A COMPUTATIONAL INVESTIGATION OF INJECTION STRATEGIES AND
SENSITIVITY ANALYSIS OF AN ETHANOL FUELLED PPCI ENGINE

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A COMPUTATIONAL INVESTIGATION OF INJECTION STRATEGIES AND
SENSITIVITY ANALYSIS OF AN ETHANOL FUELLED PPCI ENGINE

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Thesis

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ABSTRACT

An Ethanol fueled PPCI (Partially Premixed Compression Ignition) engine was computationally studied to understand the effect of injection strategies on efficiency, emissions, and noise. The CI engine selected for this study was a heavy duty single cylinder engine having a displacement of 2123 cm$^3$ with a compression ratio of 17.3 at a medium load of approximately 12 bar IMEP. CFD modelling with detailed chemistry was done using converge CFD package. All the CFD simulations presented in this study were conducted on a single engine sector to reduce the computational time and the simulations were run from Intake valve closure (IVC) to Exhaust valve opening (EVO). The injection strategy used in this study is a double injection strategy. A series of simulations were run in order to obtain the optimum injection parameters. First, the start of the first injection was changed from -60 CAD (crank angle degree) to -20 CAD (crank angle degree) by keeping the start of second injection constant at -5 CAD. Secondly, the start of the second injection was changed from -10 CAD to -2 CAD by keeping the start of first injection constant at -5 CAD. Lastly, the injection mass percentage in the first and second injection was changed from 60-40 % to 90-10 % by keeping the start of first injection and second injection constant at -50 CAD and -10 CAD.

The results obtained from these simulations give the optimum injection parameters which will have high thermal efficiency with reduced emissions and noise.
The optimum injection parameters obtained are SOFI at -50 CAD and SOSI at -10 CAD with 70 % of the fuel injected in the first injection and 30 % in the second injection.

Subsequently, the sensitivity of the engine combustion to change in inlet temperature and inlet pressure was studied by keeping the obtained optimum injection parameters. The results obtained from this showed that the engine combustion is highly sensitive to inlet temperature than the inlet pressure. Additionally, the strategies required to recover the optimum performance of the engine were explored.
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## NOMENCLATURE

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<td>Selective Catalytic reduction</td>
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<td>LNT</td>
<td>lean NOx Traps</td>
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<td>TWC</td>
<td>Three Way Catalyst</td>
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<td>UHC</td>
<td>Unburnt Hydrocarbons</td>
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<tr>
<td>CO</td>
<td>Carbon Oxide</td>
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<tr>
<td>DEF</td>
<td>Diesel Exhaust Fluid</td>
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<td>NO</td>
<td>Nitric Oxide</td>
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<td>LTC</td>
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<td>HCCI</td>
<td>Homogenous Charge Compression Ignition</td>
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<td>RCCI</td>
<td>reactivity Controlled Compression Ignition</td>
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<tr>
<td>CI</td>
<td>Compression Ignition</td>
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<tr>
<td>SI</td>
<td>Spark Ignition</td>
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<tr>
<td>OH</td>
<td>Hydroxyls</td>
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<td>DME</td>
<td>Di-Methyl Ether</td>
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<tr>
<td>LHV</td>
<td>Latent Heat Value</td>
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<td>CAD</td>
<td>Crank Angle Degree</td>
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<td>Abbreviation</td>
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<tr>
<td>CA50</td>
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<td>CDC</td>
<td>Conventional Diesel Combustion</td>
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<td>HC</td>
<td>Hydro Carbons</td>
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<td>CO₂</td>
<td>Carbon Dioxide</td>
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<td>EGR</td>
<td>Exhaust gas Recirculation</td>
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<td>DI</td>
<td>Direct Injection</td>
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<td>RON</td>
<td>Research Octane Number</td>
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<td>MON</td>
<td>Motored Octane Number</td>
</tr>
<tr>
<td>OI</td>
<td>Octane Index</td>
</tr>
<tr>
<td>IMEP</td>
<td>Indicative Mean Effective Pressure</td>
</tr>
<tr>
<td>LTHR</td>
<td>Low Temperature Heat Release</td>
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<tr>
<td>HTHR</td>
<td>High Temperature Heat Release</td>
</tr>
<tr>
<td>PPC</td>
<td>Partially Premixed Combustion</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>BTDC</td>
<td>Before Top Dead Centre</td>
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<tr>
<td>ATDC</td>
<td>After Top dead Centre</td>
</tr>
<tr>
<td>CDC</td>
<td>Conventional Diesel Combustion</td>
</tr>
<tr>
<td>RI</td>
<td>Ringing Intensity</td>
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<tr>
<td>ISFC</td>
<td>Indicated Specific Fuel Consumption</td>
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<tr>
<td>ULSD</td>
<td>Ultra-Low Sulphur Diesel</td>
</tr>
<tr>
<td>DTBP</td>
<td>Di-Tert Butyl Peroxide</td>
</tr>
<tr>
<td>PPRR</td>
<td>Peak Pressure Rise rate</td>
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<tr>
<td>EHN</td>
<td>2-Ethyl Hexyl Nitrate</td>
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<td>HD</td>
<td>Heavy Duty</td>
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<td>AMR</td>
<td>Adaptive Mesh refinement</td>
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<td>Abbreviation</td>
<td>Description</td>
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<tr>
<td>CR</td>
<td>Compression Ratio</td>
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<td>IVC</td>
<td>Inlet Valve Closing</td>
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<td>EVO</td>
<td>Exhaust Valve Opening</td>
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<tr>
<td>ABDC</td>
<td>After Bottom Dead Centre</td>
</tr>
<tr>
<td>BBDC</td>
<td>Before Bottom Dead Centre</td>
</tr>
<tr>
<td>SOFI</td>
<td>Start of First Injection</td>
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<tr>
<td>SOSI</td>
<td>Start of Second Injection</td>
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<tr>
<td>TDC</td>
<td>Top Dead Centre</td>
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CHAPTER I

