Computational study on the effects of exhaust gas recirculation on thermal and emission characteristics of HCCI diesel engine

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In this paper, a computational in-cylinder analysis of HCCI diesel engine was carried out using IC Engine FORTE (ANSYS 18.2) software package. The analysis used pre-defined industry standard CHEMKIN format for specifying a chemical reaction mechanism during the combustion duration. The investigation was carried out for the effects of various EGR mass percentages on the thermal and emission characteristics of a diesel engine running on HCCI mode of combustion. It was observed that an increase in EGR concentration resulted in the decrease in peak in-cylinder pressure and temperature and it was also found that when the EGR rates were increased beyond 75% there was no combustion happening within the cylinder. A considerable decrease in the NOx emissions was found with an increase in EGR mass percentage with almost negligible values when the EGR rates were increased beyond 50%, however there was a slight increase in un-burnt hydrocarbons.
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1 Introduction

The environmental concerns and stringent legislation regulations regarding the exhaust gas emissions from the automotive and industrial sectors using IC engines as the prime sources of power has led the researchers to look for the development of new combustion concepts to comply with these considerations and reduce the emissions. The HCCI combustion mode is having the potential to meet the stringent emission standards (EURO VI) and CO2 emission standards [1]. The homogenous charge compression ignition (HCCI) combustion is a controlled auto-ignition of homogenous fuel-air mixture during compression stroke and is characterized with lower NOx and smoke emissions along with higher thermal efficiencies [2-4]. A lot of research work has been carried out numerically as well as experimentally analyzing various HCCI combustion mechanisms. However, there are several difficulties that need to be resolved before implementation of this mode of combustion, which include the excessive heat-release rate at high loads. The HCCI combustion is predominated by the chemical kinetic mechanisms as well as the thermal conditions that the mixture goes through during the compression process [5-6]. The HCCI combustion leads to nearly instantaneous heat release resulting in rapid pressure rise rate particularly at high loads. Researchers have found that this instantaneous pressure-rise rate can be mitigated by combustion-phasing retard [7] which can reduce the maximum pressure-rise rate and prolong the combustion duration.

Various combustion-phasing control techniques have been studied which include variable compression ratio, Variable valve timing, exhaust gas recirculation and intake air heating [8-10]. The main objective of these techniques is to adjust the temperature of the compressed gases so that the air-fuel mixture auto-ignites at a desired crank angle. EGR technique is preferred to control the ignition timing and the burn rate in HCCI combustion [11]. The EGR technique has a several effects on thermal and emission characteristics of HCCI combustion. EGR influences the compression ignition combustion in three ways. The first one is thermal effect; the presence of CO2 and H2O in exhaust gas increases the specific heat capacity of the charge leading to reduced maximum combustion temperature which affects the NOx formation and the recirculation of exhaust gas increases the inlet charge temperature which is responsible for a decrease in volumetric efficiency. Secondly the chemical effect in which the combustion products in the EGR will take part in dissociation of species during combustion reactions. Thirdly, the dilution effect which leads to a decreased availability of O2 for combustion process. Based on the studies, it has been demonstrated that cooled EGR is beneficial for controlling the auto-ignition in HCCI combustion [12-15].

In the present work the effect of different EGR mass percentage rates on the thermal and emission characteristics of a single cylinder four stroke diesel engine running on HCCI mode of operation were determined numerically using an academic software package.

The introduction presents the purpose of the study and its relationship to earlier work in the field.

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2 The simulation model

The simulation for the combustion process was carried out using IC ENGINE (FORTE) module of ANSYS 18.2 software package which utilizes highly efficient coupling of detailed pre-defined industry standard chemical kinetics CHEMKIN, liquid fuel spray and turbulent gas dynamics. Direct injection HCCI Diesel engine geometry is transformed into 60o sector using periodic boundary conditions at the front and back face of the sector as shown in Figure 1 is used in order to reduce mesh size and solution time. A numerical grid shown in Figure 2 containing 218364 cells was adopted to model the combustion chamber sector geometry after accomplishing the grid-independent results.
The various engine geometry parameters are given in Table 1.

Figure 1. A 60° sector model geometry with spray cone using ANSYS Designmodeller

![Figure 1](image1.png)

Figure 2. A computational grid for the sector geometry using ANSYS Mesh

![Figure 2](image2.png)

Table 1. Engine Geometry Parameters

<table>
<thead>
<tr>
<th>No. of cylinders</th>
<th>Bore × Stroke</th>
<th>Connecting rod length</th>
<th>Compression ratio</th>
<th>Engine speed</th>
<th>Squish</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>89.9 mm × 110 mm</td>
<td>165 mm</td>
<td>15.5</td>
<td>1500 rpm</td>
<td>4.56 mm</td>
</tr>
</tbody>
</table>

The computations were carried out for the crank angle range from 180 degree BTDC (540 degree CA) to 113 degree ATDC (833 degree CA). A full Reynolds-averaged Navier-Stokes equations with the RNG (Re-Normalization Group) k-ε model is used to describe the flow field. The simulation was carried by imposing the boundary conditions and initial conditions as shown in Table 2. The modeling of combustion process was carried out for different EGR mass percentages and the effect on thermodynamic parameters and emissions was obtained.

