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Combustion and Engine – out Emission Characteristics of a PCCI Diesel Engine

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Abstract

The greatest challenge facing internal combustion engine in the 21st century is the threat of fossil fuel depletion and environmental concerns. Researches worldwide are now focused on finding out cleaner and more energy efficient engines for application in automotive applications. This dissertation describes the work undertaken at Heat power laboratory, Okayama University on a single-cylinder four stroke diesel engine operating on premixed charge compression ignition (PCCI) combustion mode.

In this study, the effects of injection parameters like injection pressure, injection timing, compression ratio and EGR rate on combustion characteristics and engine out emission of a PCCI diesel engine were investigated. PCCI combustion strategy allows for slightly well premixed air/fuel mixture with the potential of achieving simultaneously low emissions of NOx and soot. Experimental investigations were carried out both in a single-cylinder test engine and optically accessible engine. Tests were carried out under constant engine speed of 1000 rpm and intake pressure 101.3kPa with variable compression ratio, injection timing, injection pressure and EGR rates.

The exhaust emissions and in-cylinder pressure were measured under all the tested conditions when the engine was in equilibrium with no changes in the emission parameters and exhaust temperature. Analyses based on the diesel spray evolution and combustion process visualization in conjunction with engine performance and exhaust emissions was carried out. High speed video camera (NAC, Memrecam GX-1) with a resolution of 400x400pixel, frame rate of 13000fps and capable of capturing images at intervals of 0.462°crank angle was used in the experiment.

The results shows that an optimum compression ratio of 13.0 led to better indicated thermal efficiency and IMEP while achieving low exhaust emission of smoke, unburned hydrocarbons (HC) and carbon monoxide (CO) with reasonable emissions of oxides of nitrogen (NOx) without EGR at moderately early injection timing.
High injection pressure led to lower smoke, HC and NOₓ emissions but roughly the same CO emissions with the lower injection pressure. This was directly related to the fuel-air mixing which achieved better atomization. The ignition delay and injection duration was relatively short hence leading to a longer premixing time. The indicated thermal efficiency and IMEP were also superior at high injection pressure.

Higher EGR rate led to simultaneous reduction of NOₓ and smoke emissions due to the lower combustion temperatures compared to the conventional diesel combustion. However, HC and CO emissions were noted to increase due to fuel impingement, bulk quenching, and over mixing leading to an air-fuel mixture that was too lean to burn. EGR introduction was found to be very effective in the reduction of NOₓ. This also was accompanied by higher indicated thermal efficiency and IMEP.

The interaction between the spray and the piston bowl geometry played a key role in the air–fuel mixing process. This led to low smoke emissions of less than 1% for both the late and moderately early injection timings without EGR. With EGR, it was possible to achieve less than 2% smoke emissions for the PCCI combustion range considered. An optimum spray targeting spot was identified, leading to lower emissions of smoke, HC and CO but higher NOₓ without EGR. Simultaneous reduction of NOₓ and soot was achieved while utilizing the optimum spray targeting spot and applying EGR. This was accompanied by homogenous combustion and a low- luminosity flame attributed to fuel impingement on the piston bowl wall.

Under moderately early injection timing, θ_{inj} = 20° BTDC and injection pressure P_{inj} = 140 MPa, formaldehyde(CH₂O) radicals were detected in the cool flame region at θ_{inj} = 14° BTDC with the spectrometer grating number of 300l/mm, brazing number of 300nm and 2000 accumulated cycles. OH* and CH* radicals were found to be good markers of exothermic reaction in the high temperature oxidation phase. Traces of CH* radicals were detected at location 1 which is within the piston bowl cavity with the high injection pressure case taking longer to be consumed. No traces of CH* radicals were found in location 3 indicating that there was no fuel impingement at the cylinder wall. Under this condition the indicated thermal efficiency was high with low emission of smoke.
Contents

Abstract ............................................................................................................................... I

Contents ........................................................................................................................... III

List of figures ................................................................................................................. VII

List of tables ................................................................................................................... XI

Nomenclature ................................................................................................................ XII

Acknowledgement ......................................................................................................... XIV

Chapter 1  Introduction................................................................................................. 1

  1.1. Background of the present research and motivation ............................................. 1

  1.2. Main objective of the research ........................................................................... 3

  1.3. Methodology ....................................................................................................... 4

  1.4. Thesis outline ..................................................................................................... 4

  1.5. Reference .......................................................................................................... 6

Chapter 2  Fundamentals of conventional diesel engine and PCCI diesel engine ..... 7

  2.1. Introduction ........................................................................................................ 7

  2.2. Combustion in conventional diesel engines ....................................................... 7

      2.2.1. Basic combustion concept ....................................................................... 7

      2.2.2. Rate of heat release ................................................................................ 9

      2.2.3. Combustion process ................................................................................ 11

  2.3. Fundamental of PCCI combustion .................................................................. 18

  2.4. PCCI combustion implementation in diesel engine and its combustion and emission characteristics ................................................................. 18

      2.4.1. Injection timing ....................................................................................... 19

      2.4.2. Injection pressure .................................................................................. 27

      2.4.3. Injector characteristics ......................................................................... 27
Chapter 4  Effect of compression ratio and EGR on combustion and exhaust emission characteristics of a PCCI diesel engine ................................................................. 70

4.1. Introduction ...................................................................................................... 70

4.2. Experimental set up and procedure ............................................................... 70

4.3. Results and discussions .................................................................................... 71

4.3.1. Effect of compression ratio on rate of heat release ................................ 71

4.3.2. Effect compression ratio on performance ............................................... 73

4.3.3. Effect of compression ratio on specific emissions ................................. 74

4.3.4. Effect of EGR on rate of heat release...................................................... 76

4.3.5. Effect of EGR on performance .............................................................. 78

4.3.6. Effect of EGR on specific emissions ........................................................ 79

4.4. Summary ........................................................................................................... 83

4.5. References ......................................................................................................... 84

Chapter 5  Effects of spray impingement, injection parameters and EGR on combustion and emission characteristics of a PCCI diesel engine ............................. 86

5.1. Introduction ...................................................................................................... 86

5.2. Experimental set and conditions ..................................................................... 87

5.3. Results and discussions .................................................................................... 87

5.3.1. PCCI engine operating range ................................................................. 87

5.3.2. Effect of injection pressure on heat release ............................................ 87

5.3.3. Effect of injection pressure on performance .......................................... 88

5.3.4. Effect of injection pressure on ignition and combustion phasing......... 90

5.3.5. Effect of injection pressure on specific emissions ................................. 91

5.3.6. Effect of spray impingement on specific emissions .............................. 93

5.3.7. Visualisation of combustion process phenomena ................................... 96
5.3.8. Effect of EGR on heat release ................................................................. 100
5.3.9. Effect of EGR on performance ............................................................... 101
5.3.10. Effect of EGR on ignition delay and combustion phasing ............... 102
5.3.11. Effect of EGR on specific emissions .................................................. 104
5.3.12. Soot formation and oxidation in PCCI diesel engine ....................... 106
5.3.13. Optimized low emission and high efficient PCCI diesel engine ......... 113
5.4. Summary .................................................................................................. 116
5.5. References ............................................................................................... 117

Chapter 6 Spectrum Analysis of Chemiluminescence of a Low Sooting PCCI Diesel Engine Operating with Moderately Early Injection Timing ..................... 119

6.1. Introduction ............................................................................................... 119
6.1.1. Spectral characteristics of a flame ...................................................... 120
6.2. Experimental setup and conditions ......................................................... 121
6.3. Results and discussions .......................................................................... 121
6.3.1. Effect of the number of accumulated cycles on the identification of formaldehyde radicals ................................................................. 122
6.3.2. Characterization of the intermediate species in PCCI diesel engine .... 124
6.3.3. Effect of measurement location on intermediate species .................... 129
6.3.4. Effect of injection pressure on spectra of intermediate species .......... 133
6.4. Summary .................................................................................................. 137
6.5. References ............................................................................................... 138

Chapter 7 Conclusions .................................................................................. 139
List of figures

Figure 2-1 Phases of diesel combustion as function of Crank Angle (CA) in degree After Top Dead Center (ATDC)[1] ........................................................................................................ 10

Figure 2-2 A pictorial view representing Dec’s conceptual model of DI diesel combustion[11] ................................................................................................................ 11

Figure 2-3 Soot and NOx formation zones as a function of temperature and equivalence ratio (φ-T map) [12] .................................................................................. 16

Figure 2-4 NOx and soot production as a function of the equivalence ratio and temperature. The left hand side is extended with the CO production and the right hand side with UHC production. The production is obtained from a homogenous reactor simulation of n-heptane/air mixture with an ambient pressure of 6MPa and a reaction time of 2.0 ms [25]. .............................................................. 17

Figure 2-5 Injection strategy of MULDIC[34] ........................................................................ 21

Figure 2-6 Injection strategy of HiMICS system[35] .......................................................... 22

Figure 2-7 Combustion strategy of UNIBUS[4] ................................................................ 23

Figure 2-8 Operation map with UNIBUS[4] ..................................................................... 23

Figure 2-9 Multi-pulse injection of MULINBUMP[36] ..................................................... 25

Figure 2-10 Combustion regimes in MK combustion[2] ................................................. 26

Figure 2-11 Direct visualization of conventional diesel combustion and LTC (Engine speed = 1200 rpm, nitrogen dilution to simulate the EGR, using diethylene glycol diethyl ether (DGE)[68] ........................................................................................................ 32

Figure 3-1 Schematic diagram of the test engine experimental set up............................. 45

Figure 3-2(a) Schematic diagram of the optical accessible engine ................................. 47

Figure 3-2(b) Optical accessible engine ........................................................................... 48

Figure 3-3 Spectroscopic analysis experimental set up .................................................... 49

Figure 3-4 Fuel injection quantity calibration chart for Pinj = 80 and 140 MPa............ 50

Figure 3-5 Definition of the ignition delay duration. In-cylinder pressure, ROHR and pulse injection signal ............................................................ 51

Figure 3-6 Pressure calibration of the piezoelectric transducer .................................... 51

Figure 3-7 Mercury spectral calibration lamps with specific spectrum wavelength 52

Figure 3-8 Typical p-V diagram of a 4-stroke cycle engine[1] ....................................... 56
Figure 5-6 Predicted spray extreme penetration distance .................................................. 94
Figure 5-7 Spray penetration characteristics (P_{inj} = 140 MPa, m_f = 12 mg/cycle without EGR) .................................................................................................................................................................................................................................................................................................................. 95
Figure 5-8 Spray fuel impingement location at 4.2°CA ASOI .......................................... 95
Figure 5-9 Time series combustion images for different injection timing, P_{inj} = 140 MPa, without EGR (Field of view = φ62 mm) ................................................................................................................................. 97
Figure 5-10 Time-series combustion images for P_{inj} = 80 MPa, 140 MPa, without EGR. Camera frame speed = 13000 frames/second ................................................................................................................................. 98
Figure 5-11 Time-series combustion images for P_{inj} = 140 MPa, 0% and 40% EGR ...... 99
Figure 5-12 In-cylinder pressure history and rate of heat release, P_{inj} = 140 MPa, 0% EGR, \( \lambda = 4.5 \); and 40% EGR, \( \lambda = 3.0 \) .............................................................................................................................................. 100
Figure 5-13 Effect of EGR on indicated thermal efficiency, IMEP and coefficient of variance of the IMEP, P_{inj} = 140 MPa, 0% EGR, \( \lambda = 4.5 \); and 40% EGR, \( \lambda = 3.0 \) . 101
Figure 5-14 Effect of EGR on ignition delay, P_{inj} = 140 MPa, 0% EGR, \( \lambda = 4.5 \); and 40% EGR, \( \lambda = 3.0 \) .............................................................................................................................................. 102
Figure 5-15 Combustion phasing as a function of fuel injection timing ..................... 103
Figure 5-16 Effect of EGR on specific emissions, P_{inj} = 140 MPa, 0% EGR, \( \lambda = 4.5 \); and 40% EGR, \( \lambda = 3.0 \) .............................................................................................................................................. 105
Figure 5-17 Direct visualization combustion images, P_{inj} = 140 MPa, \( \theta_{inj} = 20^\circ \) BTDC, 0% EGR, \( \lambda = 4.5 \); and 40% EGR \( \lambda = 3.0 \) .............................................................................................................................................. 108
Figure 5-18 Comparison of combustion images with and without EGR conditions (images d and C in Figure 5-17)................................................................................................................................. 109
Figure 5-19 Time series of red component processed combustion images, P_{inj} = 140 MPa, \( \theta_{inj} = 20^\circ \) BTDC, 0% EGR, \( \lambda = 4.5 \); and 40% EGR, \( \lambda = 3.0 \) ................................................................. 110
Figure 5-20 Spatially integrated flame luminosity (SIFL) and rate of SIFL, P_{inj} = 140 MPa, 0% EGR, \( \lambda = 4.5 \) .............................................................................................................................................. 112
Figure 5-21 Spatially integrated flame luminosity (SIFL) and rate of SIFL, P_{inj} = 140 MPa, 40% EGR, \( \lambda = 3.0 \) .............................................................................................................................................. 112
Figure 5-22 Pressure history and rate of heat release ................................................... 114
Figure 5-23 Engine–out smoke against NOx.................................................................... 114
Figure 5-24 Time integration of spatially integrated flame luminosity (TISIFL)/IMEP and NOx/IMEP for the four cases ....................................................... 115

Figure 6-1 Spectra of cool flame at location 1 considering different values of accumulated cycles, $P_{\text{inj}} = 140$ MPa, $\theta_{\text{inj}} = 20^\circ$ BTDC, $\theta_{\text{Sp}} = 14^\circ$ BTDC ................. 123

Figure 6-2 Time series of the cool flame spectra at location 1, $P_{\text{inj}} = 140$ MPa, $\theta_{\text{inj}} = 20^\circ$ BTDC .............................................................................................................................. 123

Figure 6-3 Pressure history and rate of heat release $P_{\text{inj}} = 140$ MPa, $\theta_{\text{inj}} = 20^\circ$BTDC .................................................................................................................................. 124

Figure 6-4 Time series of spectra $P_{\text{inj}} = 140$ MPa, $\theta_{\text{inj}} = 20^\circ$ BTDC: Initial stages... 125

Figure 6-5 Time series of spectra $P_{\text{inj}} = 140$ MPa and $\theta_{\text{inj}} = 20^\circ$ BTDC: Late combustion phase .................................................................................................................................. 126

Figure 6-6 Time evolution of the CH$_2$O and CO-O recombination, CH*, OH* radicals with soot evaluated at location 1 for $P_{\text{inj}} = 140$ MPa, $\theta_{\text{inj}} = 20^\circ$ BTDC ...... 127

Figure 6-7 In-cylinder field of view and spectroscopic measurement locations..... 129

Figure 6-8 Time series of spectra at location 3, $P_{\text{inj}} = 140$ MPa and $\theta_{\text{inj}} = 20^\circ$ BTDC: Initial stages.............................................................................................................................................. 130

Figure 6-9 Time series of spectra at location 3, $P_{\text{inj}} = 140$ MPa and $\theta_{\text{inj}} = 20^\circ$ BTDC: Late combustion phases .............................................................................................................................................. 131

Figure 6-10 Time evolution of OH* radicals detected at location 1 and 3, $P_{\text{inj}} = 140$ MPa, $\theta_{\text{inj}} = 20^\circ$ BTDC .............................................................................................................................................. 132

Figure 6-11 Time series of spectra at location 1, $P_{\text{inj}} = 80$ MPa and $\theta_{\text{inj}} = 20^\circ$ BTDC: Initial stages.............................................................................................................................................. 134

Figure 6-12 Time series of spectra at location 1, $P_{\text{inj}} = 80$ MPa and $\theta_{\text{inj}} = 20^\circ$ BTDC: Initial stages.............................................................................................................................................. 134

Figure 6-13 Time series of spectra at location 1, $P_{\text{inj}} = 80$ MPa and $\theta_{\text{inj}} = 20^\circ$ BTDC: Late combustion phase .............................................................................................................................................. 135

Figure 6-14 Time evolution of OH* radicals detected at location 1, $P_{\text{inj}} = 80$ and140 MPa, $\theta_{\text{inj}} = 20^\circ$ BTDC.............................................................................................................................................. 136
List of tables

Table 3-1 Engine specification and operating conditions ................................................. 46
Table 3-2 Test fuel properties (JIS#2 diesel fuel) .............................................................. 46
Table 3-1 NAC’s Memrecam GX-1 High-speed Color Video Camera .............................. 63
Table 3-2 Optical cable specifications .............................................................................. 67
Table 4-1 Compression ratio and depth ........................................................................... 70
Table 5-1 Maximum SIFL and rate of SIFL for 0% EGR and 40% EGR .............. 111
Table 5-2 Optimized engine operating conditions .............................................................. 113
**Nomenclature**

**NOTATION**

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ATDC</td>
<td>After top dead center</td>
</tr>
<tr>
<td>BTDC</td>
<td>Before top dead center</td>
</tr>
<tr>
<td>CA</td>
<td>Crank angle</td>
</tr>
<tr>
<td>CA50</td>
<td>Crank angle of 50% heat release</td>
</tr>
<tr>
<td>CO</td>
<td>Carbon monoxide</td>
</tr>
<tr>
<td>CR</td>
<td>Compression ratio</td>
</tr>
<tr>
<td>EGR</td>
<td>Exhaust gas recirculation</td>
</tr>
<tr>
<td>HC</td>
<td>Unburned hydrocarbons</td>
</tr>
<tr>
<td>IMEP</td>
<td>Indicated mean effective pressure</td>
</tr>
<tr>
<td>LTC</td>
<td>Low temperature combustion</td>
</tr>
<tr>
<td>PCCI</td>
<td>Premixed charge compression ignition</td>
</tr>
<tr>
<td>HCCI</td>
<td>Homogeneous charge compression ignition</td>
</tr>
<tr>
<td>RPM</td>
<td>Revolutions per minute</td>
</tr>
<tr>
<td>SOI</td>
<td>Start of injection</td>
</tr>
<tr>
<td>SOC</td>
<td>Start of combustion</td>
</tr>
<tr>
<td>TDC</td>
<td>Top dead center</td>
</tr>
<tr>
<td>CoV</td>
<td>Coefficient of Variance</td>
</tr>
<tr>
<td>NO\textsubscript{x}</td>
<td>Nitrogen oxides</td>
</tr>
<tr>
<td>CO\textsubscript{2}</td>
<td>Carbon dioxides</td>
</tr>
<tr>
<td>PM</td>
<td>Particulate matter</td>
</tr>
<tr>
<td>NTC</td>
<td>Negative temperature coefficient</td>
</tr>
<tr>
<td>UV</td>
<td>Ultra violet</td>
</tr>
<tr>
<td>fps</td>
<td>Frames per second</td>
</tr>
<tr>
<td>Greek Letters</td>
<td>Description</td>
</tr>
<tr>
<td>---------------</td>
<td>---------------------------</td>
</tr>
<tr>
<td>λ</td>
<td>Excess air ratio</td>
</tr>
<tr>
<td>φ</td>
<td>Equivalence ratio</td>
</tr>
<tr>
<td>$\theta_{inj}$</td>
<td>Injection timing</td>
</tr>
<tr>
<td>η$_i$</td>
<td>Indicated thermal efficiency</td>
</tr>
<tr>
<td>θ$_{sp}$</td>
<td>Spectral timing</td>
</tr>
</tbody>
</table>
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Chapter 1

Introduction

1.1. Background of the present research and motivation

The present research has been prompted by the ever pressing concerns about fossil-fuel depletion, environmental protection, and global warming. There is an urgent need to develop and produce internal combustion engines with higher indicated thermal efficiency and lower engine-out emissions. In addition many developed and developing countries are implementing stricter emission regulations to curb the menace from the pollutants.

Internal combustion engine widely divided into compression ignition (CI) and spark ignition (SI) have had a great impact in the mobility sector since their first invention. Diesel (CI) engines are more attractive for powering light duty and heavy commercial vehicles because of their superior fuel economy, durability, reliability, and high specific power output compared to spark-ignition (SI) engines because higher compression ratio, fuel lean combustion and lack of throttling loses[1].

In terms of emissions, compression ignition engines typically produce lower carbon monoxide (CO) and unburned or partially burned hydrocarbons (HC) compared to spark ignition engines [1-2]. However, NO\textsubscript{x} which comprises of nitric oxides and nitrogen dioxides as well as particulate matter (PM) or soot are significant pollutants from compression ignition engines which require proper control strategies since they are a great threat to human health and the environment. In the presence of sunlight, NO\textsubscript{x} would reacts with volatile organic compounds (VOCs) to produce ground-level ozone or smog which is harmful to lung tissues and causes damages to vegetation leading to reduced crop yields. PM, alone or in combination with other air pollutants, causes respiratory and cardiovascular problems. Furthermore, research indicates that PM could acts as carriers of carcinogenic compounds, a potential cancer-causing agent. Environmental impacts of NO\textsubscript{x} a green house gas and PM include acid rain, climate change, water and soil quality deterioration and visibility impairment.
From this we can see that for diesel engines to maintain their relevance in the market all future diesel engines under development and subsequent production must meet the demand for lower PM and NOx emissions while maintaining or attaining higher indicated thermal efficiency.

To meet the strict performance and emission targets set for compression ignition engines, new combustion strategies, such as homogeneous charge compression ignition (HCCI), have been widely investigated. HCCI eliminates locally rich fuel–air mixtures and reduces the combustion temperature, thus simultaneously achieving low PM and NOx emissions with relatively good engine performance. However, the implementation of HCCI combustion concept still faces a lot of challenges, including a lack of combustion phase control under different operating conditions, fuels with different properties, high pressure-rise rates under high loads, and limitations in creating homogenous fuel–air mixtures [3].