INTRODUCTION

1.1 Motivation and Background

The invention of internal combustion engines revolutionized the modern society because of their simplicity and high power density. The rise in fuel costs and adverse effects of the greenhouse gases prompted researchers to look into increased efficiency from the internal combustion engine. This need for the increased efficiency made diesel engines ahead of the spark ignition engine because of their high efficiency. The recent analysis shows that the usage of diesel engines in automobiles has increased predominantly over the past few years. Unfortunately, diesel engines are also a source of particulate matter and nitrogen oxides which have serious effects on human health and environment. Because of their serious effects many countries have implemented stringent emission regulation limits over the past several years.

The diesel or the compression ignition engines depend on the autoignition quality of the fuels i.e. fuels with high autoignition quality are best suited for diesel engines. In diesel engines, air is taken from the intake stroke and is compressed, the diesel fuel is injected near the top dead center with high injection pressure and velocity with multiple orifices, which atomizes and penetrates the fuel. Due to high temperature of the compressed air, which had already persisted in the combustion chamber, the diesel fuel liquid jets break
into small droplets and vaporize, and then it autoignites. Unlike the premixed flame in the spark ignition engine, diesel engine has a high temperature diffusion flame. This high temperature promotes the formation of thermal NOx. Soot is also formed in the rich region of the fuel jet.

Emission of NOx and soot is generally controlled by various exhaust after treatment methods. These include use of Diesel Particulate Filters (DPF), Selective Catalytic reduction (SCR) and lean NOx Traps (LNT). Diesel Particulate Filter (DPF) is used to control soot emission, but it has several drawbacks. The filters which are used in the DPF get filled up with soot and need to be regenerated regularly. This process is called as Filter Regeneration. The DPF filter requires exhaust gas temperature of 600°C to remove soot which is stored on the filter walls (Dempsey, 2013). These methods increase fuel consumption and decrease the efficiency of the Diesel engine.

The NOx emissions can be reduced by using Selective Catalytic Reduction (SCR), Lean NOx Traps (LNT) and a Three Way Catalyst (TWC). The overall fuel lean operation of diesel engines makes the use of Three Way Catalyst (TWC) non-ideal. Attempts to reduce NOx by using a TWC result in pure fuel economy. The Selective Catalytic Reduction (SCR) uses a secondary fluid which is called as Diesel Exhaust Fluid (DEF), which usually is urea. Urea, when injected into exhaust, reduces to ammonia and carbon dioxide which converts NOx to nitrogen and water. Urea has to be stored in a separate tank in the vehicle and also adds to the overall fuel cost (Reitz et al, 2014). SCR reduces NOx emissions by up to 95% (Dempsey, 2013). LNT uses products of rich combustion to reduce NOx emissions to nitrogen through reactions. LNT doesn’t require a secondary fluid but the reduction of NOx is up to 70%. The engine has to be operated periodically on the rich
side to reduce NOx emissions by which the fuel efficiency is reduced, which is a drawback (Dempsey, 2013).