Table 2. Initial and Boundary Conditions

<table>
<thead>
<tr>
<th>Inlet air pressure</th>
<th>Inlet air temperature</th>
<th>Cylinder wall temperature</th>
<th>Piston top temperature</th>
<th>Cylinder Head Temperature</th>
<th>Fuel injection temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.45 bar</td>
<td>404K</td>
<td>390K</td>
<td>510K</td>
<td>460K</td>
<td>410K</td>
</tr>
</tbody>
</table>

3 Model validation

The simulation results for the HCCI diesel engine with no EGR were compared and validated with the experimental data from the engine with similar geometrical and operational specifications and imposing the same initial and boundary conditions. The comparison of the experimental and simulation results of the baseline case is shown in Figure 3.

The input parameters such as Boundary conditions, Spray modeling parameters, Turbulence modeling parameters, material and grid select of the cylinder and engine have been given to converge.

![Figure 3](image3.png)

4 Results and Discussion

The effects of EGR on the in-cylinder pressure, temperature and apparent heat release rate with varying percentage of EGR were analyzed. The results indicate that the expected trends are maintained throughout the combustion duration irrespective of the EGR concentrations. However, it can be seen that the maximum in-cylinder pressure and temperature decrease with an increase in EGR concentration, owing to an increase in the overall heat capacity and dilution effect of the charge within the cylinder.
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The variation of in-cylinder pressure due to increase in EGR concentrations in shown in Figure 4. It is observed that the in-cylinder pressure has a decreasing trend with an increase in EGR mass percentage and is reduced to the motoring pressure when the EGR rate is increased beyond 75%. The induction of EGR increases the residuals within the combustion chamber. The presence of these internal residuals due to EGR results in an increase in the burn duration by 34% and as much as 15% broadening of the temperature distribution [16]. An increased concentration of EGR increases the concentration of tri-atomic molecules such as CO2 and H2O which is responsible for increasing in the overall specific heat capacity of the gaseous charge within the cylinder. This increased heat capacity reduces the in-cylinder temperature and enhances the ignition delay. The effect of EGR concentration on the in-cylinder temperature is shown in Figure 5.

![Figure 4. Variation of in-cylinder pressure with crank angle for various EGR percentages](image1)

![Figure 5. Variation of in-cylinder temperature with crank angle for various EGR percentages](image2)

The apparent heat release rate with varying crank angle for different EGR percentages is shown in Figure 6. The result shows the delayed apparent heat release rate with an increase in EGR concentration. The start of the combustion delay and the peak value of heat release rate also decrease with an increase in EGR concentration. The increased EGR along with the instantaneous expansion of cylinder volume partially counteracts the physical chain reaction of burned gases compressing unburned gases which retards the combustion phasing resulting in decreased the heat release rates [17]. The increase of EGR concentration beyond 30% results in the delayed heat release time. This increased ignition delay and lack of oxygen deteriorates the combustion leading to a sudden increase in the specific fuel consumption.

![Figure 6. Variation of apparent heat release rate with crank angle for various EGR percentages.](image3)

The high EGR rate supplied to the engine at the expense of the suction air prevents combustion to occur due to the lack of sufficient oxygen. HCCI engines produce high levels of CO and unburned hydrocarbons which is controlled by the gas temperature and chemical reactions occurring during the combustion duration. These are mainly formed in the regions wherein the gas temperatures are lower. Figure 7 and Figure 8 show the variation of CO and unburned hydrocarbon formation with varying crank angle for different EGR mass percentages. The increased concentration of EGR is the primary cause of increased unburned hydrocarbon. EGR causes the reduction in in-cylinder temperature and increases the delay period and works as retarding ignition timing.
Figure 7. Variation of CO formation with crank angle for various EGR percentages

Figure 8. Variation of unburned hydrocarbon with crank angle for various EGR percentages

The induction of EGR into the pre-combustion mixture reduces the oxygen concentration and reduces the in-cylinder temperature thereby reducing the tendency of the formation of NOx emissions. It is observed from Figures 9, 10 and 11 that the NOx content during the combustion duration gets decreased with an increase in EGR concentration. The NOx concentrations were reduced to nearly zero as the EGR concentration was increased beyond 50%. In HCCI diesel engine the homogenous mixture gives the EGR greater opportunity to affect the combustion process. EGR is a recommended technology to mitigate the NOx formation at the expense of unburned hydrocarbon emissions, particularly at higher loads [18].

Figure 9. Variation of NO formation with crank angle for various EGR percentages

Figure 10. Variation of NO2 formation with crank angle for various EGR percentages

Figure 11. Variation of EINOX with crank angle for various EGR percentages

5 Conclusions
The effects of EGR mass percentage on the thermal and emission characteristics of a single cylinder diesel engine running on HCCI combustion mode were analyzed and the following conclusions were obtained. The pressure and temperature within the cylinder were reduced with an increase in the amount of EGR. However, the IMEP was increased leading to an increase in thermal efficiency. There is a considerable reduction in the NOx formation and is almost reduced to zero when the EGR percentage is increased beyond 50%. There is a moderate effect of EGR percentage on CO and unburned hydrocarbon emission. The formation of these emissions increases with an increase in amount of EGR.

Declaration of Conflicting Interests
The author(s) declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

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