Different combustion concepts have been developed to control the in-cylinder combustion process, in addition to the use of expensive exhaust after-treatment devices. The concept of employing in-cylinder control parameters, which is considered the most practical, least expensive, and most effective control measure, has been widely investigated. These parameters include but are not limited to injection pressure, number of injections, shape and timing of the injection, boost pressure, EGR, combustion chamber geometry, injector configurations, intake temperature and swirl ratio [4-8]. One of the most promising combustion concepts is an HCCI combustion strategy implemented in modern direct-injection diesel engines through partially premixed charge compression ignition (PCCI), where fuel and air are not fully homogenous, but the combustion event can be controlled more readily.

There are several merit and demerits of using PCCI combustion concept that have been identified in literature. Among the merits are lean mixtures, low NOx and soot, high efficiency and ability to use different type fuels while the demerits are cylinder wall wetting resulting in lubricant dilution, difficulty in mixture formation, combustion phasing problems, and high CO and HC emissions.
Several solution have been attempted to mitigate these problems including use of narrow included cone angle injector with slightly moderate injection timing, use of high injection pressure with small orifice diameter with cool EGR. Lastly to mitigate the high emissions of HC and CO higher boost pressure and multiple injections have been employed. There is still a need to investigate further these parameters while considering visualization to get the real picture and relate this with the engine-out emissions.

1.2. **Main objective of the research**

The main objective of the research work was to investigate the combustion strategy that would lead to low emissions of NO\textsubscript{x} and soot while attaining same or higher indicated thermal efficiency than the conventional compression ignition engines. To resolve the aforementioned demerits in PCCI engine the following specific objectives were identified:

1. Investigate the effects of the following key factors on combustion and exhaust emission characteristics of a PCCI diesel engine:
   - Compression ratio to resolve the problem of combustion phasing.
   - Simulated exhaust gas recirculation to resolve the problem of combustion phasing, control of NO\textsubscript{x} emissions and provide longer ignition delay to allow better premixing and hence avoid fuel rich regions.
   - Injection timing and pressure to aid in mixture preparation through better air-fuel mixing and atomization.
   - Spray impingement on soot formation and oxidation to locate the regions of soot formation and oxidation.

2. Visualization of the spray and combustion process under above mentioned parameters to understand the combustion phenomena and pollutant formation process.

3. Measurement and analysis of the spectrum of intermediate species under PCCI combustion regimes and correlate with the performance and exhaust emissions.

This research work endeavored to use diesel fuel with the specifications as shown in Table 3-2. It is recommended that future work could attempt the use other alternative fuels.
1.3. Methodology

Our research endeavored to use visualization technique to study the spray development and combustion phenomena in a PCCI diesel engine while employing measurement of the conventional parameters like in-cylinder pressure and exhaust emissions. In order to avoid cylinder wall wetting, the injection timing was varied to find the best injection timing to avoid cylinder wall wetting. In order to improve fuel – air mixing and better atomization the injection pressure was varied. To solve the combustion phasing problem simulated EGR using nitrogen gas and lower compression ratio engine were selected.

The combustion intermediate species under PCCI combustion regime were also investigated to further clarify the combustion phenomena and relate it with the performance and emission characteristics.

1.4. Thesis outline

The thesis outlines the steps taken in resolving the barriers prohibiting the implementation of PCCI combustion strategy for the low load condition. The barriers include but not limited to wall wetting leading to fuel dilution, difficulty in fuel-air mixture preparation and combustion phasing problems. Among these key factors investigated are the effect of compression ratio, injection timing and pressure, simulated exhaust gas recirculation and the spray targeting spot on the combustion and pollutant formation. Visualization of the spray development and combustion phenomena while considering the conventional parameters as in-cylinder pressure and engine-out emissions were considered. Spectroscopic analysis of intermediate species of combustion under PCCI combustion strategy was also investigated.

Chapter 1 outlines the background and motivation of the current research, the main and specific objective of the research, the methodology, the outline and the references considered.

Chapter 2 gives the literature review detailing the fundamentals of conventional diesel engine and PCCI diesel engine. The keys tools that have been used to study the combustion in diesel engine like the rate of heat release and visualization of the process
has been described in details. The main pollutant, NOx and soot that are harmful to the human and the environment emanating from diesel engine have been described. The key factors that would affect the implementation of PCCI combustion strategy like the injection pressure, injector characteristics, piston bowl geometry, compression ratio, intake temperature, exhaust gas recirculation and supercharging/turbocharging have been considered in details. The latest technology in regards to these parameters has been investigated in details.

Chapter 3 describe in details PCCI diesel engine and it’s diagnostic. The first part deals with the test and optical engine experimental setup. The second part describes the conventional engine diagnostics and optical diagnostics. The conventional engines diagnostics include the rate of heat release, engine performance and engine-out exhaust emissions while the optical diagnostics include the passive and active optical measurements. Detailed method of image acquisition and processing is also presented in this section.

In chapter 4 the effects of compression ratio and EGR on combustion and exhaust emission characteristics of a diesel PCCI engine are presented in detail.

In chapter 5 the effect of spray impingement, injection parameters and simulated EGR with nitrogen dilution on combustion and emissions characteristics of a PCCI diesel engine is presented.

In chapter 6 the study on the spectrum analysis of chemiluminescence of a low sooting PCCI diesel engine operating with moderately early injection timing is presented. The main intermediate species like CH*, OH* CH₂O, CO-O recombination that mark the different phases of the combustion process are discussed for two injection pressure and two different measurement locations.

In chapter 7 the summary outlining the conclusions arrived at in this dissertation are presented.
1.5. Reference


Chapter 2

Fundamentals of conventional diesel engine and PCCI diesel engine

2.1. Introduction

Diesel engine has had a lot history in mobility since its invention by Rudolf Diesel in 1892. It relevance in the society has continued to increase as noted in the statistics of the new registered passenger cars in western Europe, with its share standing at about 50% in 2010. Despite the high indicated thermal efficiency achieved in convention diesel combustion over the past few years it faces a lot of challenges in meeting future emission regulation in NO\textsubscript{x} and PM. For the past few decades the focus was on the performance and durability, but lately continuous improvement is needed due to stringent pollutant regulations and demand for high efficiency engines. The research trend has been to develop fuel efficient engines with less environmental impact.

PCCI combustion concept have been studied recently because of it potential to simultaneously reduce the emissions of both NO\textsubscript{x} and PM while achieving higher fuel indicated thermal efficiency and trying to make the most of combustion control, in order to minimize as much as possible the usage of aftertreatment. In this section the fundamental of PCCI engine would be explored starting from the conventional diesel engine combustion concept and its drawbacks while discussing possible solutions.

2.2. Combustion in conventional diesel engines

2.2.1. Basic combustion concept

In conventional diesel or compression ignition (CI) engines the fuel is injected into the combustion chamber and it auto ignite late in the compression stroke. The load is controlled by the amount of diesel fuel injected per cycle while the injection timing is used to control the combustion phasing. Conventional diesel engines are classified into indirect (IDI) and direct injection (DI). Indirect injection engine are equipped with a pre-
Chapter 2: Fundamentals of conventional diesel engine and PCCI diesel engine

chamber which is adjacent to the main combustion chamber. During compression the charge is forced into the pre-chamber and since the entrance is small it generate high fluid velocities. The fuel is introduced in the pre-chamber through low pressure injector as compared to the DI injectors and the turbulent air flow charge provides a rapid fuel air mixing. Recent focus has been on the direct injection system which is gaining a lot of popularity.

In DI diesel engine the fuel is injected directly into the combustion chamber late in the compression stroke. The diesel fuel spray undergoes the process of atomization, premixing with air, evaporation and self ignition due to the high in-cylinder ambient temperature at the TDC. The process of atomization can be divided into two, the primary break up or spray atomization which occurs at or in direct vicinity of the injector nozzle orifice and the spray dispersion or secondary break-up which occur slightly downstream of the nozzle tip. Spray penetration is defined as the maximum distance of the injected spray from the injector tip. The charge into the combustion chamber can be either pure air or a mixture of air and EGR.

Due to the high in-cylinder temperature at end of compression stroke, the ignition delay in conventional diesel engine is very short and hence the fuel and air charge would not mix well enough before the start of combustion. The equivalence ratio represents the actual fuel-air mass ratio divided by the stoichiometric fuel-air mass ratio given as,

\[
\phi = \frac{[F/A]_{actual}}{[F/A]_{stoichiometric}}
\]

At stoichiometric condition the amount of oxygen is just sufficient to oxidize all the fuel and \( \phi = 1 \). The local equivalence ratio at the combustion point varies greatly and this would imply that a fuel elements initially burned in fuel rich regions could later be mixed with fresh charge and further oxidized.

A lot of researches on conventional diesel engine have been focused on decreasing the exhaust emissions and at same time trying to improve on the indicated thermal efficiency. Key to this has been the stringent regulation on the emissions of NOx and soot but is really a problem in diesel engine. Among the options being studied currently is the low
temperature combustion (LTC) which has been found to have a greater potential of simultaneously reducing both emissions of NO\textsubscript{x} and soot.

In literature there are a lot of researches on the LTC concept. Among them are the Nissan modulated Kinetics (MK) combustion implemented through late injection, high swirl and heavy EGR\textsuperscript{[2-3]}. The Toyota UNiform BUlky combustion System employing dual injection system, with one early and the other close to TDC hence promoting better fuel-air mixing \textsuperscript{[4]}. Others include the New ACE PREmixed DIesel Combustion (PREDIC) which has undergone a lot of modification form naturally aspirated to highly boosted coupled with high injection pressure and application of EGR\textsuperscript{[5-6]}. The latest generation of PREDIC has considerably higher efficiency and lower emissions of NO\textsubscript{x} and soot. Premixed Compression Ignition (PCI)\textsuperscript{[7-8]}, Partially Premixed Compression Ignition (PPCI)\textsuperscript{[9-10]}, In most these combustion strategies both early and late injection timing was employed to enhance fuel air mixing while EGR was used for controlling the combustion phasing and decreasing the adiabatic flame temperature due to its dilution effect hence decrease NO\textsubscript{x} emissions. Noted in all this cases was the fact that there was an increase in the emissions of HC and CO due to the displacement of oxygen by EGR.

\subsection*{2.2.2. Rate of heat release}

From the rate of heat release a lot of information can be extracted about the combustion process. Figure 2-1 shows the rate of heat release for the conventional diesel engine. Immediately after start of injection a negative heat release is apparent. This is due to the fact that the evaporating fuel would extract some energy form the ambient charge hence lowering the in-cylinder pressure and temperature. The first phase of auto ignition starts at low temperature, around 750 K. The slow oxidation reaction of the fuel leads to a small increase in in-cylinder pressure associated with the production of free intermediate combustion radicals evidenced by the chemiluminescence of CH and formaldehyde. Due to this chemical process the temperature of the mixture increases. The time interval between the start of injection to this condition is referred to as the ignition delay.

The premixed combustion phase start immediately at the high temperature auto ignition region and is characterized by three phenomena. Firstly, the chemical kinetics enters the
high temperature reaction phase where the fuel chemistry is fast and hence the heat release increases rapidly. Final combustion products emerge with soot precursors. The second phenomenon is characterized by the appearance of incandescent soot in the spray front close to the apex of the rate of heat release. Thermal soot radiation would dominate for the rest of the combustion process even after end of fuel injection. The third phenomenon appears close to the end of this phase where a self-sustaining reaction is achieved and the flame front is established.

![Figure 2-1 Phases of diesel combustion as function of Crank Angle (CA) in degree After Top Dead Center (ATDC)][1]

In the diffusion controlled regime, the luminous flame is dominated by the thermal soot radiations since the soot particles would occupy the main part of the spray. The intensity of the thermal radiation of the soot is quite high but the chemiluminescence of the OH radicals occurs simultaneously and can be observed at the periphery of the sooting flame despite its low intensity and this can be used as a marker of the flame front. This OH radical’s radiation dominates in the region closer to the injector tip and hence defining the lift off length which determines the region where air is entrained to the spray core, upstream of the reaction zone.
2.2.3. Combustion process

Even though, rate of heat release gives very useful information on combustion it is limited since it cannot reveal fully the processes inside the burning diesel jet. Optical diagnostics carried on optically accessible engine and constant volume vessels have greatly improved the understanding of the combustion process details.

According to John Dec [11] diesel spray combustion conceptual model a lot have been brought to light about the events going on in a reacting diesel jet. In short the liquid fuel mixes with air; evaporation takes place forming combustible fuel air mixture. At auto-ignition the mixture burns rapidly in the premixed combustion phase as shown in Figure 2-1. In this phase soot tend to form if the local equivalence ratio is greater than $2^{[12-13]}$. Downstream the jet stabilizes and forms zones that describe the steps of mixing and reactions for the injected fuel components.

![Figure 2-2](image)

Figure 2-2 A pictorial view representing Dec’s conceptual model of DI diesel combustion[11]

Figure 2-2 illustrate Dec’s conceptual model of a quasi-steady jet phase. Within the jet a zone of fuel-rich premixed combustion phase is formed.

The fuel undergoes partial combustion and forms soot precursors like poly aromatic hydrocarbon (PAH). Small nuclei are then formed which gradually grows into primary
soot particles. As the jet moves downstream the soot particles stick together and form agglomerates.

Fuel amount involved in the process of soot formation and oxidation is strongly a factor of the operating conditions of the engine. The soot concentration is at the highest level at fuel rich core of the spray. At the periphery of the jet where the condition is near stoichiometric a thin reaction surface burning with high temperature diffusion flame producing CO₂ and H₂O occurs. NOₓ and OH are formed outside this flame front, where high temperature and oxygen concentration are achieved simultaneously. This condition is also favorable for the soot oxidation.

**The influence of engine set up**

Dec’s conceptual model of a reacting diesel spray during the quasi-steady portion of combustion has become a benchmark for further analysis in diesel combustion. The shape would vary significantly under transient conditions in real engine conditions. Among the factors that would have an impact on the spray are injection pressure, EGR, jet-wall interactions, swirl and the size of the nozzle diameter[11].

The most essential factor affecting the flame structure is the fuel-air mixing process. The rate of the entrained hot-air determines the in-cylinder temperature, evaporation process, the cool flame and high temperature reaction, and thus the characteristics of the combustion process. Parameters that would enhance the process of air entrainment in diesel spray are increased ambient density, high injection pressure and reduced injector orifice diameter[14]. The introduction of EGR does not affect the overall gas entrainment but higher levels of EGR means that the concentration of O₂ would be decreased leading to limited amount of O₂ entrainment into the spray.

The flame lift-off length has been found to be directly related to the fuel-air premixing process that occurs upstream of the lift-off length. To estimate the quantity of the entrained gas, an expression for the axial variation of the cross-sectional average equivalence ratio in a diesel spray is derived in [15-16]:

---

Chapter 2: Fundamentals of conventional diesel engine and PCCI diesel engine
\[
\phi(x) = \frac{2(A/F)_{st}}{\sqrt{1+16(x/x^+)^2}-1}
\]

(2)

Where \((A/F)_{st}\) is the stoichiometric air-fuel ratio by mass, for diesel is approximately 15 and \(x^+\) is a characteristic length scale defined as:

\[
x^+ = \sqrt[4]{\frac{\rho_f}{\rho_a}} \cdot \frac{\sqrt{C_a d}}{\tan(\alpha/2)}
\]

(3)

where, \(\rho_f\) and \(\rho_a\) are the fuel and ambient gas densities respectively. The area contraction coefficient, \(C_a\), and the orifice diameter, \(d\) are related to the nozzle geometry. The jet spreading angle, \(\alpha\), depends on the fuel and ambient gas densities.

The most upstream portion of the burning diesel flame is referred to as the lift-off length and is commonly determined from the OH- chemiluminescence. The lift-off length, \(H\) is derived from the following relationship:

\[
H \propto T_a^{-3.74} \rho_a^{-0.85} d^{0.34} U Z_{st}^{-1}
\]

(4)

Where, \(T_a\) is the ambient temperature, \(U\) is the fuel velocity, and \(Z_{st}\) is stoichiometric mixture fraction, which is the mass of fuel to the total mass of mixture at stoichiometric conditions.

Immediately after the lift-off length the air entrainment into the center of the jet is accelerated since the oxygen is consumed by the reactions on the periphery of the flame. The local equivalence ratio at the lift-off length is therefore critical for the combustion characteristics and the exhaust emission formation. Soot forming process in quasi-steady jet phase is believed to be affected by the air entrainment upstream the lift-off length [17-20].

The use of EGR could change the structure of the jet to a greater extent but does not have any effect on the equivalence ratio at the lift-off length region[21]. This is thought to be due to firstly, the lower \(O_2\) fraction which results in less \(O_2\) entrainment over a given distance. Secondly, the lift–off length would move slightly downstream at the same time giving the same oxygen entrainment up to the lift-off length.
Musculus, M.P.B. [22] developed an extended version of the conceptual model in 2006 considering a burning diesel jet during low temperature combustion with high levels of EGR and early injection timing. With the introduction of high levels EGR the structure of the flame was changed. Soot is formed farther downstream and only in the fuel-rich head vortex where mixing is slowest. Rather than being formed on a thin diffusion flame sheet on the jet periphery, OH and NO is formed throughout the jet cross section indicating more complete mixing and leaner mixture in the jet interior.

**Engine-out emissions in diesel engine**

The main pollutants from diesel engine are NO\textsubscript{x} and PM, where a significant contribution of PM coming from soot particles.

Soot formation occurs in the hot fuel-rich combustion zones. Soot oxidation is promoted by high temperature, lean conditions and high turbulence. If the equivalence ratio at the lift-off length is low enough it is possible to suppress the soot formation during the jet-phase. This concept is more desirable in modern diesel combustion however, it is difficult to control soot formation without affecting the soot oxidation. It is possible that the factors that suppress soot formation might promote soot oxidation. Therefore, even if the soot formation is suppressed it is not obvious that the engine-out soot emission will be reduced.

NO\textsubscript{x} formation reactions are suppressed when the in-cylinder temperature drops during the expansion stroke. Due to the fact that there is no in-cylinder oxidation of the NO\textsubscript{x} the greater part of the NO\textsubscript{x} formed would remain until the exhaust valve is opened. In order to control engine-out NO\textsubscript{x} there would be a need to suppress the formation process. This makes it important to understand the NO\textsubscript{x} formation mechanism. In literature [23] three mechanism of NO\textsubscript{x} formation that are discussed. This includes: Fuel NO\textsubscript{x} arising from fuel containing organic nitrogen. NO\textsubscript{x} can also be formed in the fuel rich regions through prompt NO\textsubscript{x} mechanism. The large bulk of NO\textsubscript{x} is formed through the reaction of the atmospheric nitrogen gas and oxygen. This mechanism is temperature sensitive and always referred to as thermal NO\textsubscript{x} mechanism. In diesel engine thermal NO\textsubscript{x} mechanism is dominant and is described by the extended Zeldovich-mechanism.
Chapter 2: Fundamentals of conventional diesel engine and PCCI diesel engine

\[ O + N_2 \leftrightarrow NO + N \]  
\[ N + O_2 \leftrightarrow NO + O \]  
\[ N + OH \leftrightarrow NO + H \]

In diesel combustion the NO₂ fraction of engine-out NOₓ is relatively low in cases without EGR but would tend to increase as the dilution levels increase and can be more than 80% for lower concentration of O₂. The increase of NO₂ at lower concentration of O₂ is attributed to the increased quenching of NO₂-to-NO reactions due to decreasing flame temperatures[23-24].

Figure 2-3 shows the \( \phi \)-T map indicating the soot and NOx formation locations. Data in Figure 2-3 is generated form a homogenous reactor simulation, implying that the reaction results are obtained at constant temperature and equivalence ratio. The reaction time is 2.0ms. As mentioned earlier the production of NOₓ is temperature dependent and would formed at temperatures > 2200K and equivalent ratio below 2.5. For soot production it takes place at \( \phi > 2 \) and peaks at about 1900K.

For a typical simplified diesel combustion without EGR the path of combustion can be described as follows. The fuel element starts at low temperature and high equivalence ratio. As the fuel mixes with air, the equivalence ratio decreases while the temperature increases. At ignition point the temperature increases at fairly constant equivalence ratio while the fuel element enters the soot formation regions. As the fuel is consumed, the mixing process continues leading to further decrease in the equivalence ratio. At this point the in-cylinder temperature increases and the NOₓ formation process starts. The peak adiabatic mixture flame temperature is achieved at an equivalence ratio slightly greater than 1. Process after this would encourage the decrease of both the equivalence ratio and temperature. In reality the stated simplified condition is far much complex since different fuel elements would undergo ignition process at very different temperatures and equivalence ratios.
Figure 2-3 Soot and NO\textsubscript{x} formation zones as a function of temperature and equivalence ratio (\(\phi\)-T map) [12]

From the \(\phi\)-T map it can be clearly seen that the regions that promote higher production of NO\textsubscript{x} provides very conducive environment for soot oxidation. This would imply that conditions that suppress formation of NO\textsubscript{x} might lead to deterioration of soot oxidation process. This results in the well known NO\textsubscript{x}/soot trade-off that is a great challenge in internal combustion engine.

There two potential paths to achieve simultaneously low emissions of soot and NO\textsubscript{x}: Firstly, promoting soot oxidation late in the combustion cycle when the in-cylinder temperature is too low for NO\textsubscript{x} formation. Secondly, avoid soot and NO\textsubscript{x} formation by operating with in-cylinder temperatures that are sufficiently low. The second alternative is the goal of PCCI combustion concept; one of the low temperature combustion concept with a penalty in the emissions of CO and HC.