The aftertreatment methods are good at reducing NOx and soot emissions but require additional fuel consumption. They are also very expensive and complex to use. So, in order to increase the engine efficiency, the engine should rely less on aftertreatment devices (Reitz et al, 2014). The future engines should be designed in such a way that they minimize the need of aftertreatment methods. Keeping this in mind, many investigations have been conducted by the researches and strategies have been developed to reduce in-cylinder production of pollutants. These strategies are usually termed as Low Temperature Combustion (LTC) strategies, such as Homogeneous Charge Compression Ignition (HCCI), Partially Premixed Compression Ignition (PPCI) and Reactivity Controlled Compression Ignition (RCCI). In LTC, because of the low combustion temperatures, which is less than 2000 K, the formation of NOx is reduced and long ignition delay eliminates the rich regions by which the formation of soot is reduced.

The LTC methods can be divided into two categories. The one in which the combustion phasing is not coupled to fuel injection event and the combustion depends on the chemical kinetic reactions. HCCI is in this category. In the second category, combustion phasing is coupled to the fuel injection event. PPCI mode is in this category. The operating regimes of HCCI, PPCI and conventional diesel mode on the local equivalence ratio - temperature map are shown in Figure 1.1.
A new method, developed recently and called as Reactivity Controlled Compression Ignition (RCCI), overcomes the limitations of HCCI and PPCI and has the potential advantages of the both modes. The three LTC techniques are briefly discussed below.

1.2. LTC strategies

LTC methods are also known as Low Temperature Combustion methods. In LTC methods, sufficient premixing occurs before the start of combustion which decreases the formation of rich regions therefore soot is reduced. The low flame temperatures which are formed by lower equivalence ratios decreases the NOx (Sage L. Kokjohn 2010).

1.2.1 Homogenous Charge Compression Ignition (HCCI)

The combination of CI engine and SI engine is HCCI engine. In HCCI, the fuel is injected very early into the combustion chamber prior to the combustion. This early
injection of the fuel makes it to mix homogenously with air, forming a well premixed fuel air mixture. This premixed fuel air mixture autoignites due to increase in temperature during the compression stroke. Unlike CI and SI engines, there is no diffusion flame and flame front propagation in HCCI engine. The equivalence ratio of the homogenous premixed charge in HCCI is less than 1. Because of early injection, the mixture is homogenous everywhere, avoiding highly rich and lean regions and decreasing the post combustion temperature, which is the key factor for producing the thermal NOx. The lean homogenous mixture eliminates the formation of Soot. Figure 1.2 shows the region of operation of HCCI engine (Bendu et al, 2013)

Figure 1.2 - Operating regime of HCCI combustion (Bendu et al, 2013).

HCCI combustion shows two stage heat release using diesel like fuels under certain conditions. The first stage relates to low temperature regime and the second stage relates to high temperature regime which is the main heat release regime. Low temperature kinetic
reactions prevail during the first stage and the oxidation of CO dominates the high temperature regime (Bendu et al, 2013). Figure 1.3 shows a typical heat release rate profile for HCCI combustion with diesel like fuels.

Figure 1.3 - Typical heat release profile of HCCI for diesel like fuels (Yao et al, 2013).

Though HCCI combustion has many advantages over the Conventional CI engines, it has to overcome the drawbacks before it is applied for the real time practical engines for mass production. The drawbacks include (i) Control of combustion phase (ii) High UHC and CO levels (iii) Knocking (iv) Starting in cold conditions (v) Homogenous mixture preparation and (vi) Narrow operating range.

1.2.2 Partially Premixed Compression Ignition (PPCI)

PPCI is developed to overcome the drawbacks of the HCCI. PPCI has better control over the start of combustion than HCCI. In PPCI, fuel is injected very early unlike conventional diesel and the HCCI engine. In the conventional diesel engine, fuel is injected
slightly before the top dead center and, in HCCI, the fuel is injected nearly at the bottom dead center. The charge distribution for PPCI and HCCI differ as HCCI is homogenous but PPCI is non-homogeneous before ignition.

Early injection with PPCI makes the fuel partially premixed. The injection event ends prior to the start of combustion making the ignition dwell positive (Kokjohn, 2012). Because of the positive ignition dwell, the charge injected into the cylinder attains partial premixing. Although the fuel is injected early in comparison to the conventional CI engines, the combustion phasing is coupled to the injection event and can be controlled with injection. The PPCI combustion can be achieved by injecting the fuel in different ways and multiple injections (Dempsey, 2013). An approach investigated by many researchers involves injecting a part of the fuel early, which helps in obtaining homogenous charge everywhere like HCCI, and direct injection of the remaining fuel to control ignition. This type of approach stratifies in-cylinder charge distribution and gives a better control over the combustion phase and duration by preventing the ignition of the charge simultaneously (Hanson, 2015). The drawbacks of the PPCI engine are increased rates of UHC and CO, combustion noise, rapid cylinder pressure rise, and difficulty in applying at high load.

