frac{E_{\text{soot}}}{RT}\right) 
\]

(2)

with \( E_{\text{soot}} = 12,500 \) cal/mole.

While the oxidation rate, assumed to be proportional to the mass of soot, \( M_{\text{soot}} \), is given by:

\[
\frac{dM_{\text{oxid}}}{dt} = \frac{6}{\rho_{\text{soot}} D_{\text{soot}}} \dot{W}_{\text{NSC}} M_{\text{soot}} 
\]

(3)

where \( \dot{W}_{\text{NSC}} \) is the oxidation rate per unit surface area (gram/sec*cm\(^2\)) of the mass of soot.

The NO emission is modeled with the Zel’довich mechanism, according to the following equations:

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

(4)

where the forward and backward equilibrium constants for the three reactions reported above are the followings:

- Reaction 1: \( k_{1f} = 7.6 \cdot 10^{13} \cdot \exp(-38,000/T) \);
  \( k_{1b} = 1.6 \cdot 10^{13} \);
- Reaction 2: \( k_{2f} = 6.4 \cdot 10^9 \cdot T \cdot \exp(-3,150/T) \);
  \( k_{2b} = 1.5 \cdot 10^9 \cdot T \cdot \exp(-19,500/T) \);
- Reaction 3: \( k_{3f} = 4.1 \cdot 10^{13} \);
  \( k_{3b} = 7.6 \cdot 10^{13} \cdot \exp(-23,650/T) \);

The steady-state approximation for \([N]\) (i.e. \(d[N]/dt=0\)) gives for the NO rate of formation the following expression:

\[
\frac{d[NO]}{dt} = 2k_{1f} \left[ O \right] [N_2] \frac{1 - \frac{[NO]^2}{K[O_2][N_2]}}{1 + \frac{k_{1b}[NO]}{k_{2f}[O_2] + k_{3f}[OH]}} 
\]

(5)

where \( K = k_{1f} k_{2f} / k_{1b} k_{3b} \) and the square brackets denote species concentrations in mole per cubic centimeter.

**ENGINE AND COMPUTATIONAL CONDITIONS**

Experiments were carried out by using a two-stroke single-cylinder direct injection diesel engine equipped with a common-rail injection system. Five different combustion chambers were tested, keeping for all of them the same operating conditions. The investigated pistons outlines are shown in Figure 1.

The first chamber was the baseline cup, while the other ones were obtained by successively introducing slight differences both on the cavities and on the fitting radius to the piston crown. The fifth chamber, from here on referred to as reflex burn, was characterized by a bowl with a double cavity to increase turbulence. All the cups were realized in such a way to keep the same compression ratio. The engine characteristics and the used operating conditions are listed in Table 1. The used injector was electronically controlled and equipped with five holes nozzle.

**Figure 1: Investigated combustion chamber profiles**

| Cylinder bore x stroke (mm) | 85 x 72 |
| Connecting rod length (mm) | 139 |
| Clearance (mm) | 1.2 |
| Compression ratio | 17 |
| Engine speed (rpm) | 1500, 4000 |
| Exhaust port closure (degrees ATDC) | -91 |
| Inlet air pressure (kPa) | 150.7 |
| Inlet air temperature (K) | 350 |
| Injection system | Common Rail |
| Number of orifice x diameter (mm) | 5 x 0.18 |
| Injection pressure (MPa) | 27.4 |
| Fuel injected (mm\(^3\)/cycle) low load | 8.16 |
Table 1: Engine characteristics and operating conditions.

The nozzle holes were characterized by a diameter of 0.18 mm and a length over diameter ratio of 6. Injection pressure was 27.4 MPa for all investigated conditions. Simulations regarded only the closed-port portion of the cycle (i.e. [-91°, +91°] ATDC). Initial condition for the velocity flow field were set by using LDV results from previous investigations in similar engines [11]. The adopted meshes, because of the existing symmetry conditions, reproduced only one-fifth of the entire combustion chamber (i.e. 72° sector) and the used grid resolution is reported in Table 2.

Table 2: Number of divisions along the radial, x, the longitudinal, y, and the axial, z, directions used to generate the computational meshes.

<table>
<thead>
<tr>
<th>Chamber</th>
<th>Nx</th>
<th>Ny</th>
<th>Nz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chamber 1</td>
<td>14</td>
<td>24</td>
<td>10</td>
</tr>
<tr>
<td>Chamber 2</td>
<td>13</td>
<td>24</td>
<td>13</td>
</tr>
<tr>
<td>Chamber 3</td>
<td>13</td>
<td>24</td>
<td>12</td>
</tr>
<tr>
<td>Chamber 4</td>
<td>14</td>
<td>24</td>
<td>11</td>
</tr>
<tr>
<td>Chamber 5</td>
<td>13</td>
<td>24</td>
<td>12</td>
</tr>
</tbody>
</table>

Table 3: BMEP measured values for the investigated conditions.