An extended version of \(\phi\)-T map with soot and NO\textsubscript{x} incorporating CO and UHC is illustrated in Figure 2-4[25] showing the reactions after 2.0 ms. Both CO and UHC originates for the lean and rich regions in the combustion chamber. For lean mixtures, a
high yield of CO is noted at temperatures between 800 and 1400 K, while in rich mixtures CO is produced at temperatures above 800 K. Below 800 K the fuel does not ignite leading to 100% production of UHC. At lean mixtures above 1200 K most of the UHC is converted to CO or is completely oxidized. At rich mixtures a high yield of UHC is noted up to temperatures approximately 2000 K. Beyond this temperature most of the UHC ends up in CO emissions[25].

Unlike emission of CO which is produced due to partial fuel oxidation, UHC need not be formed. From the number of the carbon atoms present UHC it is easy to identify its source. Heavy UHC components are believed to be associated with the liquid fuel that had no chance to react. This could be from the liquid injector dribble during the expansion stroke or liquid fuel films that did not take part in combustion process. Lighter UHC components are thought to arise from partially oxidized fuel and are linked to the source as CO emissions[26-27].

Figure 2-4 NOx and soot production as a function of the equivalence ratio and temperature. The left hand side is extended with the CO production and the right hand side with UHC production. The production is obtained from a homogenous reactor simulation of n-heptane/air mixture with an ambient pressure of 6MPa and a reaction time of 2.0 ms [25].

From the above understanding of conventional diesel combustion it is possible to control the combustion process in order to reduce the engine-out emissions. The challenge would be to avoid the regions of high emissions formation or try to enhance the oxidation of the pollutant. Practically this is not an easy task since the individual fuel elements but with highly variable values of equivalence ratio and temperatures.
2.3. Fundamental of PCCI combustion

PCCI combustion concept has shown a greater potential of simultaneously decreasing the emissions of both NO\textsubscript{x} and soot due to two basic principles: first the air-fuel is partially premixed and secondly the mixture auto ignites spontaneously within the combustion chamber due to the compression heat.

For partially premixed mixture achieved through optimizing the injection timing, the in-cylinder and temperature during compression stroke would lead to spontaneous ignition within the combustion chamber. Since the auto-ignition occurs simultaneously across the cylinder, no high temperature flame at the periphery of the spray or jet would occur like in conventional diesel combustion. This condition would lead to practically insignificant production of NO\textsubscript{x}, and due to the fuel-air being relatively well mixed without fuel rich pockets, soot formation would be avoided.

There are two limiting factors under PCCI combustion regime that would need further improvement: firstly under rich mixture or high load knocking probability increases and secondly at too lean mixtures, the local burning temperatures can be too low leading to incomplete combustion resulting in high emissions of CO and HC.

2.4. PCCI combustion implementation in diesel engine and its combustion and emission characteristics.

Homogeneity of the fuel-air charge is a key factor in the implementation of PCCI combustion in diesel engine. The fuel injection process in particular the injection timing is very crucial in the development of PCCI combustion. Some of the injection timing strategies so far used for the implementation of PCCI combustion concept in diesel engine would be reviewed below. Other factors would also be considered for instance the injection pressure, piston bowl geometry, compression ratio, intake temperature and exhaust gas recirculation (EGR) and supercharging or turbo charging while considering their effect on combustion and emission characteristics.
2.4.1. Injection timing

Considering the need for fully homogenous mixture in HCCI combustion the best candidate would have been the use of port fuel injection as in spark ignited engines then the mixture would be compressed and auto ignite like diesel combustion. Due to high boiling point range of diesel fuel and its low volatility this would lead to poor vaporization at the normal diesel intake manifold temperature. Hence this makes it practically not a viable fueling concept for the implementation of HCCI combustion in diesel engine[28]. Generally this would lead to the increase in smoke and HC emissions since the non-evaporated diesel fuel would stick on the wall of the intake manifold and the combustion chamber. Despite the fact that increasing the intake temperature would elevate the problem of poor vaporization; this would come with low engine efficiency. This fact has led to current research being focused on direct injection since it eliminates the need to heat the intake manifold to mitigate the problem of vaporization in port injection system. Hence to achieve an acceptable degree of air–fuel mixing for PCCI combustion, the injection timing is of great significance since the premixing time of air and fuel is highly dependent on when the fuel is injected into the combustion chamber. For the purpose of discussion the PCCI combustion operations would be broadly divided into three: early injection, multiple injections and late injection.

Early injection

In PCCI combustion it is a common practice to inject fuel early in the compression stroke, which would allow sufficient time for air and fuel to premix. One kind of this strategy was tested by Takeda et al under the name PREDIC (PREmixed DIesel Combustion). The engine used was a naturally aspirated DI four- stroke cycle, single cylinder with two side injectors and a central one. Different injector configurations were tested in conjunction with varying the injection timing and the excess air ratio, $\lambda$. For fixed excess air ratio in this case 2.7, the range of operational injection timing was limited by misfiring (too early) and knocking (too late). The emission of NO$_x$ were significantly lower than those of conventional diesel combustion but was accompanied with high emissions of CO and HC due to over-leaning of the mixtures. The drawbacks of the first
generation of PREDIC system include limited partial load operation and lack of ignition control timing[5-6].

More recent work have revolved around modification of the piston head geometry and narrow included angle injectors with quite some good success in improving the fuel conversion efficiency while achieving simultaneously low emissions of NOx and soot but with slight penalty on the emissions of HC and CO[29]. Under early injection timing another limitation that has been extensively research on is the problem of cylinder wall wetting leading to lubricant dilution.

Boot et al [30-32]optimized the operating condition under early injection PCCI to avoid wall wetting and investigated the use of hot EGR as a means of limiting the effect with some success but they could not eliminate it completely. It was noted that higher intake and fuel temperature at elevated pressure was advantageously in reduction of UHC emissions while narrow included angle injector led to fuel impinging on the piston bowl[30].

Martin et al. [33] considered a 15-hole, dual row, narrow included cone angle injector and this led to fuel impinging on the piston bowl wall for the injection timing beyond 69.5°BTDC. Dual row would provide for better air utilization. The confirmed that when the pool fires intensity increases the amount of NOx and soot increased while the contrary was true.

In summary, it can be concluded the early injection timing strategies promote preparation of a more premixed air-fuel before ignition than conventional diesel combustion. However, due to the lower in-cylinder temperature and density, fuel impingement on the cylinder wall would occur with the early injection strategy. To mitigate this over-penetration and cylinder wall wetting there is need to optimize the injector configuration – a narrow included cone angle injectors, combustion chamber geometry – use of Bump chamber, and air flow management – use of EGR with higher boost pressure will be critical in attaining better control for the new combustion models.
Multiple injections

The limitation of the single early injection strategy has led to subsequent development of multiple injection strategies in PCCI combustion. Some of the oldest systems featuring frequently are the MULDIC (MULTiple stage Diesel Combustion) [34] and Homogenous charge intelligent Multiple Injection Combustion System (HiMICS) [35]. The former combustion system was developed at New ACE to extend the load range of PREDIC. Shown in Figure 2-5 is the injection strategy with first early injection timing occurring at 150°BTDC and a second injection take place within the range of 2°BTDC to 30°ATDC. The first stage of combustion is premixed lean combustion with low emissions of NOx, while the second is diffusion combustion which occurs under high temperature and low oxygen condition.

![Injection strategy of MULDIC](image)

Figure 2-5 Injection strategy of MULDIC[34]

Figure 2-6 shows the injection pattern of HiMICS with a combination an advanced preliminary injection followed by an injection at around TDC and a late stage injection at approximately 30°ATDC to mitigate the emissions of smoke. Compared to the main injection and pilot injection case with conventional diesel combustion trade-off relation worsen between NOx, and fuel consumption with the well known NOx/soot trade-off in the regions of ordinary injection timing. In late injection these trade-off can be improved
for the HiMICS due to the ultra low emissions of NO\textsubscript{x}. Despite this, the combustion system has some limitations that include high emissions of HC and CO, pre-ignition and inadequate homogenization of the air-fuel mixture.

![Figure 2-6 Injection strategy of HiMICS system][35]

Toyota Motors Corporation developed a two-stage injection system named Uniform Bulky Combustion System (UNIBUS) and implemented it in a 3-l, four-cylinder DI diesel engine (1KD-FTV) commercial vehicles in August 2000. This injection strategy is shown in Figure 2-7. The first injection is done relatively early enough to allow a premixed air–fuel mixture to be attained and converted to lower hydrocarbon in the low temperature reaction. A late second injection is used to trigger combustion of all fuels, including the partially combusted fuel from the first injection and the premixed fuel from the second injection. Optimization experiments with first injection timing and quantity reveals that the early injection timing needs to be between 54°BTDC and 36° BTDC with 5 mm\textsuperscript{3}/stroke of fuel for the particular engine. The late injection timing is fixed approximately at 3°ATDC with 25 mm\textsuperscript{3}/stroke of fuel. Simultaneously low emissions of NO\textsubscript{x} and soot were realized with this combustion system. UNIBUS combustion system is limited to low load and speeds with conventional diesel combustion being utilized for the high load and speeds as shown in Figure 2-8[4].
Chapter 2: Fundamentals of conventional diesel engine and PCCI diesel engine

![Figure 2-7 Combustion strategy of UNIBUS][4]

MULINBUMP is another multiple injection concept developed by Su et al.[36] which combines premixed combustion and lean diffusion combustion through multi-pulse fuel injection and with BUMP type combustion chamber.

![Figure 2-8 Operation map with UNIBUS][4]

Through careful control of the injection pulse parameters for example the pulse injection, injection pulse number, injection period of each pulse, and the dwell in between injection
pulse, it is possible to regulate the spray tip penetration. This would lead to better mixing of the air-fuel and avoiding impingement of fuel on the cylinder liners. The main injection pulse is set very close to TDC. Figure 2-9 shows the multi-pulse injection scheduling strategy. Fuel is injected in the main injection pulse combust at higher air-fuel mixing rate than conventional diesel engine hence achieving lean diffusion combustion. A special type of BUMP combustion chamber is designed with bump rings to enhance the mixing of the air and fuel. It is possible to attain very low emissions of NO\textsubscript{x} and soot with the system despite the fact that the injection mode has to be carefully modulated for higher power output[36].

Lee and Kim [37] considered a narrow included cone angle of 60° modified from the conventional 156° injector while considering dual fuel injection system with first early injection and the second late in the compression stroke. They made comparison with the conventional diesel combustion and single early injection timing. The results indicated that the narrow included cone angle injection was very effective in NO\textsubscript{x} reduction while maintaining high fuel conversion efficiency. Dual injection with the narrow injector had also the potential of reducing CO emissions when the first and the second injection timing were optimized.

Li et al. [38] investigated the effect of two stage injections on UHC and CO in low temperature diesel combustion by varying the dwell between the two injections and the quantity of the fuel and their results indicated that with optimized dwell and injection ratio it is possible to slightly reduce the emissions of CO and UHC.

Recent studies on diesel low temperature combustion achieved through multiple injection have shown that with closely spaced split fuel injection strategy it is possible to achieve low emission of CO and HC through enhanced air-fuel mixtures with limited amount of EGR rate while maintaining reduced peak heat release for low NO\textsubscript{x} emissions and combustion noise [39-42]. While varying the engine speed Horibe et al. [43] optimized the multiple injection strategy for performance and emissions with great success.
Late injection

In late injection timing strategy, the fuel is injected just before TDC and continues till later in the expansion stroke. At this condition the in-cylinder gas temperature and density is decreasing leading to a longer ignition delay and hence an improved premixing of the air and fuel prior to combustion. When coupled with EGR the in-cylinder temperatures are further decreased leading milder combustion with lower rate of heat release peak. This condition inhibits the formation of NO\textsubscript{x} and with an increase in the ignition delay (ID) there would be adequate time for air and fuel to premix avoiding fuel rich regions and hence, lower engine-out soot emissions.

Among the late injection strategies are the Modulated Kinetics (MK) [2] developed by Nissan Motors Corporation. The first generation of MK combustion system was successfully implemented in DI diesel engine (YD25) and introduced to the Japanese market in 1998[3]. MK combustion is achieved through a large amount of EGR, retarded injection timing and high swirl ratio. EGR is used to dilute the air-fuel charge and hence decrease the adiabatic flame temperature and hence suppress the formation of NO\textsubscript{x}. The injection timing is retarded from 7°BTDC to 3° ATDC hence allow thorough mixing of the fuel and air prior to ignition and hence decrease the net soot production. This comes with a penalty in the emissions of HC. The use of high swirl ratio 3-5 is to mitigate the emission of soot and HC by enhancing the mixing of the fuel and air. This strategy is
advantageous in the reduction of the pressure rise rate since the EGR suppress the peak heat release. From Figure 2-10 it can be seen that the first generation MK combustion is limited to low load. Higher load condition would the fuel and temperature of EGR gas increases leading to longer injection duration and short ignition delay. These conditions prohibit the complete delivery of the required amount of fuel before the onset of combustion. In the second generation of MK combustion system the load range was extended by using of a slightly larger nozzle diameter coupled with higher injection pressure to decrease the injection duration. The ID delay was extended by cooling the EGR gas and decreasing the compression ratio.

![Figure 2-10 Combustion regimes in MK combustion](image)

Latest work done by Fang et al. [44] in an optically accessible diesel engine employing retarded single injection strategy shows that higher injection pressure benefit soot reduction but increases NOx emissions. Retarded injection timing simultaneously reduced the emissions of NOx and soot with longer ignition delay and flatter and wider heat release curve.
2.4.2. Injection pressure

High injection pressure has been noted to enhance mixing of the in-cylinder charge especially in conjunction with smaller nozzle diameter leading to reduction of soot emissions and slight increase in NO\textsubscript{x} [7, 45-46]. At elevated fuel injection pressure the injection velocity increases leading to a high rate of air entrainment and mixing resulting in better spray structure and combustion[14]. Investigation on constant volume chamber with optical access and fitted with common rail injection system have shown that it is possible to achieve leaner mixture at elevated injection pressure[28, 47].

Wahlin et al. [47] conducted experiments on a four-stroke, 2-liter single cylinder PCI engine considering injection timing of 50\degree to 70\degree BTDC while varying the injection pressure from 50 to 150MPa. Results showed that NO\textsubscript{x} and soot emission decrease with increase in HC and CO exhaust emissions. These results are in agreement with what Yun et al. [48] found as injection pressure was increased from 70 to 150MPa for the injection timing range of 24-34\degree BTDC.

Choi et al. [49] performed a parametric study of late injection low temperature combustion in a high speed direct injection engine while varying the injection pressure from 60 to 120MPa at 300 to 600 kPa load conditions with a swirl ratio of 3.77. At low load the findings were in agreement with those found by Wahlin et al. and Yu et al, where the peak of soot luminosity decreased with increase in injection pressure. This trend was thought to be as a result of superior early mixture preparation while under high engine load the trend was not very clear.

2.4.3. Injector characteristics

For ideal PCCI combustion with relatively well premixed air-fuel mixture the injection system should able to generate sprays with low penetration, uniform and widely dispersed with high injection rate. Previous research has shown that injectors with impinging spray nozzles are better than the conventional injectors[28, 50]. Larger
impingement angle increases the spray angle and decreases the penetration achieving a more uniform fuel concentration within the jet.

Injector nozzles with narrow included angle are design features of some of the PCCI combustion system. In a Narrow Angle Direct Injection (NADI) engine a narrow spray cone angle of less than $100^\circ$ was used to enhance mixing of fuel and air while limiting spray wall impingement under early injection strategy[51]. Kim and Lee [37] modified the typical conventional diesel engine injector with include cone angle of $156^\circ$ to $60^\circ$ in a single cylinder engine to reduce cylinder wall fuel impingement and avoid an out of bowl injection at early injection timing strategy. Lee et al. [52] investigated the effect of number of nozzle orifices on spray mixing, combustion and emission. Results indicated that increasing the number of holes significantly influences evaporation, atomization and combustion.

Karra and Kong [53] found out that convergent nozzle produced higher soot emissions than the straight-hole nozzle at higher injection pressure and this was attributed to lack of cavitation for convergent nozzle which may have a negative effect on liquid atomization. Their results showed that the ten-hole injector appeared to have a better potential for achieving low soot and NOx emissions over a wider range of injection timings and injection pressures.

**2.4.4. Piston bowl geometry**

Piston bowl geometry has been noted to play a critical role in the development of PCCI combustion. Different shapes have be considered among them are flat, shallow dish and re-entrant type[54]. Shallow dish type have been noted to reduce the formation of fuel wall-film on the surface of the piston bowl wall leading to reduced soot, HC and CO emissions compared to the standard re-entrant type. Improved indicated mean effective pressure and combustion stability have also been witnessed[55]. In PCCI combustion the BUMP combustion chamber combined with multi-pulse fuel injection has been noted to work very well[36]. With the aid of computer modeling and simulation advanced types of
piston bowl and nozzle orifice geometry have been generated and their effects on combustion and emission characteristics extensively studied [56-58].

2.4.5. Compression ratio

When the compression ratio is decreased from the conventional cases the ID is extended which enable complete injection of all the fuel to be accomplished prior to ignition. This condition is conducive for premixed combustion and a reduced maximum in-cylinder temperature at TDC. Reduction of the compression ratio from 18:1 to 16:1 was one of the strategies employed in the second generation of MK combustion which made it possible to extend the low temperature, premixed combustion to higher load conditions[3].

Laguitton et al.[59] investigated the effect of reducing the compression ratio from 18:1 to 16:1 and retarding the injection timing which led to reduced emissions of NO\textsubscript{x} and soot with a small penalty on the emissions of CO and HC when both the premixed and diffusion controlled combustion were present.

Asad and Zheng [60] investigated the means to extend the load range of low temperature combustion through decreasing the compression ratio from 17.5:1 to 13:1 and succeeded to achieve and IMEP of 1200 kPa at compression ratio of 13:1. The emission of NO\textsubscript{x} was relatively low as a consequence of high EGR and independent of the intake pressure and injection pressure. On the contrary high intake pressure and injection pressure were found to be effective in reduction of soot emissions.

2.4.6. Intake charge temperature

The intake charge temperature has been noted to affect the combustion and emission characteristics of PCCI combustion concept through two distinct processes. Firstly, under low intake temperature the ID is prolonged hence, enhancing air-fuel premixing. Secondly, the in-cylinder temperature at combustion of the fuel-air mixture at a given equivalence ratio is decreased hence suppressing the formation of NO\textsubscript{x} Lu et al.[61]
Showed that increasing the intake temperature from 31° to 54°C led to a linear increase of the emission of NO\textsubscript{x} from 10ppm to 50ppm when n-heptane fuel underwent combustion at fixed fuel delivery rate, engine speed and 30% EGR rate. This was observed to be in agreement with the work of Akagawa et al [62] in which NO\textsubscript{x} emission increased as the intake temperature was increased from 35° to 80°C. The emissions of unburned HC and CO were observed to be unaffected by the changes in the intake temperature[61].

### 2.4.7. Exhaust gas recirculation

In early injection PCCI combustion systems EGR has always been employed to extend the ignition delay hence retarding the combustion phasing. Kanda et al.[54] Conducted experiment on premixed charge compression ignition engine with heavy EGR of 54% for the purpose of retarding the combustion phasing towards TDC and this resulted in improved IMEP. Other PCI combustion systems using more than 68% EGR have shown that this is effective in controlling the start of combustion (SOC)[55]. High EGR can also be used to control pressure rise rate by altering the start of combustion. Drawbacks of high rate of EGR have been noted to problems in transient response and temperature – stability characteristics[50]. Therefore for early injection PCCI combustion concept, EGR should be coupled with other techniques like modification of the fuel properties or blending approach. For the late injection like MK combustion system, EGR is basically used as a means of controlling emissions of NO\textsubscript{x} with typical value of approximately 40%[2, 63]. NO\textsubscript{x} is reduced due to lower adiabatic flame temperature achieved by charge dilution and higher heat capacity of the in-cylinder charge when EGR is introduced.

Latest work by Idicheria and Pickett [20] in constant volume vessels shows that EGR leads to early development of cool flame after injection, an increase in the premixed-burn ignition delay which is inversely proportional to the ambient oxygen concentration and lower peak of rate of heat release as EGR increases. The timing of soot formation is strongly dependent on the amount of EGR. The time delay to soot formation from ignition was found to increase with increasing EGR.
2.4.8. Supercharging/turbocharging

To extend the load operating range in PCCI combustion concept supercharging or turbocharging have been employed frequently[64]. This is important in PCCI combustion operation since high EGR rates are typically used to control combustion phasing and decrease NO\textsubscript{x} production. The resulting dilution would limit the amount of fuel that can be added at fixed charge mass resulting in loss of engine power. To mitigate this for a given engine size, more mass of air needs to be introduced to the engine by supercharging or turbocharging. In the PREDIC combustion system described earlier on the output power was limited to half that of conventional diesel combustion under natural aspirated conditions[62]. By supercharging to 86 kPa and increasing the fuel quantity at low compression ratio of 12.5, the power output could be increased to approximately the full load of conventional, natural aspirated diesel combustion. For PCI combustion system, a boost pressure of 80 kPa resulted in an output power comparable to the full load of a conventional, natural aspirated diesel combustion engine[50].

2.5. Chemiluminescence imaging and spectral analysis

In order to understand reaction mechanism of auto-ignition and combustion mechanism in a PCCI engine, one effective way is spectrum analyses of chemiluminescence to determine the major active intermediate species. Chemiluminescence emission arises from specific molecules that are raised to an excited state by exothermic chemical reactions and then subsequently decay back to equilibrium energy level by emitting a photon. It occurs in specific wavelength bands that are characteristic of the emitting molecule. They are specific molecules responsible for the chemiluminescence change for different combustion phases and this can provide information about the nature of the reactions and the fuel/air mixture [65]. Because chemiluminescence is produced directly by exothermic reactions, it marks the location of initial combustion reactions temporally and spatially, with the limitation that the signal is integrated along line of sight. Dec and
Espey did chemiluminescence imaging of auto-ignition in diesel engine [66]. Their spectral data showed that chemiluminescence arose from formaldehyde and CH emission with no OH emission detected. In contrast, the sooting–combustion spectrum (taken after diffusion flame had formed) showed OH and “gray-body” soot emission.