1.2.3 Reactivity Controlled Compression Ignition (RCCI)

RCCI is also known as dual fuel PPCI. RCCI uses two different types of fuels at different intervals. In RCCI, a low reactivity fuel like gasoline or alcohol, which is of high octane number, is injected by using port fuel injection and a high reactivity fuel like diesel is injected directly by common rail injector using multiple injections to control the in-cylinder fuel reactivity and combustion phasing. The low reactivity fuel creates a well-mixed charge of the low reactivity fuel, and the high reactivity fuel creates reactivity
stratification which governs the onset of combustion and combustion duration. The combustion starts in the high reactivity fuel air areas and moves to low reactivity fuel air areas. This staging gives better thermal efficiencies, wide operating range, and low emissions (Reitz et al, 2014).

Apart from the novel engine combustion regimes, discussed above, significant emphasis has been placed on alternative fuels. In particular, various researchers have focused on in-tandem consideration of alternative fuels and corresponding engine combustion technologies. In the following, use of alcohols as alternative fuels is summarized with emphasis on ethanol, which is the fuel considered in the present thesis.

1.3 Alternative Fuels

Transportation has become a vital important element in day to day life. One cannot imagine the life without transportation. In U.S. and around the world, majority of the transportation vehicles rely on petroleum derived fuels i.e., gasoline and diesel which are non-renewable fuels. Gasoline, Diesel and other fuels are dangerous as they emit certain gases which have a negative impact on the environment and human health. The problem with these fuels is that they exist only in few countries and are finite in supply. Keeping in mind the future needs, we need to expand our knowledge towards the renewable and alternative fuels which have low impact on the environment. Figure 1.4 shows the use of alternative fuels in the United States.
1.3.1 Use of Alcohols as Alternative Fuels

Of all the Alternative Fuels, alcohols are most attractive and promising due to their ease of production, storage, availability and handling. Alcohols have been popular alternative fuels for many years and will play an important role in the future. Alcohols, like Ethanol and Methanol, can be used as alternative fuels. The usage of Ethanol as an alternative fuel is not new, it has been using in Brazil for the past 35 years and the situation of the oil crisis in 1970 led to use the Methanol. Both Ethanol and Methanol can be used in engines either in their pure form or by blending with conventional fuels (Ghadikolaei et al., 2015).

Alcohols are produced from agricultural feedstocks, crops and even from waste paper and grass. These can also be produced from residue of sugarcane. Alcohols are
chemically designated by the hydroxyl group (-OH) attached to one of the carbons atoms present in their structure. The alcohol fuels have many advantages which outweigh their disadvantages. The advantages are as follows (Ghadikolaei et al, 2015)

1. They can be produced from organic material such as biomass and municipal waste.
2. Alcohols have high average Octane rating than gasoline, which increases power and fuel efficiency with increase of compression ratio.
3. They release less byproduct which harms the environment because of their low evaporative emissions.
4. They have better combustion and emission characteristics
5. Soot is very low because of low carbon content and presence of oxygen in the fuel.
6. Alcohols are easily injected and atomized due to their lower viscosity.
7. They have lesser emissions because of the presence of high oxygen content, high hydrogen carbon ratio, and less Sulphur content.
8. The latent heat of vaporization of alcohols is very high.

1.3.2 Ethanol

Ethanol as an alternative alcoholic fuel is produced by fermentation of sugar from corn, sugarcane, barley, sugar beets and from residues like feedstock and waste wood. When we see the chemical structure of ethanol, it is isomeric to DME (Di Methyl Ether). They can be denoted by the same chemical formula $\text{C}_2\text{H}_6\text{O}$, $\text{C}_2\text{H}_5\text{OH}$. Though they have the same chemical formula, the chemical and thermodynamic behavior and properties are significantly different (Ghadikolaei et al, 2015). The structure of Ethanol is shown in Fig
5. It has an oxygen atom in it as shown in Figure 1.5. Because of that ethanol provides high combustion efficiency with reduction in exhaust gas emissions.

![Figure 1.5 - Structure of Ethanol](image)

The properties of Ethanol in comparison with gasoline and Diesel are shown in Table 1.1.

Table 1.1 - Properties of Ethanol in comparison to other fuels (Ghadikolaei et al, 2015).