<table>
<thead>
<tr>
<th>BMEP [Mpa]</th>
<th>Chamber</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
<td>1690 rpm</td>
<td>0.248</td>
</tr>
<tr>
<td>3500 rpm</td>
<td>0.244</td>
</tr>
</tbody>
</table>

Figure 2: Computed and measured pressure profiles for chamber 5

At low engine speed, i.e. 1690 rpm, the heat release appears clearly distinguishable into a premixed phase and a diffusive phase, while at higher speed the plot seems more continuous. From an analysis of the computed droplets SMD an independence on geometrical variations for all the investigated conditions was observed. This could be explained observing that bigger droplets speed was about 120 m/s, i.e. 10² times greater than the velocity of the flow fields acting in the chamber, which structure is determined by the piston design. Moreover, SMD computed values well agreed with data acquired during previous experimental investigations [12, 13, 14, 15].
Soot emission analysis
Soot emission diagrams are reported in Figures 5 and 6 for all the investigated piston geometries and engine speeds.

In the diagrams of the Figures 5 and 6 could be distinguished three different zones: a first linear region; a zone of transition between the end of the linear region and the maximum of the plot; and the third part from the maximum to the end. It is interesting to notice that the linear portion of the plots depends almost exclusively on the concentration of vapor fuel and, therefore, for both engine speeds, is not influenced by the bowls geometry. As it could be seen, at low engine speed, the second part of the soot prediction plots, reveals a marked dependence on the bowl geometry. Vice versa, at higher engine speed, such a dependence is less evident. According to the used model, the temporal rate of soot production is given as the difference between the soot rate of formation and of oxidation (see equation 1), thus, the second part of the soot prediction plots represents the transition from the phase in which soot formation processes dominate to that in which the particles oxidation prevails. At an engine speed of 1690 rpm the first linear region is followed by an extensive not linear part, during which soot mass grows substantially. At high engine speed, instead, the oxidation processes prevails much more quickly resulting in a lower soot production. These differences in the observed trends have to be ascribed to thermal effects, and in particular to differences in the combustion process at the two engine speeds. In fact, as it could be seen in Figures 3 at 1690 rpm, a substantial percentage of heat is released during the premixed combustion phase, when soot particles formation was still prevailing. In the phase immediately following, the curve of heat release suffers an abrupt decrease, that precedes the diffusive combustion phase, and this lowering is accompanied to a most prominent second region in the soot plots. Whereas, as shown in Figure 4 at 3500 rpm, combustion develops in a more continuous manner, and the greater percentage of heat is released earlier in the cycle accelerating the passage to the third phase in which the particles oxidation prevails. An exam of the third region of the plots in Figures 5-6 shows that soot oxidation is more relevant at low engine speed. A comparative analysis of the heat release curves and of
the predicted soot formation shows that such a dependence is due to the quantities of heat released during the expansion stroke. In fact, diagrams in Figure 5 and 6 show that soot oxidation follows the heat release curve of Figure 3 and 4, tightly, presenting a sharper slope in correspondence of the higher rate of heat released, and gradually decreasing to an asymptotic value, as soon as the heat release plot goes to zero. In general, at 1690 rpm, where a greater percentage of the total heat is released during the diffusion combustion phase, a better soot particles oxidation is observed, whereas at 3500 rpm the soot oxidation rate is clearly lower due to the greater percentage of heat released during the earlier part of the cycle where the soot formation process was still in act. It is interesting to notice the effect of the fitting radius to the piston crown by comparing results obtained for the chambers 2 and 3. Figures 7 and 8 show KIVA graphic outputs at 21° crank angle degrees ATDC and at 3500 rpm. Such conditions were chosen in correspondence of the point in which the courses of the soot curves of Figure 6 begin to separate. Chamber 3, which is characterized by a smoother fitting radius to the piston crown, during the first part of the expansion stroke, shows a big vortex that brings "fresh" air from the upper side of the cylinder to the piston bowl, where high soot concentrations and temperatures regions are located. The simultaneous presence of high temperatures regions and oxygen rich mixture facilitate particles oxidation. Vice versa chamber 2, because of the sharper fitting radius to the piston crown produces a flow field with a small vortex located in the upper side of the cylinder. In this region oxygen concentration was already diminished by the presence of combustion nuclei, whereas, the unburned mixture, present in the bowl concavity, was pushed by the generated flows toward the squish region thus not being able to reenter the piston bowl where the soot particles and the high temperature region were located. It turned in a less effective oxidation. Another interesting effect produced by the geometry on the soot emission is given by the different behavior of the chambers 2 and 4 at 3500 rpm.