Upatnieks and Mueller [67-68] investigated the influence of nitrogen dilution and charge-gas temperature on in-cylinder combustion processes and engine-out NOx and smoke emissions. Engine-out measurements of NOx and smoke emissions and in-cylinder images of natural luminosity were obtained for charge-gas oxygen concentrations from 9% to 21%. The results show that soot incandescence can be negligible for fuel-rich local mixture stoichiometries that would result in intense soot incandescence under undiluted operating conditions, as shown in Figure 2-11 [68]. Figure 2-11 shows that the flame color of LTC is blue due to very low flame temperatures. Finally, the two results all demonstrate that low temperature combustion with near-zero engine-out smoke and NOx emissions can be achieved using a traditional direct injection strategy.

Figure 2-11 Direct visualization of conventional diesel combustion and LTC (Engine speed = 1200 rpm, nitrogen dilution to simulate the EGR, using diethylene glycol diethyl ether (DGE)[68]

Kashdan and Bruneaux studied HCCI using conventional injector with optimized multi-hole nozzle (NADI™ concept) producing narrow angle jet[69]. Their study was on the
effect of piston geometry on the in-cylinder fuel/air mixture distribution and combustion development of late injection strategy. Fuel employed for the experiment was n-decane a surrogate of diesel fuel.

With the aid of a high speed digital video camera, Fang et al. [44, 70-71] investigated combustion processes in an HSDI diesel engine applying different injection strategies. For early pre-TDC injection strategies, a two-stage low temperature combustion heat release rate pattern was observed including HCCI combustion and fuel film combustion (pool fire). For multiple injections, very high soot combustion left over from the first injection was observed with pool fires during the second injection process. By further advancing the first injection and retarding the second injection, the pool fires from the first injection can be eliminated.

Wontec et al. [72] studied the spectroscopic and chemical kinetics analysis of the phases of HCCI auto-ignition and combustion for single and two stage ignition fuel fuels. In their study they considered iso-octane and primary reference fuel mixture PRF80 as fuels. They observed that for both fuels the spectrum during ITHR (Intermediate temperature heat release) was dominated by formaldehyde chemiluminescence. The two stage fuel showed LTHR (low temperature heat release) with weak spectrum of formaldehyde. The HTHR (High temperature heat release) for both fuels was dominated by broad CO continuum with some contribution from HCO, CH and OH.

Mancaruso et al. [73] considered spectroscopic measurements using single late injection across TDC using conventional large cone angle injector with piston bowl without dome. CH was detected near the bowl wall where fuel impinged. OH was widely distributed in the chamber and during the whole combustion. They noted that OH was a marker of premixed combustion. The entire aforementioned researcher concentrated on primary reference fuel for the experiments and not real fuel in internal combustion engines.

The complexity of the auto-ignition process and the small amount of detailed experimental data demonstrate that more investigations with good temporal and spatial resolution are necessary to achieve a better understanding of the physical and chemical processes involved in PCCI diesel engines. Optical diagnostic techniques have played an
important role in the measurement and understanding of combustion phenomena in internal combustion engines in the past [66, 74]

Most researches involving spectral analysis have been applied to SI and HCCI combustion using surrogate fuels [69, 72], dimethyl ether (DME) [75], MK combustion or late injection [73] due to their low soot emissions. Data for PCCI combustion with moderately early and early injection have not been recorded.
2.6. Summary

From the literature survey it has been noted that there are several key factors that affect performance and exhaust formation in PCCI combustion concept that need to be addressed. These factors can be subdivided three; firstly mixture preparation- injection timing, injection pressure, injector nozzle configuration and combustion chamber geometry that would affect the spray targeting spot. Secondly, physical properties- in-cylinder pressure, temperature and density that can be altered by the compression ratio, EGR, intake temperature and boost pressure and thirdly, chemical properties of the fuel – cetane and octane number that can be altered by the choice of fuel and additives. Optimizations of these parameters are necessary to achieve simultaneous reduction of NOx and soot while maintaining or attaining higher indicated thermal efficiency. As noted, when the in-cylinder temperature decreases due to high EGR, this would lead to high emissions of HC and CO. Mixture preparation would play a vital role with higher boost intake pressure to ensure there is sufficient oxygen to allow for complete oxidation of the fuel while still operating at low temperature combustion.
2.7. References


Chapter 2: Fundamentals of conventional diesel engine and PCCI diesel engine


Chapter 2: Fundamentals of conventional diesel engine and PCCI diesel engine


Chapter 2: Fundamentals of conventional diesel engine and PCCI diesel engine


Chapter 3

PCCI diesel engine and its diagnostics

PCCI diesel engine has been researched extensively as solution to the conventional diesel engine problem of high NOx and soot emissions with the advantage of attaining similar or greater performance. The present investigation aims to study in depth the parameters that would have a great impact in the performance and exhaust emissions of a PCCI diesel engine. Tests were carried out both in the test engine and optical engine. This chapter would give a detailed description of the experimental set up and the engine diagnostics employed in this investigation.

3.1 Engine

3.1.1 Test engine

A four-stroke, single-cylinder, direct-injection supercharged diesel engine with a displacement of 781.7 cm³ was used for the investigation. Table 3-1 shows the engine specifications and the operating conditions. Table 3-2 shows the specification of the low-sulphur JIS #2 diesel fuels used in the experiment, which is commonly available in Japan. A schematic diagram of the test engine is shown in Figure 3-1. A common rail injection system capable of developing an injection pressure of 180 MPa was used. A valve-covered orifice (VCO) injector with four 0.1-mm-diameter holes placed symmetrically in the nozzle tip was used.

The top dead centre (TDC) signals and every half-degree crank angle (CA) were detected by photo interrupters and coupled with a controller to control the injection timing and injection duration. In-cylinder pressure was measured with a piezoelectric pressure transducer (6052C, Kistler) coupled with a charge amplifier (5011B, Kistler). The pressure history was analysed to obtain the heat release rate to investigate the combustion characteristics. Exhaust emissions were captured using a NOx– CO analyser (Horiba, PG-240), HC analyser (Horiba, MEXA-1170HFID), and smoke meter (Horiba, MEXA-600s). The data for each engine condition were captured when the engine was in
equilibrium, during which there was almost no change in the emission parameters and exhaust temperatures.

Figure 3-1 Schematic diagram of the test engine experimental set up
### Table 3-1 Engine specification and operating conditions

<table>
<thead>
<tr>
<th>Specification</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine type</td>
<td>4-stroke, single-cylinder, water cooled</td>
</tr>
<tr>
<td>Bore x Stroke</td>
<td>96x108 mm</td>
</tr>
<tr>
<td>Swept volume</td>
<td>781.7 cm³</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>13</td>
</tr>
<tr>
<td>Combustion system</td>
<td>PCCI, direct injection</td>
</tr>
<tr>
<td>Combustion chamber</td>
<td>Derby hat</td>
</tr>
<tr>
<td>Engine speed</td>
<td>1000 rpm</td>
</tr>
<tr>
<td>Intake pressure</td>
<td>101 kPa</td>
</tr>
<tr>
<td>Injection system</td>
<td>Common rail system</td>
</tr>
<tr>
<td>Fuel injection pressure</td>
<td>80 MPa, 140 MPa</td>
</tr>
<tr>
<td>Fuel injection quantity m_f</td>
<td>12.2 mg/cycle</td>
</tr>
<tr>
<td>Straight-hole injector</td>
<td>φ 0.1 mm x 4 holes</td>
</tr>
<tr>
<td>Included cone angle</td>
<td>140°</td>
</tr>
<tr>
<td>Injection timing sweep</td>
<td>2 - 40°BTDC</td>
</tr>
<tr>
<td>EGR rate</td>
<td>0 , 40%</td>
</tr>
<tr>
<td>Intake temperature</td>
<td>40°C</td>
</tr>
<tr>
<td>Coolant temperature</td>
<td>80°C</td>
</tr>
<tr>
<td>Lube oil temperature</td>
<td>80°C</td>
</tr>
</tbody>
</table>

### Table 3-2 Test fuel properties (JIS#2 diesel fuel)

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cetane number</td>
<td>57-60</td>
</tr>
<tr>
<td>Density (@15°C g/cm³)</td>
<td>0.8217</td>
</tr>
<tr>
<td>Lower heating value (kJ/kg)</td>
<td>42.9</td>
</tr>
<tr>
<td>Sulfur mass (ppm)</td>
<td>&lt;10</td>
</tr>
<tr>
<td>Flash point (°C)</td>
<td>64</td>
</tr>
</tbody>
</table>
3.1.2 Optical engine

The use of optical engine helps to gain insight into the combustion chamber by making some of the parts with transparent materials. Different materials are used but the most commonly used are the sapphire and quartz. The amount of optical access varies from engine to engine. Figure 3-2(a) and (b) shows the schematic diagram and pictorial view of the optical accessible engine used in this work. It has access from below through the piston crown. To achieve this cylinder head is lifted up; the piston is extended with a 45° angled mirror installed at the bottom of the piston extension.

Figure 3-2(a) Schematic diagram of the optical accessible engine
The purpose of using optically accessible engine is to be able to gain understanding of the combustion processes in the all-metal (test engine) and hence it is desirable to make a small change in the engine as much as possible. The combustion process might be affected by the changes in heat transfer and flow pattern.

In this work a single cylinder optical accessible engine was used. The engine was warmed up to by circulating heated coolant maintained at 80°C as the test engine. To avoid the risk of sapphire window failure due to thermal and mechanical stress the engine was operated on skip fire mode. The maximum field of view was 62 mm diameter in a bore of 96 mm. Combustion images were obtained at a frame rate of 13,000 fps with a resolution of 400×400 pixels; thus, images could be taken at crank angle (CA) intervals of 0.462°.

In order to measure the spectra of intermediate species in PCCI diesel engine under moderately early injection timing two spectrometers were used namely: SR163i with a
spectral range of 250 – 800 nm and a centre wavelength of 423 nm and while for the short wavelength and higher resolution MS257 with the centre wavelength of 390 nm and spectral range of 350-450 nm was used.

The experimental setup comprised of three key components namely: the spectrometer connected to the engine using the fibre optics probe, pulse generator to synchronize the engine and the spectrometer, data acquisition and storage in the computer. Two different diameters of optical fibre were considered namely: 200 μm for the lower resolution and 400 μm for the high resolution spectrometer. Figure 3-3 shows the spectroscopic measurement experimental set. The flame emission time series was detected with the spectrometer in the range of 250 to 800 nm with an exposure time of 3° crank angle or 0.5ms.

Figure 3-3 Spectroscopic analysis experimental set up
3.2 Calibration and definitions

In order to be sure of the quantity of fuel injected per cycle a calibration test was carried out. The test was done to determine the energizing time for each injection cycle at the two injection pressures of 80 MPa and 140 MPa chosen. This was performed in order to be sure of the injection quantity per cycle for each condition considered. Figure 3-4 shows the injected amount of fuel as a function of the energizing time for single injection mode.

Ignition delay is defined as the duration between the start of injection (SOI) and start of combustion (SOC). In our experiment an injection delay of 1.5°CA was noted between the start of actuation (SOA) and start of injection. This was accounted for in the estimation of the ignition delay. During the ignition delay the fuel and air would premix before the onset of combustion. Figure 3-5 shows the definition of ignition delay adopted in our study. As shown in Figure 3-5 SOC corresponds to the second derivative of the rate of heat release first positive peak. This point corresponds to the start of the high temperature combustion. Throughout the thesis the start of actuation would be considered as fuel injection timing.

![Figure 3-4 Fuel injection quantity calibration chart for $P_{\text{inj}} = 80$ and 140 MPa](image)

**Figure 3-4** Fuel injection quantity calibration chart for $P_{\text{inj}} = 80$ and 140 MPa
Figure 3-5 Definition of the ignition delay duration. In-cylinder pressure, ROHR and pulse injection signal

Figure 3.6 show pressure transducer calibration curve. To ensure that the pressure transducer was giving the accurate measurement frequent calibration was done. The constant of proportionality between the in-cylinder pressure and voltage was found to be 10.2 for the current experimental work.

Figure 3-6 Pressure calibration of the piezoelectric transducer
The main purpose of the spectrograph is to split the incoming light spectrum into its specific component wavelength. The most essential parameter of the spectrograph is the grating, which can be moved to cover different ranges of wavelengths. The resulting light spectrum is captured by a CCD camera for further analysis.

In order to determine the accurate wavelengths of the light spectrum, the spectrograph and CCD camera have to be calibrated. A Mercury (Hg) spectral calibration lamp with several distinct peaks in the range of 250 – 550 nm was used for that purpose. The calibration lamp was attached to a fiber optic adapter and the light spectrum was captured by the CCD camera. The peaks in the spectrum were then assigned specific wavelength values corresponding to the calibration lamp specification. Based on this information, the CCD controller software automatically determined the wavelength values of the other pixels in the camera. The same procedure was repeated for different grating positions to cover all the wavelength range of interest. Figure 3-7 shows the light spectrum of the calibration lamp for different grating positions. The calibration lamp emission is characterized by several sharp peaks in the UV and visible wavelength region.

![Figure 3-7 Mercury spectral calibration lamps with specific spectrum wavelength](image)
3.3 Rate of heat release (ROHR).

If the pressure inside the cylinder as function of volume is known, the apparent rate heat release can be calculated. The in-cylinder volume as function of crank angle, $\theta$, can be expressed as [1],

$$V = V_c \left\{ 1 + \frac{1}{2} (r_v - 1) \left[ R + 1 - \cos \theta - \left\{ R^2 - \sin^2 \theta \right\}^{0.5} \right] \right\}$$

where, $V_c$ is the clearance volume, $r_v$ is the compression ratio, $R$ is the ratio between the connecting rod and the crank radius. The apparent rate heat release gives information about the combustion process and is a useful tool in combustion engine diagnostics. The following is a description of the heat release theory in [1-2]. In heat release analysis the cylinder is considered a thermodynamic system with uniform pressure and temperature. According to the first law of thermodynamics the energy balance of such a system can be expressed as

$$\frac{dQ}{dt} = \frac{dU}{dt} + \frac{dW}{dt} + \sum_i m_i h_i$$

where $dQ/dt$ is the heat added to the system, $dU/dt$ is the change in internal energy, $dW/dt$ is the work performed by the system, $m$ is the mass, and $h$ is the enthalpy for an element, $i$, that enters the system. The internal energy, $U$, can be expressed as

$$U = mC_v T$$

where $C_v$ is the specific heat at constant volume and $T$ is the temperature. If the mass in the system is constant the derivative of $U$ is

$$\frac{dU}{dt} = mC_v \frac{dT}{dt}$$

From the ideal gas law
\[ pV = mRT \] 

(5)

where \( V \) is the volume and \( R \) is the specific gas constant, it follows that

\[ \frac{dT}{T} = \frac{dV}{V} + \frac{dp}{p} \] 

(6)

Considering \( R \) and \( m \) are taken to be constant. Using Eq. 5 and 6, Eq. 4 can be rewritten in the form

\[ \frac{dU}{dt} = \frac{C_p}{R} \left\{ p \frac{dV}{dt} + V \frac{dp}{dt} \right\} \] 

(7)

The work performed by the system can be expressed as

\[ \frac{dW}{dt} = p \frac{dV}{dt} \] 

(8)

Neglecting mass exchange and using Eq. 7 and 8, Eq. 2 can be rewritten as

\[ \frac{dQ}{dt} = \frac{C_v}{R} \left\{ p \frac{dV}{dt} + V \frac{dp}{dt} \right\} + p \frac{dV}{dt} \] 

(9)

The specific gas constant can be expressed as

\[ R = C_p - C_v \] 

(10)

where \( C_p \) represent the specific heat ratio at constant pressure and \( C_v \), specific heat ratio at constant volume. Eq. 10 and the ratio
\[
\gamma = \frac{c_p}{c_v}
\] (11)

can be used to simplify Eq. 9 into

\[
\frac{dQ}{dt} = \frac{\gamma}{\gamma-1} p \frac{dV}{dt} + \frac{1}{\gamma-1} V \frac{dp}{dt}
\] (12)

Since both the volume and pressure trace are more commonly expressed as a function of Crank Angle Degree (CAD), \(\theta\), Eq. 12 is more useful in the form

\[
\frac{dQ}{d\theta} = \frac{\gamma}{\gamma-1} p \frac{dV}{d\theta} + \frac{1}{\gamma-1} V \frac{dp}{d\theta}
\] (13)

This equation is referred to as the apparent heat release. The above procedure assumes zero mass transport across the system boundary. In reality this is not the case. To handle the mass losses mathematically correct requires Eq. 4 to be rewritten which affects the subsequent steps. It is, however, more common to assume that the mass losses are small enough to be handled in a separate term

\[
\frac{dQ}{d\theta} = \frac{\gamma}{\gamma-1} p \frac{dV}{d\theta} + \frac{1}{\gamma-1} V \frac{dp}{d\theta} + \frac{dQ_{losses}}{d\theta}
\] (14)

where, \(dQ_{losses}\) consists of mass losses combined with heat losses. The losses decrease the in-cylinder pressure and if they are not considered, the calculated heat release is lower than the actual heat release. The mass losses mainly consist of leakage over the piston rings. This phenomenon is referred to as blow by.
3.4 Engine performance

With known in-cylinder pressure and cylinder volume the indicated work and pumping work can be evaluated. Figure 3-8 shows the PV diagram for the 4-stroke diesel engine.

\[
W_{c,i} = \int p \, dV = \text{Area } A + \text{Area } C
\]  

(15)

The indicated work per cycle \( W_{c,i} \), is obtained by integrating around the curves to obtain the area enclosed by the p-V diagram.

The pumping work can be obtained by integrating around the p-V diagram over the exhaust and intake strokes.

\[
W_p = \int p \, dV = \text{Area } B + \text{Area } C
\]

(15)

Whereas the gross indicated work per cycle is calculated from the compression and expansion strokes

\[
W_{kg} = \int p \, dV = \text{Area } A + \text{Area } C
\]

(16)

For four stroke engine, the net indicated work per cycle is work delivered over the entire four stroke cycle.
Chapter 3: PCCI diesel engine and its diagnostics

\[ W_{ln} = \int pdV = (\text{Area A} + \text{Area C}) - (\text{Area B} + \text{Area C}) = \text{Area A} - \text{Area B} \quad (17) \]

This means that net indicated work per cycle equals the gross indicated work minus the pumping work. When discussing indicated quantities like “indicated” work per cycle or power it is recommend that you state explicitly whether it is gross or net [1]. For the purpose of our discussion in this thesis we will consider the net indicated output since in our experiments we dealt with naturally aspirated conditions.

The indicated power per cylinder is related to the indicated work per cycle by

\[ P_i = \frac{W_i N}{n_R} \quad (18) \]

where \( n_R \) is the number of crank revolutions for each power stroke per cylinder at normally taken as 2 for four-stroke engine. \( N \) is the engine crank shaft speed rev/s. The net indicated power output represent the summation of useful work available at the shaft and the work required to overcome all the engine losses. Brake power output can be measured by the dynamometer and this allows the evaluation of friction power (friction power = indicated power – brake power) and the actual useful work available at the wheels.

From the p-V diagram we can also determine the indicated mean effective pressure (IMEP), an essential parameter which is a good indicator of the performance of the engine.

\[ \text{IMEP} = \frac{W_i}{V_d} \quad (19) \]

Hence, indicated thermal efficiency would be given by,

\[ \eta_i = \frac{\text{Work per cycle}}{\text{Input energy}} = \frac{\text{IMEP} \times V_d}{m_f Q_{LHV}} \quad (20) \]
where \( m_f \) is the mass of fuel inducted per cycle and \( Q_{\text{LHV}} \) the low heating value of the fuel. In our case we considered the low heating value was 42.9MJ/kg. In our experiment the density of the fuel was found to be very critical and was selected as shown in table 3-2. The cyclic variation of diesel engine can be estimated form the coefficient of variance (COV) of the individual IMEP values. COV is defined as the ratio of the standard deviation in IMEP and the mean IMEP.

\[
\text{COV} = \sqrt{\frac{\sum_{1}^{n}(\text{IMEP} - \overline{\text{IMEP}})^2}{\text{IMEP}}} / (n-1)
\]

(20)

where \( n \) is the number of cycle. In our experiments we sampled 84 cycles for each case.

### 3.5 Emissions measurement

One of the objectives of internal combustion engine researches is geared to minimizing the exhaust emissions to the environment due to the ever stringent emission regulation hence; the measurement of the exhaust emissions becomes very essential. Whereas optical diagnostics and rate of heat release analysis are performed to analyze the combustion process, exhaust emission measurement gives more details on the operating conditions. Among the most harmful exhaust emissions from diesel engines are PM, NO\(_x\), unburned hydrocarbon (UHC), and carbon monoxides (CO). PM consist of both solid and liquid components. A larger part of it is made of soot particles.
3.5.1 Smoke

Smoke and smoke opacity meter has been used to measure the optical properties of diesel exhaust. The instruments are designed to quantify the visible black smoke emissions by utilizing such physical properties as the extinction of a light beam by scattering and absorption.

\[
\text{Opacity} = 1 - \frac{E}{E_0} = 1 - \exp[-KL]
\]

where:

\begin{align*}
E_0 &= \text{light intensity before the smoke sample cell, W/cm}^2 \\
E &= \text{light intensity after the smoke sample cell, W/cm}^2 \\
K &= \text{extinction coefficient, 1/cm} \\
L &= \text{light path length, cm.}
\end{align*}

Opacities are typically expressed in percentage values where 0% value represents clear air and 100% opacity represents the infinite smoke. In general opacities of 2% are not visible to the naked eye whereas opacities higher than 5% present clearly visible plumes.
of smoke. The results of the opacity measurement can be also given as the extinction coefficient K. Opacity meters typically have a resolution of $K = 0.01 \text{ m}^{-1}$. Opacity meters and principles are defined by ISO 11614 standard.