<table>
<thead>
<tr>
<th></th>
<th>Ethanol</th>
<th>Methanol</th>
<th>Gasoline</th>
<th>Diesel</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Formula</strong></td>
<td>CH₃CH₂OH</td>
<td>CH₃OH</td>
<td>C₇H₁₆</td>
<td>C₁₄H₃₀</td>
</tr>
<tr>
<td><strong>Molecular Weight</strong></td>
<td>46.07</td>
<td>32.04</td>
<td>100.2</td>
<td>198.4</td>
</tr>
<tr>
<td><strong>Density</strong></td>
<td>0.785</td>
<td>0.972</td>
<td>0.737</td>
<td>0.856</td>
</tr>
<tr>
<td><strong>Normal Boiling Point</strong></td>
<td>78</td>
<td>64</td>
<td>38-204</td>
<td>125-400</td>
</tr>
<tr>
<td><strong>LHV (KJ/g)</strong></td>
<td>26.87</td>
<td>19.99</td>
<td>43.47</td>
<td>43.16</td>
</tr>
<tr>
<td><strong>Carbon Content</strong></td>
<td>52.2</td>
<td>37.5</td>
<td>85.5</td>
<td>87</td>
</tr>
<tr>
<td><strong>Sulfur Content</strong></td>
<td>0</td>
<td>0</td>
<td>200</td>
<td>250</td>
</tr>
</tbody>
</table>
The advantages of Ethanol are as follows:

1. It helps in reducing greenhouse gases
2. It can be easily mixed with gasoline
3. It can be used as an oxygenate in gasoline.
4. Ethanol burns more cleanly and the exhaust gases are cleaner.
5. Ethanol is an anti-freeze. Even in freezing cold conditions, fuel will not freeze.

Ethanol and methanol are the two alcohol fuels which are being and will be used as prominent alternative fuels for internal combustion engines.

In this chapter, various novel engine combustion technologies were briefly described along with an introduction of ethanol as an alternative fuel. These strategies are reviewed in detail in Chapter 2. The motivation of the present work is to explore the PPCI strategy based on ethanol. This is also presented in Chapter 2.
CHAPTER II

LITERATURE REVIEW

2.1 Introduction

As discussed in Chapter 1, LTC strategies reduce in-cylinder NOx and soot production without losing thermal efficiency. The main difference in these LTC strategies in comparison to the conventional CI (Compression Ignition) combustion is that they sufficiently premix fuel and air and keep post combustion temperature low to avoid NOx and soot formation, which is not achieved in conventional diesel engines. To achieve clean combustion, the peak equivalence ratio should be less than 2 and the peak temperature should be less than 2000 K. In the following, the relevant literature on HCCI, PPCI and RCCI is reviewed in detail.

2.2 HCCI Literature

The HCCI combustion is the simplest method of achieving LTC combustion. In HCCI, fuel is injected in the intake manifold or nearly at the bottom dead center, which gives sufficient time for proper mixing of fuel and air. The overall equivalence ratio of this mixture is fuel lean (generally less than 0.5). The mixture is then compressed and combustion occurs when it reaches its autoignition temperature. In HCCI, the combustion is controlled purely by chemical kinetics of the fuel. The HCCI combustion has nearly zero NOx and soot emissions and high thermal efficiency due to shorter combustion duration. Though HCCI
combustion offers good thermal efficiency and zero NOx and soot emissions, there are major drawbacks. In HCCI, the control of combustion is very difficult since it depends purely on chemical kinetics, which is influenced by initial temperature, initial pressure and composition of fuel and air mixture. The rate of heat release is very rapid in HCCI combustion and it is not controllable, which results in high pressure rise rate. This high pressure rise rate gives high peak cylinder pressures. Because of high cylinder pressure, the HCCI operating regime is confined to medium load. At high loads HCCI combustion gives high peak pressures, noise and vibration and at low loads misfire occurs because of the extended ignition delay which is a result of low equivalence ratio and low gas temperatures (Dempsey, 2013).

Many researches have studied HCCI to understand its operation and limitations. These studies also proved that HCCI can be realized using different types of fuels. The present focus on HCCI research is to extend its operating range while decreasing the pressure rise rate and noise.

(Onishi et al, 1979) were the first ones to investigate HCCI combustion. They found that rapid ignition of charge could reduce emissions and improve fuel economy. An experimental spectroscopic analysis study was conducted by (Naguchi et al, 1979). From their work, they noted that ignition occurs at several points simultaneously. Inside the cylinder, they found CH₂O and HO₂ which are the key indicators of low temperature autoignition chemistry before ignition, and after ignition they found CH, H and OH radicals which indicate the high temperature chemistry. From these works, it can be conclude that there is no flame propagation in HCCI engine combustion and the combustion is purely
dependent on chemical kinetics, which is controlled by pressure, temperature and composition, unlike flame propagation in SI engines and fuel/air mixing in Diesel engines.

(Flowers et al, 2002) investigated CO and HC emissions in isooctane HCCI engine using multizone simulations. They developed a detailed chemical kinetic model to simulate HCCI engine. Their research indicated CO and HC emissions smaller by an order of magnitude. They divided the entire computational domain into small chemical kinetic zones. The results indicated that most of the HC and CO emissions are from the unreacted mixture in the crevice region and boundary layer in the squish region.