These chambers are characterized by the same fitting radius to the piston crown, whereas chamber 4 presents a deeper bowl cavity as shown in Figure 1. As can be seen from the plots in Figure 6, the fourth geometry produces a relatively smaller quantity of soot during the formation phase and also oxidizes more efficiently soot particles. As can be seen from the Figure 9, due to its particular shape, chamber 4 produces a flow which enters down into the bowl, pushing up the unburned charge from the cavity to the upper side of the cylinder, where high temperature and soot particles are located. As regards the reflex burn geometry, Figure 10 shows that the upper concavity generates a second charge motion which prevents the unburned flow rising from the lower cavity to reach the zone where soot particle are located. The result is that both the flows are constricted to reenter into the bowl and therefore soot oxidation is limited.
Figure 8: Iso-contours for soot, temperature and velocity for chamber 3 at 3500 rpm and 21 crank angle degrees ATDC

**Figure 11 and 12 represent predicted nitrogen oxides emission for all investigated pistons geometry and engine speeds. In general, increasing engine speed from 1500 rpm to 4000 rpm, both a reduction of the NOx emission level and a reduction of the influence of the bowls geometry was observed.** This second effect could be explained by the increasing of the air-flow velocity with the increase of the engine speed. Air-flow velocity increases because of the combined effect of the burned mixture expansion and of the more rapid piston motion. The reduction of the NOx emission level with the increase of the engine speed, observed also in [16, 17, 18], could be justified both with the decreasing of the mixture residence time at high temperature and with the increase of the mixing processes that tend to homogenize the temperatures within the cylinder charge.

**Nox emission analysis**

In particular, chambers 1 and 4 do not show substantial differences increasing engine speed. Chamber 1, characterized by a wide mexican-hat bowl, does not change significantly the morphology of the in-cylinder flow field by increasing the engine speed and, therefore, the mixing processes between the hotter gases and unburned mixture are somehow comparable. Similarly, chamber 4, characterized by a deep reentrant bowl, is able to well direct the in-cylinder flow field also at all engine speeds and therefore substantial differences in the mixing process were not observed. Vice versa, the reflex burn chamber seems to be strongly affected by engine speed. In fact, going from 1690 rpm to 3500 rpm NOx emission level was reduced of a factor three. This behavior is justified by the fact that the double concavity determines a different flow fields according to the engine regime. As results by an analysis of the velocity flow field at 1690 rpm the smaller upper bowl concavity is not able to
Yet, it is interesting to notice that with engine speed also the percentage of mass at a given temperature reflex the flow back to the piston bowl, making it to flow out in the squish zone, thus not contributing to the mixing process between the unburned and burned gases, confined in the inferior part of the bowl by the vortex generated by the bottom bowl concavity. On the other hand, at 3500 rpm, the upper bowl concavity because of the higher piston speed is able to reflect the flow toward the central part of the piston. Because of this flow the entrainment of fresh air in the high temperature zones is facilitated, reducing in such a way peak temperatures.
increases as shown in Figures 13 and 14 for the 1690 rpm and 3500 rpm, respectively. By comparing the Figures 11-14, it is evident that NO emission are not determined only by thermal effects, in fact, while NO emission are drastically reduced increasing engine speed, mass fraction with a temperature greater than 2500 K is substantially augmented. This can be explained by observing that the characteristic time,

\[ \tau_{NO} = \left( \frac{1}{\frac{d[NO]}{dt}} \right)^{-1} \]

for the NO formation process described by Eq. (4) at a temperature of 2700 K (computed core flame temperature) is \( \tau_{NO} = 0.6 \text{ ms} \). It means that to reach equilibrium conditions 13 and 6 crank angle degrees, for an engine speed of 1690 and 3500 rpm, respectively, are needed. The relatively long residence time also explains why NO chemistry is so sensitive to the first stage of the combustion process. However, the significantly long characteristic time is not sufficient to explain differences in the NO emission for the different combustion chamber geometries.

Although the NO formation process is mainly temperature-controlled (Figures 13 and 14), a certain influence, as predicted by Eq. (5), of the oxygen concentration is also observed. An evidence of this dependence is shown in Figure 15 where contour plots for temperature, oxygen and NO are depicted. In the upper panel are clearly visible two high temperature zones, that could potentially produce NO. However, as shown by the oxygen and NO contour plots only one falls in a relatively oxygen rich zone and therefore is able to form NO. The effect of oxygen concentration on the NO formation rate is estimated to be of the same order of magnitude of the temperature effect.

CONCLUSION

The emission characteristics of five different pistons geometry for a range of engine speed varying between 1500 rpm and 4000 rpm were investigated and the following conclusion can be drawn:

1. The effect of bowl geometries on emissions was found to be more relevant at the lower engine regimes.

2. The effect of the fitting radius to the piston crown (chamber 2 and 3) was investigated. Results showed that a smoother radius at higher engine speed generates a more ordinate flow with the presence of big vortices that facilitate mixing between burned and unburned gases, thus assuring a higher oxygen concentration as well as lower peak temperatures in the hot gas regions. This improved soot oxidation and increased NOx emissions.

3. The effect of the bowl re-entrance (chamber 3 and 4) was also found to affect engine emissions characteristics. Highly re-entrant bowl turned to be less sensitive to the engine speed. However spray angle and injection timing are critical parameter to be optimized. Best results are obtained with the spray aiming at the bottom part of the bowl concavity.

4. NOx emissions were found to decrease as engine speed increases. The high characteristic time for
the NO formation process, $\tau_{NO}$, partially justifies such a dependence on engine speed.

5. A strong dependence of NO emissions on local oxygen concentration was proved by numerical simulation. Using the Zel’dovich NO mechanism of formation this effect was estimated to be of the same magnitude of that due to temperature dependence.

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REFERENCES