### 3.5.2 Nitrogen oxides (NO$_x$)

NO$_x$ measurement is achieved through the chemiluminescence technique. Chemiluminescence is the light emission from an atom or molecule that is electronically excited by a chemical reaction. Ozone O$_3$ generated by the chemiluminescence detector (CLD) instrument reacts with the nitric oxide (NO) resulting in an electronically excited NO$_2$ nitrogen dioxide and O$_2$. When the excited NO$_2$ returns to the ground state it emits a photon (in terms of light - $h\nu$) with a wavelength between 600 and 3000nm.

$$\text{NO} + \text{O}_3 \rightarrow \text{NO}_2^* + \text{O}_2 \rightarrow \text{NO}_2 + \text{O}_2 + h\nu$$  \hspace{1cm} (22)

A photomultiplier is used to measure the light and is amplified before it is converted to the concentration of NO. Since CLD only measure NO, the nitrogen dioxide is passed through a catalyst that converts NO$_2$ to NO then measure. Detection before and after the catalytic converter corresponds to the emissions of NO and total NO$_x$, where the difference gives the value of the NO$_2$. Regular calibration with known concentration of NO and NO$_2$ of the CLD is required [references].

### 3.5.3 Unburned hydrocarbon

Unburned hydrocarbon (UHC) found in gas phase of diesel exhaust are a mixture of many hydrocarbon species derived from diesel fuel and from lubricating oil. UHC is measured with the Flame Ionization Detectors (FID). The exhaust gas is burned in a carbon free flame, normally hydrogen–helium environment i.e. 40% hydrogen and 60% helium and fed between two electrodes with an applied voltage. The UHC in the exhaust results in ionized carbon and free electrons. The carbon ions are positive and are subsequently pulled to the negative electrode. The resulting current is proportional to the number of carbon atoms in the UHC. The calibration of FID should be accomplished with a zero UHC gas for example nitrogen gas and a gas containing a known UHC concentration on a regular basis [references].
### 3.5.4 Carbon monoxide(CO) and carbon dioxide(CO$_2$)

Infrared analyzers are commonly used for measurement of the concentration of CO and CO$_2$. Their principle of operation is based on the absorption of infrared radiation (IR) of these gases. The instrument consists of one sample cell, one reference cell and one detector cell. The exhaust gas flows through the sample cell while the reference cell contains air. The sample and reference cell are illuminated with IR radiation and the transmitted radiation is measured or detected. The detector is comprised of a third cell filled with the gas to be measured either CO or CO$_2$. The detector is subdivided in two sections with a membrane in between. One side of the membrane collects the transmitted radiation through the sample cell while the other through the reference cell. If the exhaust contains the analyzed gas the sample cell will absorb some of the radiations implying that the sample cell side of the detector will then collect fewer radiations. The gas on the opposite side of the detector cell will expand in proportion to the absorbed radiations. The membrane would bulge in the sample side of the detector and the bulge is in relation to the concentration of the measured gas. The amount of the radiation absorbed is given by the Beer’s law,

$$a_\lambda = 1 - \exp(-C_iQ_\lambda L)$$  \hspace{1cm} (23)

Where, $C_i =$ the concentration of species i

$Q_\lambda =$ the absorption efficiency

$L =$ the optical path length

Carbon monoxide absorbs radiation at about 4.6$\mu$m while carbon dioxide at about 4.2$\mu$m wavelengths. The use of optical filters eliminates absorption from gases with interference absorption spectra. The NDIR requires regular calibration using a gas with zero CO or CO$_2$ for example nitrogen gas and a gas containing known concentrations of CO or CO$_2$.

### 3.1 Optical diagnostics

Different optical diagnostics techniques can be used depending on the purpose of the optical engine. Optical measurement techniques can be classified as either passive or
active. In passive optical measurement technique the combustion phenomenon is imaged as it is without interference. Therefore all the passive optical measurements give a line-of-sight perspective of the combustion chamber. Among the limitation of this technique is the fact that it is difficult to image the inside of a reacting flame and only intermediate species that radiate naturally can be imaged.

In active optical measurement technique, an external radiation source is utilized to actively generate the radiation from the measurement volume. This gives the advantage of investigating the interior of the flame and more intermediate species can be studied. Depending on the accessibility of the combustion chamber the active optical measurement technique can allow for measurement on point, a long a line, in a plane or in three dimensions.

### 3.1.1 High speed video camera

The use of high speed camera is classified as a passive optical diagnostic technique. This can enable you to record the natural combustion radiation like soot luminosity and chemiluminescence from different gas molecules. The soot luminosity is normally dominant and emits radiation of hot soot particles characterized by a continuous broadband spectrum as a black body radiator. Chemiluminescence arises from excited combustion radicals due to exothermic chemical reactions occurring during the auto-ignition process. Generally the soot luminosity is comparable or of greater magnitude than the chemiluminescence after ignition. When specific radicals are studied the camera can be equipped with a band-pass spectral filter that would isolate the specified radical wavelength.

Hydroxyl radical (OH), an important intermediate combustion species in high temperature chemistry are commonly imaged at a wavelength of 308nm. The images of OH radicals give information on where the high temperature reactions occur.

Table 3.1 shows the specification of the high speed video camera used in our investigation. Figure 3-10 shows the high speed video camera used in this investigation.
## Table 3-1 NAC’s Memrecam GX-1 High-speed Color Video Camera

<table>
<thead>
<tr>
<th>Recording method</th>
<th>CMOS sensor technology</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resolution</td>
<td>1280 X 1024 pixels,(depend on camera speed)</td>
</tr>
<tr>
<td>Frame storage</td>
<td>Over 100 frames</td>
</tr>
<tr>
<td>Color, Gradations</td>
<td>&gt;20,000 ISO monochrome, &gt;5,000 ISO color</td>
</tr>
<tr>
<td>Recording speed</td>
<td>50fps to 200,000fps</td>
</tr>
<tr>
<td>Exposure time</td>
<td>adjustable</td>
</tr>
<tr>
<td>External trigger In</td>
<td>TTL (positive/negative), switch closure</td>
</tr>
<tr>
<td>Trigger mode</td>
<td>Set trigger point at any desired frame</td>
</tr>
<tr>
<td>Recording format</td>
<td>8-bit dedicated format, BMP, AVI</td>
</tr>
</tbody>
</table>

![High-speed video camera (GX-1, nac Image Technology)](image)

Figure 3-10 GX-1 NAC Image Technology
3.1.2 Spectrograph

In order to understand reaction mechanism of auto-ignition and combustion mechanism in a PCCI engine, one effective way is spectrum analyses of chemiluminescence to determine the major active species. Chemiluminescence emission arises from specific molecules that are raised to an excited state by exothermic chemical reactions and then subsequently decay back to equilibrium energy level by emitting a photon. It occurs in specific wavelength bands that are characteristic of the emitting molecule. They are specific molecules responsible for the chemiluminescence change for different combustion phases and this can provide information about the nature of the reactions and the fuel/air mixture [3]. Because chemiluminescence is produced directly by exothermic reactions, it marks the location of initial combustion reactions temporally and spatially, with the limitation that the signal is integrated along line of sight. Dec and Espey did chemiluminescence imaging of auto-ignition in diesel engine[4]. Their spectral data showed that chemiluminescence arose from formaldehyde and CH emission with no OH emission detected. In contrast, the sooting–combustion spectrum (taken after diffusion flame had formed) showed OH and “gray-body” soot emission.

3.1.2.1 Shamrock SR163i Spectroscope with ICCD:

The luminescence spectrum of the premixed flame of the diesel fuel in the end gas region was measured by using spectroscope - Shamrock SR163i manufactured by the ANDOR TECHNOLOGY® with ICCD. The wavelength resolution is lower with an approximate value of 1.57nm depending on the grating. It is possible to measure 200nm to 800nm wavelength range and at same time set the wavelength at the centre manually. Figure 3-11 shows the Shamrock SR163i spectroscope with ICCD used in this research.

3.1.2.2 MS257 Type Imaging Multichannel Spectroscope:

The MS257 1/4 m Monochromator is a completely automated, efficient 1/4 m instrument, with enough versatility to satisfy most spectroscopy applications. Stray light is negligible, and there is no re-entrant spectrum. Four gratings are installed in the MS257 type imaging multi channel spectroscope. The wavelength precision is ±0.1 nm, and the
wavelength resolution is high. Figure 2-12 shows the MS257 type imaging multichannel spectroscope.

Figure 3-11 Shamrock SR163i spectroscope with ICCD

Figure 3-12 MS257 type imaging multichannel spectroscope
Calibration lamp

Frequent calibration of the spectrograph was done to ensure accurate measurement of the spectrum could be achieved using an UVP 90-0019-01 Mercury spectrum calibration lamp. Lamp's lighted length is 2.12" (53.8mm) and outer diameter to 0.375" (9.5mm). Lamp’s quartz tube is covered with a blue filter to absorb visible light. Lamp emits Mercury spectrum with the primary energy at 254nm. The principal emission is at 365nm wavelength (long wave) by converting the power from 254nm. The Hg calibration lamp is powered by a DC power supply to ensure constant light intensity throughout the whole calibration process. The spectral calibration lamp is mounted in a fiber optic adapter and the emitted light is transferred to the spectrograph using an UV-VIS optical fiber. Figure 3-13 shows the UVP standard pen-ray mercury lamp.

![UVP's standard Pen-Ray® Mercury Lamp](image)

**Figure 3-13** UVP's standard Pen-Ray® Mercury Lamp

Optical fibre

In order to collect the light emitted during combustion process from the cylinder an optical access to the cylinder is required. DIAGUIDE optical fiber is made of silica glass and is especially well suited for applications with high power laser beam guide. SI (Step Index) type fiber uses pure silica core with Aramid Fiber Yarn Reinforced PVC Sheathed Fiber. The high OH silica in the fiber is capable of transferring light from UV to visible (250 to 800 nm).
Figure 3-14 shows the DIAGUIDE optical cable and Table 3-2 shows the optical cable specifications.

![DIAGUIDE optical cable](image)

**Figure 3-14 DIAGUIDE optical cable**

**Table 3-2 Optical cable specifications**

<table>
<thead>
<tr>
<th>Type</th>
<th>Product</th>
<th>Core Dia. (μm)</th>
<th>Fiber Dia. (μm)</th>
<th>Outer Dia. (mm)</th>
<th>Allowable Tension Strength (N)</th>
<th>Allowable Bending Radius (mm)</th>
<th>Color</th>
</tr>
</thead>
<tbody>
<tr>
<td>SI</td>
<td>STU200-FV</td>
<td>200/400</td>
<td>500</td>
<td>4</td>
<td>80</td>
<td>100</td>
<td>Black</td>
</tr>
</tbody>
</table>

### 3.2 Image acquisition and processing

The raw images were captured with a high speed video camera from the bottom view of the optically accessible engine. The image intensity before fuel injection was subtracted from the image intensity at a specific time during combustion. This eliminated background light so that only the magnitude of the light emitted from the flame could be plotted. The resultant colour image was then separated into its corresponding red, green, and blue (RGB) components. The red component was representative of the soot forming regions in the flame and plotted as a final processed image. This was achieved through in-house programming in MATLAB. Figure 3-15 shows image processed from raw data to processed one.
3.3 Experimental conditions

The experimental conditions for the present research varied according to the specific experiment conducted. This would be shown on the specific part of the thesis.
3.4 References
Chapter 4

Effect of compression ratio and EGR on combustion and exhaust emission characteristics of a PCCI diesel engine

4.1. Introduction

The aim of reducing the compression ratio is to reduce the in-cylinder temperature and thus the adiabatic flame temperature during combustion to suppress NO\textsubscript{x} emissions. However, major reductions have not been achieved to date because of the associated negative effects on cold-start capability [1]. Lower compression ratio has been found to be effective in extending the ignition delay due to the low compression pressure and reduced charge temperature[2]. Recent studies done by Asad et al. [3] shows that lower compression ratio could aid in extending the engine load of PCCI combustion concept, while a combination of both intake boost and injection pressure is essential to maintain low-NO\textsubscript{x} and low-soot emissions and to mitigate the indicated thermal efficiency penalty. In this section effects of compression ratio and EGR on combustion and exhaust emission characteristics of a Diesel PCCI engine would given in detail.

4.2. Experimental set up and procedure

The experimental set up is as shown in Figure 3-1. For this particular experiment the engine speed and intake pressure was kept constant at 1000rpm and 101kPa. The injection pressure chosen was 80 MPa. This was to chosen to isolate the effect of compression ratio easily.

![Figure 4-1 Piston-head configuration](image)

Table 4-1 Compression ratio and depth

<table>
<thead>
<tr>
<th>CR</th>
<th>Depth (d) mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>11.2</td>
</tr>
<tr>
<td>14</td>
<td>12.6</td>
</tr>
<tr>
<td>13</td>
<td>14.25</td>
</tr>
<tr>
<td>12</td>
<td>16.25</td>
</tr>
</tbody>
</table>
The injection timing and EGR rate was varied while all the measurements of exhaust emissions and in-cylinder pressure were carried out when the engine was believed to be in a stable condition.

Real EGR contains CO$_2$, H$_2$O, N$_2$ and O$_2$ in thermodynamically significant quantities and CO, THC, NO$_x$ and soot in thermodynamically insignificant quantities. The effect of real EGR can be divided into three namely; dilution effect, thermal effect and chemical effect. Ladommatos et al. [4] Abd-Alla G.H. [5] and Zheng et al. [6], have noted that the dilution effect is substantial compared to the chemical and thermal effect on combustion and exhaust emissions. This has been found to be effective in extension of ignition delay and reduction of NO$_x$ at the expense of higher particulate and unburned hydrocarbon. The real EGR system would be considered in future work. In this work we considered the effect of nitrogen dilution, which has been studied previously [7] in our laboratory. The baseline tested compression ratio (CR) was 15 with a Derby hat piston-head configuration. A reduction in the compression ratio was obtained using different piston heads with different bowl depths (varying the value of d), while the same bowl shape was maintained, as shown in Figure 4-1 and Table 4-1. The Derby hat piston-head configuration was chosen to allow spray to be guided into the piston bowl, thus promoting the mixing of the air and fuel within the piston bowl, avoiding cylinder-wall wetting under moderately early injection timing. Recent research [8] on diesel engines has focused on narrow-angle wall-guided sprays when considering late injection timing. While it is a promising technology, a flexible system that can enable an easier transition to conventional diesel combustion is still needed. For an easier transition from the PCCI regime at moderately early injection timing to conventional diesel combustion, a slightly narrowed angle of 140° with the Derby hat piston geometry was used in this study.

4.3. Results and discussions

4.3.1. Effect of compression ratio on rate of heat release

In order to understand the combustion characteristic of a PCCI engine operated with varying compression ratios, the rate of heat release was investigated for all the cases. Figure 4-2 shows the pressure history and the rate of heat release (ROHR) for the
different compression ratios (CRs) at an injection timing of 20° BTDC. The in-cylinder pressure decreased as the compression ratio was reduced from 15 to 12. The same trend was observed with the ROHR. This is consistent with the expected trend because the in-cylinder temperatures would decrease as the compression ratio is decreased [2]. Under conditions of CR12, the ignition delay was increased compared with CR15 because of the lower in-cylinder compression pressure and charge temperature. With CR14 and above, a knocking phenomenon and in-cylinder pressure fluctuations were noted. CR13 was observed to have normal combustion with a smooth pressure curve.

To further clarify trends in the PCCI combustion regime, the rate of heat release under CR13 was investigated in detail. Figure 4-3 shows the rate of heat release at different injection timing for CR13. Late injection timing leads to predominantly premixed combustion, with a slight proportion of diffusion-controlled combustion. This combustion is slightly different from conventional diesel combustion because a large portion was premixed. Early injection timing of $\theta_{\text{inj}} \geq 20°$ BTDC exhibited a two-stage ignition, with the first stage representing the low-temperature oxidation (LTO) and the second stage, the high-temperature oxidation (HTO) phenomenon, predominant in PCCI combustion.

![Graph showing in-cylinder pressure and ROHR for different compression ratios at $\theta_{\text{inj}} = 20°$ BTDC](image)

Figure 4-2 Pressure history and ROHR for the tested compression ratios at $\theta_{\text{inj}} = 20°$ BTDC
Chapter 4: Effect of compression ratio and EGR on combustion and exhaust emission characteristics of a PCCI diesel engine

4.3.2. Effect compression ratio on performance

To understand the relationship between the compression ratio and engine performance within a diesel PCCI engine, indicated thermal efficiency, IMEP, and coefficient of variance of IMEP were analyzed in detail. Figure 4-4 shows the effect of compression ratio on indicated thermal efficiency and IMEP. As the injection timing was advanced, it was noted that the indicated thermal efficiency and IMEP decreased for all the compression ratios tested, but with greater decreases for higher compression ratios. A compression ratio of 14 and above led to lower indicated thermal efficiency and IMEP under moderately early injection timing. This was thought to be due to poor fuel combustion and higher negative work. Of all the cases investigated, CR13 showed superior values, more so with moderately early injection timing without EGR i.e. in the PCCI regime.
4.3.3. Effect of compression ratio on specific emissions

To further understand the relationship between different compression ratios and specific engine emissions in a diesel PCCI engine, a detailed investigation was conducted. Figure 4-5 shows the specific emissions as function of injection timing for various compression ratios. CO and HC showed similar trends in that as the injection timing was advanced, the emissions increased. This could be attributed to low in-cylinder temperature, density and pressure leading to higher fuel-spray penetration, causing fuel to be deposited on the cylinder wall and hence, incomplete combustion.

Figure 4-4 Indicated thermal efficiency and IMEP as a function of injection timing for the tested compression ratios
NO\textsubscript{x} increased drastically as the injection was advanced to a maximum at 20° BTDC, and then decreased thereafter. Smoke emission showed lower values under the retarded condition, but increased as the injection was advanced. For all the cases considered, CR12 had the highest emissions of smoke, HC, and CO with the lowest emission of NO\textsubscript{x}, whereas CR15 had the highest emission of NO\textsubscript{x} with the lowest emissions of HC, smoke, and CO. Of all the test conditions considered, CR13 had approximately the same emissions of HC, CO, and smoke as CR15, but with slightly lower emissions of NO\textsubscript{x}. This observation leads us to conclude that there is an optimum value of compression ratio below which the exhaust emission deteriorates. In this case, CR13 was noted to be the optimum compression ratio for exhaust emissions.
A tradeoff was observed between smoke and NO\textsubscript{x} emissions. An increase in NO\textsubscript{x} was accompanied by a corresponding decrease in smoke. Higher in-cylinder temperatures enhanced production of NO\textsubscript{x} but lead to rapid oxidation of smoke, and the converse is also true. Lower temperatures led to a longer ignition delay, which gives the air–fuel mixture sufficient time to premix, thus avoiding fuel-rich zones, which burn with soot while at the same time inhibiting the formation of NO\textsubscript{x}. CR12 clearly had the highest emissions of smoke, which was considered a limiting factor despite the low NO\textsubscript{x} emissions, whereas CR14 and above led to knocking and high pressure fluctuations with lower fuel conversion efficiency and IMEP. Of all the investigated compression ratios, CR13 was considered the most appropriate because it had the best indicated thermal efficiency, IMEP, and exhaust emissions. This compression ratio was selected for further analysis of combustion characteristics and exhaust emissions under different amounts of EGR rate.

### 4.3.4. Effect of EGR on rate of heat release

EGR has been noted in the literature to improve IMEP and to extend the ignition delay[9-10]. In conventional diesel combustion, it has been used to control emissions of NO\textsubscript{x} through charge dilution and lowering the adiabatic flame temperature. In this section, an in-depth analysis of the effects of EGR on performance and emissions will be presented.

The in-cylinder pressure history and ROHR with and without EGR are shown in Figure 4-6. Late injection timing led to typical diesel combustion, dominated by premixed combustion and a small diffusion-controlled combustion proportion. The injection duration was 9.2° CA, which ended during the premixed-combustion phase. Advancing the injection timing beyond 20° BTDC, the heat-release pattern exhibited PCCI combustion with two-stage heat release. The first was attributed to low-temperature combustion, and the second to high-temperature combustion, separated by a short delay due to the negative temperature coefficient (NTC) ignition behavior of the mixture. At 30° BTDC, a decrease in peak in-cylinder pressure and ROHR was noted as a result of the leaner mixture formed because ignition delay was prolonged due to the low charge
temperature at the time of injection.

Under EGR conditions, the ignition timings of both LTO and HTO were greatly affected due to the dilution effect. A greater influence of EGR was seen with \( \theta_{\text{inj}} = 10^\circ \) and \( 15^\circ \) BTDC, where the start of combustion was delayed into the expansion stroke where the in-cylinder temperature was rapidly decreasing, and the rate of heat release was slowed down.

![Graphs showing in-cylinder pressure history and rate of heat release with 0% and 40% EGR rates.](image)

Figure 4-6 In-cylinder pressure history and rate of heat release with 0 and 40% EGR rates.
The combustion characteristic at $\theta_{\text{inj}} = 15^\circ$ BTDC is typical of the modulated kinetics of combustion proposed by Kimura et al.[11], although we achieved this without employing heavy EGR and high swirl as they did. For moderately early injection timing, the LTO and HTO phases were clearly seen despite the fact that they were phasing before TDC. With the introduction of EGR, the ignition delay was prolonged and this promoted the air-fuel mixing before combustion.