(Lee et al, 2015) conducted a study to increase the operating range and to control the combustion timing. In order to extend the operating range, EGR stratification, asymmetric injection and open valve injection were used. By using these methods the maximum load at 1500 and 2000 rpm increased by 10% and 28 %, respectively. In this study they used peak pressure value and pressure rise rate as the variables to judge the stabilization of combustion.

The two main parameters which control the autoignition timing and the combustion control in the HCCI combustion is the time – temperature history and the autoignition characteristics of the fuel. The control methods of time - temperature history include initial pressure, initial temperature, use of EGR and variable compression ratio. These methods are used to control before intake valve closure, and when the intake valve is closed the fuel injection strategies control the combustion and autoignition timing (Dempsey, 2013).

(Das et al, 2015) studied HCCI-DI engine using dual injection strategy with EGR. They varied the premix ratio from 0 to 1 and realized that by increasing the premix ratio,
the peak pressure and the pressure rise rate is increased and combustion is advanced from the base condition. As the premix ratio increases, more amount of fuel is introduced in the early stage which makes the fuel to undergo pre-flame chemical reactions which in turn increases peak pressure and pressure rise rate. So they used EGR along with dual injection to decrease NOx emissions, pressure rise rate and peak pressure.

(Yang et al, 2011) conducted a study to increase the high load limit of the HCCI engine using fuel stratification of gasoline and methanol. In this study, gasoline was injected early to make homogenous charge and the methanol was injected directly. Due to high latent heat and the direct injection of methanol, the temperature decreases during atomization before combustion and there is reduction in the peak pressure and pressure rise rate. An increase in fuel stratification increased the combustion duration, thereby increasing the operating regime of the high load limit.

Though Diesel HCCI combustion gives nearly zero NOx and soot emissions, but its practical implementation is limited to low loads only. Because of its auto ignition quality and shorter combustion duration, it is not acceptable at medium and high loads. Even with the implementation of new research methods to the Diesel HCCI, the operating regime cannot be extended.

(Shibata et al, 2005) studied the influence of fuel properties on HCCI combustion and proved that both the low temperature and high temperature chemistry is important in understanding the HCCI combustion and the low temperature reactions are very important in the combustion phasing. In precedence to the above work, (Kalghatgi 2010) studied HCCI combustion with fuels having different octane numbers. (Bessonette et al, 2009)
also studied the influence of fuel reactivity on the HCCI combustion. Both works are capable of achieving zero NOx and soot emissions and an increase in the extension of operating range. From these works we understand that the best fuel for HCCI combustion to operate at medium and high loads is a low cetane number fuel (i.e. high octane number).

(Zheng et al, 2015) studied butanol HCCI combustion using a single cylinder engine with high compression ratio and compared with diesel HCCI combustion. In this study, butanol HCCI combustion offered low NOx and soot levels with minimum requirement of EGR. Because of low reactivity of butanol, the combustion phasing and thermal efficiency was way better than that of Diesel HCCI. At high loads, EGR and pressure boost was required to decrease pressure rise rate.

Similar to the previous studies, (Zhang et al, 2015) studied combustion characteristics and performance of methanol fueled HCCI engine. The key findings from this work were those combustion phasing and heat release rates are sensitive to intake temperature, while thermal efficiency depends on the equivalence ratio. At CA50 (Crank angle for 50% heat release) of 7.5 CAD (Crank angle in degree) and combustion duration of 11 CAD, the maximum thermal efficiency was achieved.

(Maurya et al, 2014) experimentally studied combustion characteristics and performance of methanol and ethanol fueled HCCI engine using a four cylinder four stroke engine at different speeds and compared them with the Gasoline HCCI. From their results, methanol and ethanol are better than gasoline In HCCI combustion.

In order to control autoignition timing and the extension of the operating range, many researches have studied the effect of various parameters like EGR, control of fuel
injection, fuel modification and boosting. (Ogawa et al, 2003) used DME as the main fuel and various reaction suppressors like Methanol, Methane, Ethanol, Hydrogen and water. From their study they were able to extend the operating range with low exhaust gas emissions. In a follow-up work, (Liu et al, 2009) investigated the influence of fuel properties and operating conditions using different fuels with research octane number (RON) greater than 90 using a multicylinder direct injected diesel engine. Their results showed that the effect of fuel properties on HCCI combustion depends on the operating conditions, i.e. different fuels have different effects at different operating conditions. The sensitive fuels (Fuels with greater difference between Research and Motor Octane Numbers) are very good at extending the load range. In order to extend the low load range, high inlet temperature is needed, and high inlet pressure is needed to extend high load range for sensitive fuels.