### 4.3.5. Effect of EGR on performance

To understand the effects of EGR on performance in the diesel PCCI engine, an investigation was carried out. Figure 4-7 shows the effect of EGR on indicated thermal efficiency, IMEP, and the coefficient of variance of IMEP ($\text{COV}_{\text{IMEP}} (%)$). As the injection timing was advanced, the indicated thermal efficiency and IMEP gradually decreased with or without EGR. The highest IMEP corresponded to phasing close to the TDC ($-2^\circ$ ATDC) without EGR. With the introduction of 40% EGR, higher indicated thermal efficiency and IMEP were observed across the injection sweep, apart from late injection, where a marked reduction was observed. This could have been due to over-mixing, leading to an air–fuel mixture that was too lean to burn or fuel wall quenching. In conventional diesel combustion, advancing the injection timing leads to higher pressure-rise rates but drastically reduces in PCCI combustion regime. This could be attributed to the fact that in conventional diesel combustion, the premixed part burns very fast, whereas in PCCI, a longer premixing time and a lower in-cylinder temperature results in milder combustion. As the amount of EGR introduced increases, the pressure-rise rate drastically declines because of the dilution effect, leading to extended ignition delay and milder combustion. The combustion phasing was noted to retard with the introduction of EGR, correspondingly leading to improvement in the IMEP because the in-cylinder temperature was reduced, resulting in milder combustion coupled with the fact that negative work was greatly minimized. The $\text{COV}_{\text{IMEP}}$ was not affected with or without EGR for the injection timings considered. The values were in the range of 1–3%, indicating that the combustion process was stable under these conditions.
4.3.6. Effect of EGR on specific emissions

In PCCI combustion, it is common to use EGR to lower the adiabatic flame temperature. This reduces NOx at the expense of increased emissions of HC and CO. Figure 4-8 shows the effect of EGR on smoke, NOx, CO, and HC emissions. In cases without EGR, as the injection timing was advanced, NOx emissions drastically increased, up to a maximum at 20° BTDC, and then declined drastically in more advanced conditions. This could be due to the high temperature, which promotes NOx emissions and a very short time for fuel–air mixing prior to combustion. PCCI conditions with early
injection above 30° BTDC and all cases with 40% EGR achieved very low emissions of \( \text{NO}_x \). This was attributed to the reduced local flame temperature and reduced concentration of oxygen in the intake charge.

Early injection timing, \( \theta_{\text{inj}} = 30° \) BTDC and above, without EGR was observed to lead to excessive smoke emissions. This could be attributed to a low in-cylinder temperature that did not allow the soot formed from the rich fuel impinging on the surface of the piston to be oxidized. Smoke emissions below 2% were achieved for \( \theta_{\text{inj}} = 2 \) to 30° BTDC with 40% EGR and with no EGR. When the injection timing was advanced, the in-cylinder temperature, density and pressure decreased, and fuel-spray penetration was enhanced, leading to fuel deposits on the surface of the piston, providing a source of fuel-rich zones and promoting smoke emission. The emission of smoke in conventional diesel combustion is less than that in PCCI combustion regime. The major purpose of PCCI combustion is not to completely eliminate smoke but to reduce it to acceptable levels. It has been noted by many researchers that it is possible to obtain simultaneous reduction of \( \text{NO}_x \) and soot by incorporating a very large amount of EGR (>67%)[12-13], but this comes at the expense of higher fuel consumption and increased emissions of CO and HC. With 40% EGR, injection timing between \( \theta_{\text{inj}} = 15 \) to 25° BTDC was found to achieve less than 0.5% smoke. This was attributed to the fact that the air–fuel mixture could be well premixed without creating fuel-rich pockets hence, leading to better combustion. The application of EGR increased ignition delay and offered sufficient mixing time for fuel and air before the start of combustion. Figure 4-9 shows the relationship between smoke and \( \text{NO}_x \) without and with 40% EGR. It can be seen that as \( \text{NO}_x \) decreased, the smoke increased, but with the introduction of EGR, it was possible to achieve simultaneous reduction of both emissions under a PCCI combustion regime.

Furthermore, as the injection timing was advanced, CO emissions increased dramatically. Higher EGR led to higher CO. Under a retarded condition with 40% EGR (\( \theta_{\text{inj}} = 10° \) BTDC) CO emissions were slightly higher. This condition could be related to the HC emissions; it could be attributed to the lower temperature and insufficient oxidant for complete combustion. When injection timing is too early, higher emissions could also be associated with piston-bowl wall wetting.
Chapter 4: Effect of compression ratio and EGR on combustion and exhaust emission characteristics of a PCCI diesel engine

Figure 4-8 Effects of EGR on specific emissions

Figure 4-9 Smoke vs. NOx without and with 40% EGR
As the injection timing was advanced, a corresponding increase in HC emissions was observed. This trend was also seen with 40% EGR. This could be attributed to the availability of only a limited amount of oxygen to complete combustion. At $\theta_{\text{inj}} = 10^\circ$ BTDC with 40% EGR conditions, the HC emissions were higher than without EGR. This could be attributed to two effects: over-mixing, where the mixture is too lean to burn, and flame quenching in the expansion stroke. This result is consistent with the work of Han et al. [14] and Colban et al. [15]. To mitigate this problem, it would be desirable to increase the available air mass through supercharging while maintaining the EGR levels.
4.4. Summary

In this section the effects of compression ratio and EGR on the combustion characteristics and exhaust emissions in a diesel PCCI engine has been investigated. A single-cylinder test engine was used. Simulated EGR, consisting of N₂ gas, was used to achieve lower NOₓ. The following are the summary of the findings.

1. PCCI combustion at all the tested compression ratios was achieved with moderately advanced injection timing without using EGR- injection timing of > 20° BTDC. This resulted in lower indicated thermal efficiency and IMEP. A compression ratio of 13 was noted to have lowest emissions of smoke, HC, and CO, reasonable amounts of NOₓ, and better indicated thermal efficiency and IMEP.

2. The introduction of EGR enabled combustion phasing to occur closer to and after TDC with milder reaction rates, thus achieving higher indicated thermal efficiency and IMEP. A 40% EGR rate was found to be sufficient to achieve simultaneously low NOₓ and soot emissions with a slight penalty in HC and CO emissions.
4.5. References


Chapter 5

Effects of spray impingement, injection parameters and EGR on combustion and emission characteristics of a PCCI diesel engine

5.1. Introduction

The interaction between the spray and the combustion chamber plays a critical role in the performance and emissions characteristics of an internal combustion engine. When the fuel impinges on the relatively cold cylinder liner the effects would be increase in unburned HC, CO, smoke and dilution of the lubricating oil. These are very serious problems that need to be addressed to achieve better indicated thermal efficiency with minimum exhaust emissions in internal combustion engines.

In that case the fuel spray phenomena would play an important role in the combustion characteristics and exhaust emissions formation process of a direct injection diesel engine in which the fuel spray is directly injected into the combustion chamber. In addition, the quality of the fuel-air mixture formation would also be affected, this being a very important factor in reducing emissions. Therefore, the spray and atomization characteristics have to be considered to reduce exhaust emission and improve the combustion performance.

To clearly understand the combustion mechanism inside the combustion chamber in PCCI combustion mode there is need to study the effect of spray impingement, injection timing, injection pressure and EGR rate in the preparation of air – fuel mixture, the heat release process and the formation of soot, NO\textsubscript{x} and other combustion products. Visualization of the spray development and combustion process becomes a necessary tool to observe the phenomena and relate this to engine-out emissions. This study shares more understanding in the relationship between injection parameters, mixture formation and combustion process in PCCI combustion mode.
This section would seek to address the effect of spray impingement, injection pressure and EGR on combustion characteristics and formation of exhaust emissions in PCCI engine in detail.

5.2. Experimental set and conditions

The experimental setups used for this study are shown in Figure 3-1 and 3-2. Two injection pressures were chosen 80MPa and 140MPa with a slightly narrow included cone angle of 140° to avoid cylinder wall wetting at moderately early injection timing and low compression ratio of 13. Lower in-cylinder temperature, density and pressure at TDC would allow extension of the ignition delay that would lead to better premixing of fuel and air without EGR. The injection timing was varied to estimate the operating range of PCCI combustion. The in-cylinder pressure and exhaust emission were measured. Visualization of the spray development and combustion phenomena was carried out.

5.3. Results and discussions

5.3.1. PCCI engine operating range

PCCI engine operating range determination is very important in order to be able to know the most suitable range to run the engine. It has been noted by past researcher that there is no precise demarcation boundary between PCCI and standard diesel combustion [8]. In that case reasonable assumptions have to be made. Combustion characteristics in the past have been used to distinguish the difference. PCCI combustion is characterized with short combustion duration and moderately early injection timing with two stage heat release curve. In order to achieve PCCI combustion the premixing time is a critical parameter and should be long enough to allow thorough premixing of the fuel and air to be achieved before start of combustion. The operating range for our experiment for PCCI combustion was achieved with injection timing between 20 -30° BTDC without EGR while with EGR between 10° – 30°BTDC.

5.3.2. Effect of injection pressure on heat release

Rate of heat release and the in-cylinder pressure were used in this study to evaluate the combustion characteristics of the PCCI combustion mode. Figure 5-1 shows
the in-cylinder pressure history and rate of heat release for the injection timings sweep for $P_{\text{inj}} = 80$ MPa and 140 MPa. Each pressure curve was obtained by averaging 84 individual pressure traces. The higher injection pressure, $P_{\text{inj}} = 140$ MPa, led to a higher in-cylinder pressure. In case of retarded conditions, a single heat-release peak was 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. The higher injection pressure resulted in a higher heat-release peak with a rapid burn rate. The higher injection pressure also led to shorter combustion duration.

![Figure 5-1 In-cylinder pressure history and rate of heat release, $P_{\text{inj}} = 80$ and 140 MPa, 0% EGR, $\lambda = 4.5$](Image)

5.3.3. Effect of injection pressure on performance

Indicated mean effective pressure and fuel conversion efficiency has been used in many researches as a mean to evaluate the performance of the engine under the specified operating conditions[1-2]. Figure 5-2 shows the effect of injection pressure on indicated
thermal efficiency, indicated mean effective pressure (IMEP), and the coefficient of variance of the IMEP. For conventional diesel combustion, advancement of the injection timing led to a simultaneous reduction in the indicated thermal efficiency and IMEP, with $P_{\text{inj}} = 140$ MPa being superior to $P_{\text{inj}} = 80$ MPa. This could be due to the short injection duration and hence longer premixing time before the onset of combustion, as well as the higher fuel exit velocity, leading to better atomisation for the higher injection pressure. Stable indicated thermal efficiency values and IMEP were realised with a phasing close to TDC because there was minimum negative work done. There was an optimal injection timing for which a higher indicated thermal efficiency and IMEP were achieved. This was realised between $15^\circ$ and $20^\circ$ BTDC and was thought to be related to the spray targeting position and fuel impingement on the piston bowl wall, which would be discussed in the spray analysis and combustion images in the subsequent section. The coefficient of variance of the IMEP for the tested condition was less than 3%, implying that combustion was stable.

![Image](image_url)

Figure 5-2 Effect of injection pressure on indicated thermal efficiency, IMEP and Coefficient of variance of the IMEP, $P_{\text{inj}} = 80$ and $140$ MPa, 0% EGR, $\lambda = 4.5$
5.3.4. Effect of injection pressure on ignition and combustion phasing

The ignition delay is an important parameter used to assess the time which the fuel and air would premix before ignition. The combustion phasing (CA50) is the time in crank angle when 50% heat release is achieved and this would help to know where maximum work is obtained. Figure 5-3 shows the effect of injection timing on ignition delay. Advanced injection timing depicted long ignition delay. Under the condition tested the injection pressure had a very small effect on ignition delay with the higher injection pressure of $P_{\text{inj}} = 140$ MPa showing slightly shorter ignition delay due to better fuel-air mixing and atomization. Ignition delay is affected by the in-cylinder temperature, pressure, chemical property of the fuel. The in-cylinder condition considering low compression ratio would not be favorable for self auto ignition of the fuel despite having been mixed well. This would imply under same injection timing and different injection pressure, chemical kinetics of the fuel would have more effect than the injection pressure. The effect of the pressure would be minimal as compared to temperature and in-cylinder pressure.

Figure 5-4 shows the combustion phasing at CA50 against the injection timing. It is noted that for advanced injection timing the CA50 phasing is advanced and this translate to lower IMEP. Lower injection pressure indicated more retarded combustion phasing than the higher injection. This could be related to the mixing and atomization of the fuel. Higher pressure leads to better atomization than lower cases.
5.3.5. Effect of injection pressure on specific emissions

Figure 5-5 shows analysis conducted to understand the effect of injection pressure on specific emissions. The in-cylinder temperature for the higher injection pressure was higher than that of the lower injection pressure. Under all conditions, smoke emissions were lower for the higher injection pressure. This could be attributed to the short injection duration, leading to a long premixing time and better fuel atomisation; hence, it
would be possible to avoid a fuel-rich zone that burns with soot emissions. An injection timing of $\theta_{\text{inj}} = 30^\circ$ BTDC and earlier resulted in higher smoke emissions, with lower injection pressures displaying higher values. This phenomenon was observed despite the fact that the premixing time was longer. This could be related to the fact that under this condition, there was fuel impingement on the piston surface, and hence some could be splashing to the crevices, which becomes a rich-fuel zone that would burn with soot emissions.

With a late injection timing of $\theta_{\text{inj}} = 2^\circ$ to $15^\circ$ BTDC with $P_{\text{inj}} = 140$ MPa, NO$_x$ emissions were higher compared to $P_{\text{inj}} = 80$ MPa; however, the opposite occurred in the PCCI combustion regime with $\theta_{\text{inj}} = 20^\circ$ to $40^\circ$ BTDC. This implies that the combustion transitioned to PCCI and the in-cylinder temperature decreased, leading to lower NO$_x$ emissions for the higher injection pressure. The higher injection pressure created better atomisation and vaporisation, which in turn increased the premixed burned fraction and the local combustion temperature, leading to higher NO$_x$ emissions and a rapid pressure-rise rate due to the rapid combustion. In PCCI regime, the in-cylinder temperature is relatively low and the premixing time is relatively long, leading to mild combustion. The higher in-cylinder temperature led to the oxidation of soot but also promoted higher NO$_x$ emissions. The injection pressures of $P_{\text{inj}} = 140$ MPa and $P_{\text{inj}} = 80$ MPa had roughly the same CO emissions under all injection-timing conditions. With early injection timing, CO emissions increased drastically. This could be attributed to fuel impingement on the surface of the piston, leading to incomplete fuel combustion. As the injection timing was advanced, HC emissions for both injection pressures were identical, with slightly higher values for the lower injection pressure of $P_{\text{inj}} = 80$ MPa. For conventional diesel combustion ($\theta_{\text{inj}} = 5^\circ$ to $15^\circ$ BTDC) and a moderately early injection timing/PCCI regime ($\theta_{\text{inj}} = 20^\circ$ to $25^\circ$ BTDC), it is possible to achieve less than 2 g/kW\text{h}, while at $\theta_{\text{inj}} = 30^\circ$ BTDC and earlier injection timings, the lower injection pressure led to higher HC emissions compared to the higher injection pressure. This could be due to fuel impingement on top of the piston surface, leading to incomplete fuel vaporization and oxidation with a significant variation in the equivalence ratio, creating either over-rich or over-lean regions.
5.3.6. Effect of spray impingement on specific emissions

Spray targeting spot plays a critical role in the formation of CO and soot. As stated by Lee and Reitz [8] these points depend on the included spray angle and the injection timing. Figure 5-6 shows the furthest distance a spray can travel before hitting the piston surface, the upper most edge of the Derby hat groove and the wall of the Derby hat groove. It is noted that from 30°BTDC to 23° BTDC the spray would impinge on the piston surface while from 23°BTDC to TDC it would impinge inside the Derby hat wall.
In order to obtain the spray development images in the optical accessible engine, a high speed camera was used. The spray tip penetration based on the diesel spray development analysis is represented in Figure 5-7. Spray tip penetration is defined as the maximum distance of the injected spray from the injector hole. In this work, the spray tip penetration is averaged from five spray movies. As shown the diesel spray penetration at early injection timing (30°BTDC) is longer than that at late injection timing (10°BTDC). This could be explained from the perspective that late injection near TDC, the spray encountered higher temperature, density and pressure which led to the evaporation of the spray and hence smaller quantity impinging on the Derby hat wall. The injection duration was less than 7.4 deg CA under this condition.

The increase in injection pressure induced an increase in spray tip penetration due to the increase injection velocity. At a given constant injection quantity the higher injection pressure induced short injection duration. This indicated that the spray at high injection pressure ended sooner than those at low injection pressure causing momentum loss to start early. This is in agreement with Shao and Yan [3]. From the spray tip penetration it can be noted that for 30°BTDC the spray by postulation impinges on the top surface of the piston because from Figure 5-7 (our bottom view optical limitation was φ62mm) the spray is noted to be penetrating further after 4° crank angle after SOI.

Figure 5-6 Predicted spray extreme penetration distance
Chapter 5: Effect of spray impingement, injection parameters, and EGR on combustion and exhaust emission characteristics of a PCCI diesel engine

A further analysis from the spray development images clearly shows where the fuel spray impinges. Figure 5-8 shows the spray impingement location for the injection sweep considered. At 10°BTDC it impinges on the wall of the Derby hat. This is substantiated by the predicted value which shows it clearly that below 23°BTDC the spray impinges on the wall of Derby hat wall in Figure 5-8.

Spray would impinge on the surface of the piston with injection timing of $\theta_{\text{inj}} = 30°\text{BTDC}$, while for the cases from 10-23° BTDC on the Derby hat wall. The best spray targeting spot for lower emission of smoke was found to be between 15-25° BTDC injection timing.
5.3.7. Visualisation of combustion process phenomena

Combustion images at $P_{\text{inj}} = 140$ MPa without EGR, varying injection timing.

To clearly understand the exhaust emission trend, in-cylinder visualisation of the combustion process was done. Figure 5-9 shows the time series combustion images at different injection timing, $P_{\text{inj}} = 140$MPa without EGR. At advanced injection timing 25 – 30$^\circ$BTDC premixed combustion was achieved with non luminous flames, the ignition delay was longer leading to better mixing but due to some fuel impinging on both the wall of the Derby hat and piston surface some low intensity luminous flame could be seen evidence of fuel rich zones burning with some soot. Under moderately late injection timing of 15 – 20$^\circ$ BTDC luminous combustion flame was seen. This could be attributed to the impinged fuel since the ignition delay was long enough to allow for premixed combustion to be achieved with blue flame being noticed in the initial stages of combustion. 10$^\circ$BTDC showed very high intensity of luminosity. The ignition delay was short because the in-cylinder temperature remained high and the impinged fuel on Derby hat wall burned with increased luminosity. Diffusion controlled combustion occurred at this stage. This was confirmed both by rate of heat release and combustion images. The impinged fuel on the Derby hat wall burned producing smoke. The smoke produced was re-oxidized in the high temperature regions resulting in less engine-out smoke for the high injection pressure but increase for the lower injection pressure. From the spray penetration analysis it was noted that between 15$^\circ$BTDC and 25$^\circ$BTDC the injected spray targeted the upper part of the piston bowl and the spray progress in a radial way to the bottom edge leading to better mixing within the combustion chamber.
Chapter 5: Effect of spray impingement, injection parameters, and EGR on combustion and exhaust emission characteristics of a PCCI diesel engine

Figure 5-9 Time series combustion images for different injection timing, $P_{\text{inj}} = 140$ MPa, without EGR (Field of view = $\phi62$mm)
Combustion images at $\theta_{\text{inj}} = 25^\circ$ BTDC for $P_{\text{inj}} = 80$ MPa & 140 MPa without EGR

Figure 5-10 shows the time-series of combustion images at injection timing of 25$^\circ$BTDC for the injection pressure of $P_{\text{inj}} = 80$ MPa and 140 MPa, the intensity of the flame luminous decreased as the injection pressure was increased. This could be attributed to better atomization and higher injection velocity, hence higher momentum of fuel targeting the upper edge of the Derby hat wall leading to better mixing of the air with fuel. Well premixed fuel burned with non luminous flames. Combustion flame kernel appearance was advanced for the low pressure case. Blue flame was detected for both injections at the initial development stage of combustion.

a) $P_{\text{inj}} = 80$ MPa, $\theta_{\text{inj}} =25^\circ$ BTDC

b) $P_{\text{inj}} = 140$ MPa, $\theta_{\text{inj}} =25^\circ$ BTDC

Figure 5-10 Time-series combustion images for $P_{\text{inj}} = 80$ MPa, 140 MPa, without EGR. Camera frame speed = 13000 frames/second
Chapter 5: Effect of spray impingement, injection parameters, and EGR on combustion and exhaust emission characteristics of a PCCI diesel engine

Combustion images at $\theta_{\text{inj}} = 20^\circ$ BTDC for $P_{\text{inj}} = 140$ MPa with EGR

Figure 5-11 shows the time-series combustion images at constant injection pressure $P_{\text{inj}} = 140$ MPa with and without EGR, $\theta_{\text{inj}} = 20^\circ$ BTDC. It is noted that first appearance of the flame is retarded for EGR cases. The luminosity intensity decreases with EGR. Some parts would burn with soot as indicated by scattered luminous flames. This could be attributed to fuel impingement on the wall of Derby hat.

![Combustion Images](image)

a) $P_{\text{inj}} = 140$ MPa, $\theta_{\text{inj}} = 20^\circ$ BTDC, 0% EGR

![Reflections](image)

b) $P_{\text{inj}} = 140$ MPa, $\theta_{\text{inj}} = 20^\circ$ BTDC, 40% EGR

Figure 5-11 Time-series combustion images for $P_{\text{inj}} = 140$ MPa, 0% and 40% EGR
5.3.8. Effect of EGR on heat release

Considering the improvements achieved while utilizing higher injection pressure of $P_{\text{inj}} = 140$ MPa without EGR, further advancements in performance and exhaust emissions were sought by introduction of EGR. In this section, the effects of EGR on combustion characteristics and exhaust emissions will be explored in detail. Figure 5-12 shows the in-cylinder pressure history and heat release rate at $P_{\text{inj}} = 140$ MPa with and without EGR. The peak in-cylinder pressure and heat release rate decreased with the introduction of EGR. With EGR, the ignition delay was longer, and the combustion phasing was retarded for all conditions. This was attributed to the lower in-cylinder temperature due to the dilution effect of EGR. Enhanced air–fuel mixing before ignition due to a longer ignition delay led to a milder combustion process. Late injection timing was dominated by premixed combustion with only one peak. The injection duration was 7.4° CA. Advancing the injection timing led to a two-stage heat release: the first stage was attributed to low-temperature reactions and the second stage was attributed to high-temperature reactions separated by a short delay due to the negative temperature coefficient (NTC) ignition behaviour of the mixture.

![Figure 5-12 In-cylinder pressure history and rate of heat release, $P_{\text{inj}} = 140$ MPa, 0% EGR, $\lambda = 4.5$; and 40% EGR, $\lambda = 3.0$](image-url)
5.3.9. **Effect of EGR on performance**

Many researchers in the past have used EGR to improve the indicated thermal efficiency and IMEP, as well as extend the ignition delay, thereby controlling the combustion phasing and pressure rise rate [4-5]. In conventional diesel combustion, EGR has been traditionally used to control NOx emissions through charge dilution and by lowering the adiabatic flame temperature [6-9]. In this section, an in-depth analysis of the effects of EGR under higher injection pressure on the engine performance will be presented. Figure 5-13 shows the effect of EGR on the indicated thermal efficiency, IMEP, and coefficient of variance of the IMEP at $P_{\text{inj}} = 140$ MPa. With a retarded injection timing of $\theta_{\text{inj}} = 2–10^\circ$ BTDC, the indicated thermal efficiency and IMEP without EGR was superior to cases with 40% EGR. This was thought to be related to either fuel quenching or over-mixing, leading to the formation of a mixture that was too lean to allow complete combustion. However, at $\theta_{\text{inj}} = 15^\circ$ BTDC, the indicated thermal efficiency and IMEP reached a maximum value and then gradually decreased. The highest indicated thermal efficiency and IMEP corresponded to a phasing after TDC with a longer ignition delay. Introducing 40% EGR improved indicated thermal efficiency and IMEP for $\theta_{\text{inj}} = 15–20^\circ$ BTDC. This was the same injection timing that improved performance with different injection pressures, implying that there is optimal injection timing at which both the higher injection pressure and EGR achieve improved performance.
5.3.10. **Effect of EGR on ignition delay and combustion phasing**

The ignition delay plays a greater role in the fuel air mixing and hence impact very much on the combustion and emissions formation in internal combustion engines. Combustion phasing in this case considered as the time in crank angle corresponding to 50% burn of the fuel also plays a critical. Too advanced combustion phasing leads to higher amount of negative work done and hence lower indicated thermal efficiency while late combustion phasing would lead to maximum power attainment.

Figure 5-14 shows the effects of EGR on ignition delay. EGR had a significant impact, achieving a longer fuel–air premixing time well before ignition, which translated...
into better performance and lower soot emissions. This was thought to be directly related to the dilution effect of EGR.

Figure 5-14 Effect of EGR on ignition delay, $P_{\text{inj}} = 140$ MPa, 0% EGR, $\lambda = 4.5$; and 40% EGR, $\lambda = 3.0$

Figure 5-15 Combustion phasing as a function of fuel injection timing

Figure 5-15 shows the combustion phasing against the injection timing. Cases with 0% EGR rate, the combustion phasing (CA50) was observed occurs in the compression stroke thus leading to more negative power which has an impact on the
Chapter 5: Effect of spray impingement, injection parameters, and EGR on combustion and exhaust emission characteristics of a PCCI diesel engine

performance. For the 40% EGR case combustion phasing was near TDC and after TDC for most of the cases. This condition led to higher indicated thermal efficiency and higher IMEP.

5.3.11. Effect of EGR on specific emissions

PCCI combustion utilizes EGR to lower the adiabatic flame temperature and oxygen concentration, resulting in controllable combustion phasing and pressure-rise rate. This also leads to a reduction in NO\textsubscript{x} emissions but an increase in HC and CO emissions. Figure 5-16 shows the effects of EGR on the maximum in-cylinder temperature (T\textsubscript{max}), as well as smoke, NO\textsubscript{x}, CO, and HC emissions. For all the tested conditions without EGR, the maximum in-cylinder temperature was higher than with EGR. A retarded injection timing had a lower maximum in-cylinder temperature, while advancing the injection timing led to a gradual rise in the in-cylinder temperature until $\theta_{\text{inj}} = 15^\circ$ BTDC, which drastically reduced in-cylinder temperature for PCCI combustion regime. The in-cylinder maximum temperature, both with and without EGR, was less than 1500 K. Excessive smoke emissions were produced for $\theta_{\text{inj}} = 10^\circ$ and $30^\circ$ BTDC with 40% EGR and for an early injection timing of $\theta_{\text{inj}} = 35^\circ$ BTDC and above without EGR. This could be attributed to the low in-cylinder temperature, density and pressure that did not allow complete oxidation of the soot formed from the rich fuel impinging on the surface of the piston. Smoke emissions of less than 2% were achieved for $\theta_{\text{inj}} = 2–30^\circ$ BTDC with 40% EGR and without EGR. As the injection timing was advanced, the in-cylinder temperature decreased and fuel penetration was enhanced, leading to fuel impingement on the surface of the piston, providing a source of fuel-rich zones that burned with smoke emissions. The smoke emissions of conventional diesel combustion were lower than those in the PCCI regime. PCCI combustion is not meant to completely eliminate smoke emissions but rather reduce them to acceptable levels. Many researchers have noted that it is possible to obtain a simultaneous reduction in NO\textsubscript{x} and soot by incorporating large amounts of EGR [9-10], but this comes at the expense of high fuel consumption and increased CO and HC emissions. It was possible to achieve less than 0.5% smoke emissions with EGR at an injection timing between $\theta_{\text{inj}} = 15^\circ$ and $25^\circ$ BTDC. This was thought to arise from the fact that the spray struck the piston bowl wall and the fuel–air
was premixed well without creating fuel-rich pockets so that better combustion was achieved. This agreed with the results obtained by Fang et al. [11] for narrow-angle wall-guided spray combustion.

For conventional diesel combustion without EGR, NOx emissions drastically increased as the injection timing was advanced up to a maximum at $\theta_{\text{inj}} = 15^\circ$ BTDC, after which they decreased drastically in the PCCI combustion regime. This could be attributed to the high in-cylinder temperature, which promotes NOx emissions, and a short duration for fuel–air mixing prior to combustion. EGR effectively reduced NOx emissions. This was attributed to the reduced oxygen concentration and the decrease in flame temperature in the combustible mixture. A moderately early injection of $\theta_{\text{inj}} = 30^\circ$ BTDC and above led
to low NO\textsubscript{x} emissions without EGR due to the reduced in-cylinder temperature but also led to an increase in smoke emissions.

As the injection timing was advanced, CO emissions increased drastically. EGR led to higher CO emissions. Under retarded conditions of $\theta_{\text{inj}} = 10^\circ$ BTDC with 40% EGR, the CO emissions were high. This could be attributed to the low temperature and insufficient oxygen for complete combustion. When the injection timing was too early, higher emissions could also be associated with piston surface/cylinder wall wetting.

HC emissions increased as the injection timing was advanced. The trend was the same with and without EGR. This could be attributed to the limited amount of oxygen available for complete combustion. In the PCCI combustion regime of $\theta_{\text{inj}} = 10^\circ$ BTDC with 40% EGR, HC emissions were relatively high compared to the case without EGR. This could be attributed to two effects: over-mixing, where the mixture was too lean to burn, and flame quenching during the expansion stroke. This result agreed with the findings of other researchers [12-13]. To mitigate the problem, it is desirable to increase the available air mass through supercharging while maintaining the same EGR levels.

5.3.12. Soot formation and oxidation in PCCI diesel engine

To clarify emission trends in the test engine, the combustion process was visualised in an optically accessible engine using bottom-view images. The four spray plumes penetrated at an angle of 90° relative to each other, but the first on-set of the flame kernel occurred between the spray plumes. This phenomena was attributed to the fact that when the spray strikes the Derby hat wall the spray tend to move inward towards each other and gets well mixed up in between where ignition occurs. In this section, the results of an in-depth study of the combustion process, carried out under the condition for which simultaneous low NO\textsubscript{x} and soot emissions were achieved, are presented. Figure 5-17 shows the time-series direct-visualisation combustion images for $P_{\text{inj}} = 140$ MPa and $\theta_{\text{inj}} = 20^\circ$ BTDC, with and without EGR, together with the in-cylinder pressure history. The upper images correspond to the case without EGR, while the lower images represent the case with 40% EGR. Early combustion occurred $-6.1^\circ$ after top dead centre (ATDC) for the case without EGR, and injection was complete at $-11.05^\circ$ ATDC. There was a
short premixing time. The early flame locations were more downstream of the spray and located near the piston bowl corner. A blue flame (images b–e) was observed during early flame development; the flame quickly filled the bowl region uniformly due to the higher injection velocity. Some pockets of more luminous flame were observed between the spray directions (images c and d), but these burned out quickly late in the combustion cycle. The spray impingement location near the piston bowl wall was observed, but these weak local flames disappeared gradually when the burning rate of the film flame was low. The regions with high luminous flames indicated some non-homogeneities in the air–fuel mixture in the piston bowl.

With the introduction of EGR, more homogenous combustion phenomena were observed. For this case, the injection ended near the same CA as the case without EGR, but the first sign of a flame appeared at about 0.5° ATDC. The early flames were located further downstream near the piston bowl wall. The combustion was evenly distributed in the combustion chamber. The luminosity of the flame was significantly reduced, and the flame was more homogenous. Because the premixing time was long, the fuel that struck the piston bowl wall tended to premix well with air and fuel, burning with low luminosity. At 5.6° BTDC, some weak local flames due to fuel impingement were observed near the piston bowl; these burned longer at a lower rate.
Chapter 5: Effect of spray impingement, injection parameters, and EGR on combustion and exhaust emission characteristics of a PCCI diesel engine

Figure 5-17 Direct visualization combustion images, $P_{\text{inj}} = 140$ MPa, $\theta_{\text{inj}} = 20^\circ$ BTDC, 0% EGR, $\lambda = 4.5$; and 40% EGR $\lambda = 3.0$

To clarify the differences in the combustion images with and without EGR, a detailed investigation was carried out on two typical images for the two conditions. Figure 5-18 compares these combustion images with and without EGR. Blue and highly luminous flames were evident for the case without EGR, while the 40% EGR case was characterised by blue and weak luminous flames. Low engine soot emissions were observed for these conditions ($\theta_{\text{inj}} = 20^\circ$ BTDC, 0% and 40% EGR).
Further analysis of the raw images was carried out to isolate the components that represent soot formation and oxidation location. Figure 5-19 shows a time series of the processed red-component combustion images for $P_{\text{inj}} = 140$ MPa and $\theta_{\text{inj}} = 20^\circ$ BTDC, both with and without EGR, coupled with the in-cylinder pressure history. In the case without EGR, the soot formation regions were further downstream and located between the fuel sprays, where they impinged and deflected inwards towards each other. This was thought to be due to the high moment of inertia of the fuel coming out of the injector and striking the piston bowl wall, hence enhancing the mixing of the air and fuel, coupled with the fact that the in-cylinder temperature at this point was about 1500 K, promoting oxidation so that the engine soot emissions at the exhaust pipe were a minimum. With the introduction of EGR, the soot locations were uniformly distributed in the combustion chamber and further downstream. Due to the long ignition delay, the fuel and air had a longer premixing time, and hence no pockets of fuel-rich zones formed, preventing sources of soot. This case could burn with only a small quantity of soot formed, which was subsequently oxidised. The images indicate that at $\theta_{\text{inj}} = 20^\circ$ BTDC with EGR, it was possible to simultaneously achieve low engine soot and NO$_x$ emissions.
The red component of the spatially integrated flame luminosity (SIFL) was obtained by summing the pixel values of the bottom-view images. Previous research demonstrated that SIFL is strongly correlated with the engine soot emissions [11]. Figures 5-20 and 5-21 show the SIFL and rate of SIFL with and without EGR at \( P_{inj} = 140 \) MPa. A high SIFL was observed with late injection timing, while moderately early injection timing led to a lower SIFL. Flame luminosity is typically dependent on the local temperature and soot concentration. Under similar temperature distributions, higher flame luminosity indicates higher soot formation [14]. The oxidation rates correlated well with the maximum in cylinder temperature. Higher temperatures led to higher soot oxidation rates, as noted at \( \theta_{inj} = 10^\circ \) BTDC without EGR, and therefore less engine soot at the exhaust pipe. As the injection timing was advanced, the in-cylinder temperature decreased along with the corresponding SIFL peak, leading to a low oxidation rate and slightly more engine soot emissions.
Chapter 5: Effect of spray impingement, injection parameters, and EGR on combustion and exhaust emission characteristics of a PCCI diesel engine

Table 5-1 shows the maximum SIFL and rate of SIFL for all the conditions considered. Cases without EGR had higher values compared to those with EGR.

<table>
<thead>
<tr>
<th>Injection timing</th>
<th>SIFL (max)</th>
<th>Rate of SIFL (max)</th>
<th>SIFL (max)</th>
<th>Rate of SIFL (max)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0% EGR</td>
<td>40% EGR</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10° BTDC</td>
<td>9.29E+06</td>
<td>1.92E+06</td>
<td>7.19E+03</td>
<td>2.85E+03</td>
</tr>
<tr>
<td>15° BTDC</td>
<td>5.23E+06</td>
<td>8.71E+05</td>
<td>1.01E+04</td>
<td>4.26E+03</td>
</tr>
<tr>
<td>20° BTDC</td>
<td>1.56E+06</td>
<td>3.84E+05</td>
<td>1.11E+05</td>
<td>1.54E+04</td>
</tr>
<tr>
<td>25° BTDC</td>
<td>2.28E+05</td>
<td>5.96E+04</td>
<td>6.89E+04</td>
<td>1.07E+04</td>
</tr>
<tr>
<td>30° BTDC</td>
<td>1.26E+05</td>
<td>1.90E+04</td>
<td>4.62E+03</td>
<td>2.29E+03</td>
</tr>
</tbody>
</table>

To some extent, the derivative of the flame luminosity (rate of SIFL) showed the soot formation rate and oxidation rate during the combustion process. In general, cases without EGR showed higher positive peaks compared with EGR cases. This indicates faster combustion and soot formation processes. Late injection timing showed the highest peak for the cases considered. The negative peaks were much higher for the late injection timing without EGR, implying a higher oxidation rate. Cases without EGR indicated higher in-cylinder temperatures compared to those without EGR. Engine soot emissions for the late and moderately early injection timings without EGR ($\theta_{inj} = 10–30°$ BTDC) were less than 1%, and the temperature was above 1400 K. This confirms that a higher in-cylinder temperature resulted in higher soot oxidation rates. The soot oxidation process plays an important role in determining the engine exhaust emissions at the tailpipe. Cases with EGR resulted in lower rates of SIFL, but the trends were similar to those without EGR. The soot oxidation process was faster than soot formation; hence, the engine soot emissions were also relatively low.
Chapter 5: Effect of spray impingement, injection parameters, and EGR on combustion and exhaust emission characteristics of a PCCI diesel engine

Figure 5-20 Spatially integrated flame luminosity (SIFL) and rate of SIFL, $P_{\text{inj}} = 140$ MPa, 0% EGR, $\lambda = 4.5$

Figure 5-21 Spatially integrated flame luminosity (SIFL) and rate of SIFL, $P_{\text{inj}} = 140$ MPa, 40% EGR, $\lambda = 3.0$
5.3.13. Optimized low emission and high efficient PCCI diesel engine

In order to understand clearly the best PCCI combustion strategy a further analysis of the performance and emission characteristics under the optimum condition of $\theta_{inj} = 20^\circ$BTDC with various operating conditions were carried out. Table 5-2 shows the optimized engine operation conditions considered.

Table 5-2 Optimized engine operating conditions

<table>
<thead>
<tr>
<th>Case number</th>
<th>Rail pressure (MPa)</th>
<th>Injection timing (°BTDC)</th>
<th>EGR (%)</th>
<th>IMEP (bars)</th>
<th>Indicated thermal efficiency (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>80</td>
<td>20</td>
<td>0</td>
<td>2.77</td>
<td>41.5</td>
</tr>
<tr>
<td>Case 2</td>
<td>80</td>
<td>20</td>
<td>40</td>
<td>2.86</td>
<td>43</td>
</tr>
<tr>
<td>Case 3</td>
<td>140</td>
<td>20</td>
<td>0</td>
<td>3.12</td>
<td>46.7</td>
</tr>
<tr>
<td>Case 4</td>
<td>140</td>
<td>20</td>
<td>40</td>
<td>3.17</td>
<td>47.3</td>
</tr>
</tbody>
</table>

Figure 5-22 shows the pressure history and the rate of heat release. It was noted that higher injection pressure led to advanced and high peak of the in-cylinder pressure and ROHR with high emission of NO$_x$ and low emission of smoke. On the other hand the introduction of EGR led to retarded and lower peak of in-cylinder pressure and ROHR but with slightly longer combustion duration. The amount of negative power was greatly reduced. It can be clearly seen that the higher injection pressure of $P_{inj} = 140$ MPa with 40% EGR achieved higher indicated thermal efficiency with simultaneously low emission of both NO$_x$ and smoke as shown in Figure 5-23 and Table 5-2.

Figure 5-23 shows the relationship between smoke and NO$_x$ for the optimum condition. It can be noted that at higher injection pressure of $P_{inj} = 140$ MPa, the emission of NO$_x$ was high but the smoke emission was the minimum. When EGR is introduced the inverse proportionality occurred where the emission of NO$_x$ was reduced drastically with a slight increase in smoke. This was noted to be related to the in-cylinder temperature.
Figure 5-22 Pressure history and rate of heat release

Figure 5-23 Engine–out smoke against NO$_x$
Figure 5-24 shows the time integration of spatially integrated flame luminosity (TISIFL)/IMEP and NO\textsubscript{x}/IMEP for all the cases considered. A lower value showed lower in-cylinder temperature and lower sooting combustion. Higher injection pressure led to drop in TISIFL/IMEP and NO\textsubscript{x}/IMEP (case 1 to case 3). The introduction of EGR led to further reduction (case 3 to case 4). Lower TISIFL/IMEP and NO\textsubscript{x}/IMEP was noted to represent the optimum indicated thermal efficiency and engine-out emission.
Chapter 5: Effect of spray impingement, injection parameters, and EGR on combustion and exhaust emission characteristics of a PCCI diesel engine

5.4. Summary

In this section an in-depth analysis of the effects of spray impingement, injection parameters, and EGR on the combustion characteristics and exhaust emissions of a PCCI diesel engine were investigated using a single-cylinder test engine and an optically accessible engine. Late and moderately early injection timings were considered, leading to the following conclusions.

Under late and early injection timings, the higher injection pressure, $P_{\text{inj}} = 140$ MPa, led to better indicated thermal efficiency and IMEP compared to the lower injection pressure, $P_{\text{inj}} = 80$ MPa. The coefficient of variance of the IMEP was less than 3% for the higher injection pressure. Correspondingly, smoke and HC emissions were lower, while CO emissions remained relatively unchanged. For a late injection of $\theta_{\text{inj}} = 2–15^\circ$ BTDC, NO$_x$ emissions were higher for the lower injection pressure, but for $\theta_{\text{inj}} = 20–40^\circ$ BTDC, the higher injection pressure led to lower NO$_x$ emissions.

The use of EGR led to a simultaneous reduction in soot and NO$_x$ emissions at the best injection timing of $\theta_{\text{inj}} = 20^\circ$ BTDC, for which the spray struck the piston bowl wall at an optimum targeting spot, leading to improved fuel–air mixing. The indicated thermal efficiency and IMEP were superior to cases without EGR but also led to increased HC and CO emissions. EGR was effective in reducing NO$_x$ emissions for the cases considered.

The interaction between the spray and the piston bowl geometry played a key role in the air–fuel mixing process. This led to low smoke emissions of less than 1% for both the late and moderately early injection timings without EGR. With EGR, it was possible to achieve less than 2% smoke emissions for the same range. Both homogenous combustion and low luminosity flames were observed for the low-soot-forming conditions. Low luminosity flame spots were attributed to fuel spray impingement on the wall of the piston bowl and deflection towards the space between the sprays. $\theta_{\text{inj}} = 20^\circ$ BTDC with EGR was the optimum injection timing that gave simultaneously low soot and NO$_x$ emissions.
References


Chapter 6

Spectrum Analysis of Chemiluminescence of a Low Sooting PCCI Diesel Engine Operating with Moderately Early Injection Timing

6.1. Introduction

In order to understand reaction mechanism of auto-ignition and combustion mechanism in a PCCI engine, one effective way is spectrum analyses of chemiluminescence to determine the major active species. Chemiluminescence emission arises from specific molecules that are raised to an excited state by exothermic chemical reactions and then subsequently decay back to equilibrium energy level by emitting a photon. It occurs in specific wavelength bands that are characteristic of the emitting molecule. They are specific molecules responsible for the chemiluminescence change for different combustion phases and this can provide information about the nature of the reactions and the fuel/air mixture[1]. Because chemiluminescence is produced directly by exothermic reactions, it marks the location of initial combustion reactions temporally and spatially, with the limitation that the signal is integrated along line of sight.