Based on the work of (Ogawa et al, 2003), (Yao et al, 2009) extended their work to dual fuel engine to know the emissions and combustion performance using DME/Methanol as fuel. A reduced chemical kinetic mechanism of DME and Methanol comprising of 27 species and 35 reactions was used to simulate. The simulation results were in well accordance with the experimental ones. They noted that the UHC emissions are mainly because of the unburnt fuel in the piston crevice region and the CH₂O is from cylinder liner wall. The majority of CO emissions are from the top part of the piston. The CO, UHC, and CH₂O emissions are very low when temperature in the cylinder is above 1400 K.

From the literature discussed above, it can be concluded that HCCI engines are good at reducing NOx and soot emissions to near zero levels without any reduction in thermal efficiency, but HC and CO emissions can be high.
To decrease these, several studies have been conducted by changing the nozzle diameter, using narrow spray cone angle, increasing the number of holes. All these methods are good at achieving near zero emissions and increase in thermal efficiency but they are restricted to low and medium loads and by crossing the limit, the exhaust gas emissions increase drastically due to rapid burning of the premixed fuel. To improve exhaust gas emissions from HCCI combustion, (Kim et al, 2007) investigated a narrow spray cone angle and dual injection strategy using a common rail diesel engine at various fuel injection parameters. The key factors from their results indicate that when the injection angle is decreased from 156 to 60 degree, wall wetting problems are decreased and dual injection with narrow angle fuel injection by optimizing the first and second injection is an effective method in decreasing NOx and CO emissions without a reduction in thermal efficiency.

The conventional engines must use only a specific fuel like gasoline in SI engine and Diesel in CI engine. HCCI can use wide range of fuels (Christensen et al, 1999). (Epping et al, 2002) reported that the fuel should have high volatility in order to form homogeneous charge.

To further investigate various types of fuels used in HCCI combustion, Yao et.al. (2004) investigated the influence of octane number on performance and emissions of HCCI combustion. The results showed that the operating range can be extended by using different fuels at different loads. They further investigated using gasoline, PRF, PRF and Ethanol fuels. The test results showed that CA50 is not sensitive to the Research Octane Number (RON) and Motor Octane Number (MON), but relates with the Octane Index (OI). With an increase in OI, the resistance to autoignition increases and higher IMEP can be reached.
Along with the use of different fuels in HCCI combustion to overcome its limitations, there are some chemical components which increase or decrease the heat release rate with their addition to the fuel. (Aceves et al, 2003) investigated different fuel additives and ranked them for HCCI combustion based on their ability to advance ignition. (Shibata et al, 2005) also investigated different fuels and their effect on Low Temperature Heat Release (LTHR) and High Temperature Heat release (HTHR). EGR is also one of the methods of fuel modification. Addition of EGR decreases temperature in the cylinder, controls heat release rate and delays autoignition, which decreases peak cylinder pressures.

2.3 PPCI Literature

Though there are many advantages with HCCI combustion, but the lack of direct control of the start of combustion in HCCI and the lack of coupling between fuel injection and combustion event is the major problem. In addition, the literature on HCCI combustion proves that it is very sensitive to pressure, temperature and EGR. Theoretically all these parameters can be controlled, but on a cycle to cycle to basis it is difficult to control them, which made the engine research community to look forward for other alternative methods like early or late injection of the fuel. These Methods are technically known as Partially Premixed Combustion (PPC) or Partially Premixed Compression Ignition (PPCI). In general, PPCI stands in between DICI and HCCI combustion since the fuel is directly injected into the combustion chamber like the DICI and, like HCCI, it is injected early or late which promotes mixing. The early injection of fuel in the PPCI can lead to high pressure rise rates and limit its maximum operating load similar to that of HCCI.

The PPCI concept has been investigated by many researchers but the pioneering work was done by (Kalghatgi et al, 2007). In his study, he compared the gasoline fuel with
RON of 95 and a diesel fuel for change in different parameters like EGR levels, load and start of injection timings in a single cylinder heavy duty engine. The results showed that gasoline fuel has lower levels of NOx and smoke than the diesel fuel at all operating conditions. Due to its high resistance to autoignition and consequent increase in the ignition delay, gasoline allowed longer time for fuel and air to mix and achieve low emissions of NOx and smoke.

Further, to know the fuel octane effects on PPCI engines, they compared four fuels with different octane numbers (91, 84, 78, 72) which are in the gasoline boiling range, with diesel fuel at low load and high load using a single injection by changing different parameters in a single cylinder light duty compression ignition engine. The results showed that gasoline fuel has very low smoke and NOx levels compared to diesel and the best fuel found was in between 75-85 RON for the used operating conditions and compression ratio (Kalghatgi et al, 2009).