One strategy to determine combustion emissions is to correlate them with the presence and distribution of certain chemical species in the combustion flame. It has been established that certain intermediary radical species in the flame such as OH*, H₂CO, CH*, C₂* and CN* (when there is nitrogen content in the fuel) are involved in the chain reaction mechanisms, and play important roles in the formation of combustion emissions such as NOₓ and particulate matter (PM) [1].

Auto ignition process in PCCI combustion exhibits two-stage heat release. The first always referred to as the cool flame is governed by the low temperature oxidation and takes place at temperature range between 700 to 900 K and the raises the temperature high enough to lead to the second stage thermal flame. In between the two stages is a region referred to as the negative temperature coefficient (NTC) in which the ignition delay duration increases with the increasing initial temperature. This behaviour is clearly
shown by the heat release in the cool flame region being reduced as the initial temperature increases. The thermal flame or high temperature oxidation is achieved by the activation of the decomposition reaction of H$_2$O$_2$ accumulated in the cool flame region to OH radicals. The mechanisms involved in the high temperature oxidation are relatively simple and typically occurs when the in-cylinder temperature of 1100 K is attained irrespective of the engine operating condition and the fuel structure [2]. A more recent study has also indicated that there could be some dependence on the in-cylinder pressure and fuel structure[3]. Shibata and Urushihara [3] concluded that the initiation and progression of low temperature heat release (LTHR) is primarily dependent on chemical components in the fuel, and the temperature and pressure at the start and end of LTHR differ notably depending on the fuel. On the contrary, the decomposition of H$_2$O$_2$ that has accumulated during LTHR triggers high temperature heat release (HTHR) and the HTHR start is unrelated to fuel composition.

6.1.1. Spectral characteristics of a flame

The combustion of a fossil fuel is a complex chemical/thermal reaction. The characteristics of the flame can be identified by the nature and degree of the spectral emissions from fuel molecules/particles participating in the exothermic reactions. The emission spectra given off by the flame contain two different elements, i.e., emission lines from the species participating in the chemical processes (discrete or band spectra) and the underlying blackbody curve (continuous spectra). The continuous spectra in the flame are generally observed in the luminous region where radiative energy emitted by soot and other solid particles is distributed in a common manner over a broad spectral range, and complies with the Planck radiation theory. The discontinuous spectra are attributed to isolated atoms or free radicals (intermediate species) in the flame. When the fuel reacts with oxygen at high temperature, a number of free radicals are produced in excited electronic states, and are characterised by strong spectral bands. The spectral bands of hydrocarbon flame emissions in the 250- 800nm spectral region are dominated by OH* (308nm), CN* (387nm), CH* (431.5nm), C$_2$* (514nm)[4], CO-O recombination (350 - 450 nm) and formaldehyde, H$_2$CO (370 - 480 nm) which are the interests of this investigation.
6.2. Experimental setup and conditions

In this study, the spectrum of chemiluminescence of combustion in the range of 200nm to 800nm wavelength was acquired by an ICCD detector coupled with a spectrometer. Two types of spectrometers were used for this experiment namely; SR163i for the low resolution and measurement range between 250 to 800nm wavelength and MS257 for the high resolution and a measurement range between 350nm to 550nm wavelengths. The spectral analyses of chemiluminescence for the moderately early injection timing for two injection pressures $P_{\text{inj}} = 80$ and 140 MPa considering two measurement locations was carried out. The main goal of this study is to characterise the main intermediate species across the different phases of PCCI combustion while using diesel fuel. Detailed measurement was also undertaken in the cool flame region for higher injection timing to isolate the weak emission of formaldehyde through increasing the grating value from grating 150lines/mm/ brazing 300nm to grating 300line/mm/ brazing 300nm under higher gain number.

6.3. Results and discussions

In order to understand the chemical reaction in PCCI engine the spectra of chemiluminescence of intermediate species were measured using two spectrometers and the results are presented and discussed in this section. Auto ignition can be generally divided into three well-known durations according to the essential reactions involved. The first stage, the LTO period which last from the beginning of compression to the end of cool flame. The next is the period starting from the end of cool flame to the beginning of the HTO referred to as the $\text{H}_2\text{O}_2$ period or thermal combustion preparation. The final part is referred to as $\text{H} + \text{O}_2$ period or late burn. This has a great influence on the flame speed and other post-ignition phenomena[5].
6.3.1. Effect of the number of accumulated cycles on the identification of formaldehyde radicals.

Formaldehyde plays a key role in the cool flame region in PCCI combustion. Its production is noted in the low temperature oxidation region (LTO). Figure 6-1 shows the spectrum of species in the low temperature oxidation region while considering different values of the accumulated cycles.

In order to understand the spectrum of chemiluminescence in the low temperature oxidation (LTO) region the resolution of the spectrometer was increased and the number of accumulated cycles increased. In Figure 6-1 the spectra of CH$_2$O in LTO region was measured considering higher grating value of 300 lines/mm with a brazing number of 300 nm and a gain of 150. The accumulated cycles were varied to clearly isolate the low intensity of the formaldehyde (CH$_2$O) radicals. 2000 accumulated cycles was noted to precisely detect the presences of the CH$_2$O in the range of 350 – 480 nm wavelengths due to the high resolution of the spectrometer.

In order to understand the detailed history of chemical reaction in the LTO region, a crank angle resolved measurement with 0.6° crank angle interval was considered. Figure 6-2 shows the time series of the cool flame from the start to the end. Under this condition, $P_{\text{inj}} = 140$ MPa, the cool flame was noted to start from $\theta_{sp} = 14^\circ$ BTDC and end at $\theta_{sp} = 12.2^\circ$ BTDC where spike of CH* radical was noted. At low temperature T< 800 K chain branching occur leading to the production of CH$_2$O and OH* radicals through the process of H atom abstraction from the fuel. Once the CH$_2$O is formed, it consumes OH* radicals though the reaction.

$$\text{HCHO} + \text{OH} \rightarrow \text{HCO} + \text{H}_2\text{O}$$  \hspace{1cm} R1

Under this condition the HCO would readily react with O$_2$ to produce CO + HO$_2$, leading to the chain termination of the reaction since OH* radicals production would diminish.

The symbol $\theta_{sp}$ was used to denote the spectral measurement timing in this work.
Figure 6-1 Spectra of cool flame at location 1 considering different values of accumulated cycles, \( P_{\text{inj}} = 140 \text{ MPa} \), \( \theta_{\text{inj}} = 20^\circ \text{BTDC} \), \( \theta_{\text{sp}} = 14^\circ \text{BTDC} \)

Figure 6-2 Time series of the cool flame spectra at location 1, \( P_{\text{inj}} = 140 \text{ MPa} \), \( \theta_{\text{inj}} = 20^\circ \text{BTDC} \)
6.3.2. Characterization of the intermediate species in PCCI diesel engine

The intermediate species in internal combustion engines plays a major role in the performance and emission formation. Figure 6-3 shows pressure history and rate of heat release (ROHR) for injection pressure $P_{\text{inj}} = 140 \text{ MPa}$ at injection timing $\theta_{\text{inj}} = 20^\circ \text{BTDC}$ respectively. The low temperature oxidation (LTO) and high temperature oxidation (HTO) locations which are typical with PCCI combustion can be clearly seen from the figures.

![Figure 6-3](image_url)  
Figure 6-3 Pressure history and rate of heat release $P_{\text{inj}} = 140 \text{ MPa}$, $\theta_{\text{inj}} = 20^\circ \text{BTDC}$

In order to understand the trend of the intermediate species evolution under PCCI combustion mode, time series of spectra was considered. Figure 6-4 and 6-5 shows the time series of the spectra for $P_{\text{inj}} = 140 \text{ MPa}$ and $\theta_{\text{inj}} = 20^\circ \text{BTDC}$. From $\theta_{\text{sp}} = 20^\circ$ to $14^\circ \text{BTDC}$ the spectra was weak but at $\theta_{\text{sp}} = 11^\circ \text{BTDC}$ spikes of OH* and CH* radicals were noted being markers of the high temperature exothermic reaction. Under this condition the flame front consumes the fresh air and fuel leading to the local temperature
increasing. Excited OH* radicals were formed in the primary combustion zone by the chemiluminescence reaction of

\[ \text{CH} + \text{O}_2 \rightarrow \text{CO} + \text{OH} \]  

An inverse proportionality was noted where the CH* radical decreased as the OH* radicals increased. The presence of CH* radical was noted to extended to \( \theta_{sp} = 5^\circ \text{BTDC} \) with a range of about 6° crank angle or 1ms. This was thought to relate to the spray targeting spot where the fuel struck the wall of the Derby hat with higher momentum and then spread out towards the centre of the piston bowl hence, leading to the fuel mixing well with the air and hence resulting in better atomisation under this condition.

Thereafter the luminance flame spectrum was noted with the formation and oxidation of soot (670 - 690 nm wavelengths).

Figure 6-4 Time series of spectra \( P_{\text{inj}} = 140 \text{ MPa}, \theta_{\text{inj}} = 20^\circ \text{BTDC} \): Initial stages
The analysis of time evolution of the major intermediate species was carried out. Figure 6-6 shows time evolution of CH$_2$O, CO-O recombination and CH*, OH* radicals detected at location 1 for $P_{\text{inj}} = 140$ MPa and $\theta_{\text{inj}} = 20^\circ$BTDC. It can be clearly seen that in the LTO region the production of CH$_2$O increases drastically until the start of the high temperature oxidation. The value of OH* radicals start to increase just after the end of LTO but reaches the maximum at the peak of the ROHR then decreased thereafter. The same trend was displayed also by the CH* radicals and CO-O recombination which reached the maximum at the peak of the ROHR then drastically reduced. The only difference was the production levels where OH* emission had a higher intensity indicating a more homogenous spatial distribution of this radical in the chamber under this condition.
At peak of the ROHR, the emission of soot was relatively low implying that higher \(\text{OH}^*\) radical emission led to faster oxidation of the formed soot because of the high temperature in the HTO region. It is noted that high temperature and \(\text{OH}^*\) radical in the late combustion phase led to faster oxidation of the soot formed resulting in significantly reduced engine-out soot emission and higher indicated thermal efficiency.

\(\text{OH}^*\) radical was noted to be a good marker of premixed combustion and start of the high temperature oxidation. \(\text{CH}^*\) radical was also found to be good marker of fuel-rich regions within the Derby hat piston head cavity. This region was noted to move towards the centre of the piston bowl. This confirms the fact that the fuel would first strike inside the Derby hat wall and spread inwards towards the centre of the piston bowl.

Figure 6-6 Time evolution of the \(\text{CH}_2\text{O}\) and CO-O recombination, \(\text{CH}^*\), \(\text{OH}^*\) radicals with soot evaluated at location 1 for \(P_{\text{inj}} = 140\) MPa, \(\theta_{\text{inj}} = 20^\circ\) BTDC
hence, leading to better mixing of the fuel and the air. From visualization data combustion was noted to start at the edge of the Derby hat piston head and while it is approaches the piston bowl centre the fuel would have evaporated due to high temperature generated by combustion under this condition.

After the disappearance of the CH* radicals and the strong OH emissions; the burned gas is also characterised by broadband emission from the UV to visible. This is related to carbon monoxide reaction, \( CO + O \rightarrow CO_2 + hv \) responsible for the CO continuum chemiluminescence emissions. This is predominant with flames at low temperature or reduced in-cylinder pressure[1]. The HTO is also characterised by the decomposition of \( H_2O_2 \) build up during the cool flame period in the low temperature region between 600 and 700K. In the thermal preparation for the HTO the main route of the chain reaction cycle is:

\[
\begin{align*}
HCHO + OH & \rightarrow CHO + H_2O & \text{R3} \\
CHO + O_2 & \rightarrow HO_2 + CO & \text{R4} \\
HO_2 + HO_2 & \rightarrow H_2O_2 + O_2 & \text{R5}
\end{align*}
\]

This is achieved during the LTO period but in thermal flame region the \( H_2O_2 \) is decomposed to OH* radicals which promote ignition through reaction R6. This requires high temperature above 1100 K for the reaction to proceed. High production levels of \( H_2O_2 \) leads to high fuel reactivity.

\[
H_2O_2 + M \rightarrow 2OH + M & \text{R6}
\]
6.3.3. Effect of measurement location on intermediate species.

The spray impingement location is a very essential parameter in the formation of emission in PCCI engine. It is paramount to measure the evolution of the intermediate combustion radical in this region in order to relate it with the engine-out emissions. Figure 6-7 shows the spectroscopic measurement locations considered in this study. Its effect would be analysed in detail in this section.

Figure 6-7 In-cylinder field of view and spectroscopic measurement locations.
In order to understand the effect of changing the measurement location on the chemiluminescence spectrum of PCCI combustion with moderately early injection timing the locations were varied from 1 to 3. Figure 6-8 and 6-9 shows the time series spectra for $P_{\text{inj}} = 140$ MPa and $\theta_{\text{inj}} = 20^\circ$ BTDC at location 3 for the initial and late combustion phases of PCCI engine. Some weak spectrum of formaldehyde was detected at $\theta_{\text{sp}} = 11^\circ$BTDC but at $\theta_{\text{sp}} = 8^\circ$BTDC, OH* radicals with a broadband of CO-O recombination and no traces of CH* radicals were detected. This meant that at this measurement point located at the end gas region, all the fuel had atomized with no fuel impingement at the cylinder wall. This could be one of the reasons why under this condition the indicated thermal efficiency was sufficiently high with very low emission of smoke as noted in chapter 5 [6].

![Figure 6-8 Time series of spectra at location 3, $P_{\text{inj}} = 140$ MPa and $\theta_{\text{inj}} = 20^\circ$ BTDC: Initial stages](image_url)
Figure 6-9 Time series of spectra at location 3, $P_{\text{inj}} = 140$ MPa and $\theta_{\text{inj}} = 20^\circ$ BTDC:
Late combustion phases
Figure 6-10 the time evolution of the OH* radicals at position 1 and 3 for $P_{\text{inj}} = 140$ MPa. The OH* emission intensity was lower for location 3 compared to location 1 but the evolution trend was similar with location 3 case diminishing faster. In case of the high injection pressure the intensity of the luminous flame dies fast compared to the lower injection pressure. OH* radicals also follow the same trend indicating that there is a relationship between this and the engine-out emission of soot, which is noted to be higher for the lower injection pressure case[7].

Figure 6-10 Time evolution of OH* radicals detected at location 1 and 3, $P_{\text{inj}} = 140$ MPa, $\theta_{\text{inj}} = 20^\circ$ BTDC
6.3.4. Effect of injection pressure on spectra of intermediate species

In moderately early injection timing it was noted in chapter 5 that this parameter affects the emission formation and engine performance. Higher injection timing led to lower emissions and higher indicated thermal efficiency and IMEP. In order to understand the effect of pressure on the spectrum of chemiluminescence under PCCI combustion strategy two injection pressure were chosen; $P_{\text{inj}} = 80$ and 140 MPa. Figure 6-11, 6-12 and 6-13 shows the time series of the spectra for $P_{\text{inj}} = 80$ MPa and $\theta_{\text{inj}} = 20^\circ$BTDC. From $\theta_{\text{sp}} = 20^\circ$ to $14^\circ$BTDC the spectra was weak but at $\theta_{\text{sp}} = 11^\circ$BTDC spikes of OH* and CH* radical were noted being markers of the high temperature exothermic reaction.

In case of higher injection pressure, $P_{\text{inj}} = 140$ MPa the presence of CH* radical was extended to $\theta_{\text{sp}} = 8^\circ$BTDC as shown in Figure 6-4. This was thought to relate to the spray targeting spot where the fuel struck the wall of the Derby hat with higher momentum and then spread out towards the centre of the piston bowl hence, leading to the fuel mixing well with the air and hence resulting in better atomisation for the case of $P_{\text{inj}} = 140$ MPa. In the case of $P_{\text{inj}} = 80$ MPa higher concentration of the fuel might have remained at the Derby hat wall after the impact. Higher injection pressure led to better atomisation of the fuel and air.

Under lower injection pressure condition the maximum emission of OH* radicals is reached at $5^\circ$BTDC while for the high injection pressure is $8^\circ$BTDC. This was thought to be related to the onset of thermal ignition for both the cases. Higher injection pressure had advanced onset of high temperature oxidation when the air and fuel is very well premixed given that the short injection duration and ignition delay.
Figure 6-11 Time series of spectra at location 1, $P_{inj} = 80$ MPa and $\theta_{inj} = 20^\circ$ BTDC: Initial stages

Figure 6-12 Time series of spectra at location 1, $P_{inj} = 80$ MPa and $\theta_{inj} = 20^\circ$ BTDC: Initial stages
Figure 6-14 shows the time evolution of OH* radicals detected at location 1, $P_{\text{inj}} = 80$ MPa and $\theta_{\text{inj}} = 20^\circ$ BTDC. The intensity of the spectra was noted to increase when the injection pressure was increased with slight increase in the late combustion phase. This was found to lead to the oxidation of the smoke in the case of higher injection pressure. As previously noted high OH* is directly related to high temperature and this promotes the oxidation of soot formed.
Figure 6-14 Time evolution of OH\(^*\) radicals detected at location 1, \(P_{\text{inj}} = 80\) and 140 MPa, \(\theta_{\text{inj}} = 20^\circ\) BTDC
6.4. Summary

This section states the summary of the findings in the chemiluminescence spectral analysis of moderately injection timing PCCI diesel engine as follows:

1. The spectrums of formaldehyde (CH$_2$O) radicals were detected in the cool flame regions; a proof that the combustion concept studied (PCCI) had two-stage heat release. Higher grating of 300 lines/mm, brazing number of 300 nm with 2000 accumulated cycles gave precise measurements because of its high resolution.

2. At location 1 the OH$^*$ radicals were found to be good markers of the start of the exothermic reaction and premixed phase of combustion. CH$^*$ radical was found to be a good marker of the fuel-rich region within the piston bowl cavity. The peak of CO-O recombination and the ROHR were found to be related.

3. The soot formation within the piston cavity was noted to arise from the fuel impingement on the Derby hat wall but was oxidized thereafter. Higher OH$^*$ radicals led to faster oxidation of the soot in the late combustion phase.

4. Higher injection pressure led to higher emission of OH$^*$ radicals in the initial and the late combustion phase and hence to low emission of smoke at the exhaust due to the high temperature promoting the oxidation of soot.
6.5. References


Chapter 7

Conclusions

The key factors that affect combustion and pollutant formation in internal combustion engine were investigated under PCCI combustion mode. These in-cylinder parameters that were critical to the analysis were varied. These parameters included compression ratio, injection pressure, injection timing and EGR. The in-cylinder pressure was measured and used to calculate the ROHR which was critical for the combustion characteristic analysis. The engine-out emission were measured at the exhaust and used to evaluate the exhaust emission characteristics. Visualisation of the spray development and combustion phenomena was also done under the tested conditions to clearly understand the spray impingement and its relation to exhaust emission trend. The following are the key finding in this research.

1. PCCI combustion was achieved at moderately early injection timing without EGR. The transition point was found to be at 20° BTDC. Too early injection timing resulted in lower indicated thermal efficiency and IMEP with high exhaust emission of smoke, HC, and CO while the emission of NOx was relatively low for all the considered compression ratios. CR 13 had superior performance and the lowest emissions.

2. Advanced injection timing led to low in-cylinder pressure, low ROHR, low IMEP and indicated thermal efficiency with high emissions of smoke, CO and HC but low NOx emissions. This was thought to be caused by the fact that the fuel impinged on the cylinder wall and poor fuel-air mixing occurred.

3. Injection timing of $\theta_{\text{inj}} = 15 - 25°$ BTDC was found to be the optimum spray targeting spot for better performance and emissions. At this timing it was found out that the fuel strikes the walls of the Derby hat piston bowl and hence enhancing the premixing of the fuel and air within the piston bowl cavity.

4. Higher injection pressure of $P_{\text{inj}} = 140$ MPa led to higher indicated thermal efficiency, IMEP, low NOx, smoke and HC and but comparable CO with the low injection pressure $P_{\text{inj}} = 80$ MPa
5. EGR led to higher indicated thermal efficiency, IMEP and flameless combustion with near zero emissions of NO\textsubscript{x} with a slight increase in smoke, CO and HC emissions.

6. The interaction between the spray and the piston bowl geometry played a key role in the air–fuel mixing process. This led to low smoke emissions of less than 1% for both the late and moderately early injection timings without EGR. With EGR, it was possible to achieve less than 2% smoke emissions for the same range. Both homogenous combustion and low luminosity flames were observed for the low-soot-forming conditions. Low luminosity flame spots were attributed to fuel spray impingement on the wall of the piston bowl and deflection towards the space between the sprays. \( \theta_{\text{inj}} = 20^\circ \text{BTDC} \) with EGR was the optimum injection timing that gave simultaneously low soot and NO\textsubscript{x} emissions.

7. Under moderately early injection timing, \( \theta_{\text{inj}} = 20^\circ \text{BTDC} \) and injection pressure \( P_{\text{inj}} = 140 \text{ MPa} \), formaldehyde was measured in the cool flame region while OH* and CH* radicals were found to be good markers of exothermic reaction in the high temperature oxidation phase. Also CH* radicals were noted to be good marker of the fuel-rich regions within the piston bowl cavity. No trace of CH* radicals were found in location 3 indicating that there was no fuel impingement at the cylinder wall. Under this condition the indicated thermal efficiency was high and with low emission of smoke.

8. Soot formation due fuel impingement at the Derby hat wall and its fast oxidation under high injection pressure was noted for both the initial and late combustion phase evidenced by high emission of OH* radicals.