These results (Kalghatgi et al, 2007) show that the best fuel for the PPCI combustion should be the fuel which is having high octane number as gasoline and also early or late injection of the fuel in PPCI results in high thermal efficiency as the Combustion Phasing (CA50) occurs after the top dead center and the injection of the fuel before combustion results in low levels of smoke and NOx emissions.

Further work conducted by (Kalghatgi et al, 2010) by using split injection with gasoline and diesel showed that the usage of pilot injection resulted in the appearance of Low Temperature Heat Release (LTR) in the Heat Release curve. The LTR initiated low temperature chemistry and the High Temperature Heat Release (HTHR) initiates the main
combustion event. Due to this major change in heat release curve, the soot emissions were very high in gasoline split injection due to lack of proper air fuel mixing before combustion, but the use of split injection with gasoline in PPCI engine increased the load limit to 17 bar IMEP with low NOx and Soot emissions.

Research at the Lund University showed that the emissions from Diesel PPCI were under emission limits when compared with the conventional diesel. In order to achieve this, EGR rate should be in excess of 70 % which is impractical to achieve in practical operation. Since the appropriate level of premixing cannot be achieved with Diesel fuel as it has high cetane number, which makes it highly reactive to autoignite rapidly, which in turn increases the peak cylinder temperature and results in increased NOx and Soot levels. Wall wetting is the major problem of the Diesel PPCI engines because of its high boiling point. Because of these issues associated with diesel PPCI engines, diesel fuel is not considered as the best fuel for PPCI operation.

The usage of different Octane number fuels in the PPCI engines was extensively studied by (Manente et al, 2009) at Lund University. They did many studies on PPCI engines using different higher octane number fuels and ethanol from low load to high load and compared with diesel. Their work demonstrated that the best fuel to fit for the compression ignition engine should be the one with the higher octane number.

(Manente et al, 2009) conducted a study to understand the behavior of the Octane Number fuels which are in the gasoline boiling with Research Octane Number ranging from 69 to 99 in a single cylinder engine at 1300 and 1000 rpm with 50 % EGR for the load range of 1 to 12 bar IMEP. The compression ratio used for this study was 18.3. The
injection strategy used was split injection with pilot injection at -60 CAD. Their results showed that usage of gasoline like fuels in CI engines could achieve high efficiency with emissions below the target levels. The limiting factor for this study was that they could not go beyond the 12 bar IMEP because of high compression ratio.

In continuation of the above work to increase the load range, they conducted a study using seven fuels with octane number ranging from 69 to 99 with a load sweep from 5 to 18 bar IMEP in a single cylinder Scania D12 engine with compression ratio of 14.3. Their results showed that the gross indicated efficiency of 54 to 56 % could be achieved with a reduction in heat transfer and exhaust losses, but with a high boost pressure. EGR level of 50 % has to be used to achieve NOx below the target levels at high load of 18 bar IMEP. The usage of 50% EGR, for loads higher than 7 bar IMEP, achieved combustion efficiency of 98 % resulting in low HC and CO emissions. The Peak Pressure Rise Rate, which is the major problem of the PCCI engine at higher loads, can be eliminated by separating the end of main injection and the start of combustion (Manente et al, 2009).

Use of gasoline in CI engines, with operating conditions similar to diesel injection strategy, resulted in high heat loss. So the rules used for Diesel PPCI can no longer be applicable while using gasoline in CI engine. This led to the thinking of a new injection strategy when gasoline like fuels are used in CI engines. (Manente et al, 2009) developed an advanced injection strategy for gasoline at high load with the injection of 54.5% of the fuel in the pilot injection at -60 CAD and the remaining around TDC with the appropriate EGR %. This advanced injection strategy was compared with diesel by keeping CA50, EGR and amount of fuel constant. The results showed that the emission levels and the gross fuel consumption of the gasoline was lower than diesel. In the same study, gasoline, ethanol
and diesel were compared at 14.8 bar IMEP with 25 % EGR. Gasoline and ethanol showed low soot and NOx levels than diesel due to longer ignition delay while higher HC and CO emissions.

The unique properties of the Ethanol make it a good potential fuel for PPCI engines. To obtain high efficiency with low emissions, one has to apply a strategy which results in appropriate in-cylinder temperature with a fuel which has the properties for effective combustion. So, in order to know the effects of ethanol in PPCI engines, a sensitivity study was conducted by (Manente et al, 2013) in a single cylinder heavy duty engine at medium and low loads with split injection strategy by varying different parameters like intake temperature, EGR level and Injection pressure. They showed that EGR rate less than 45 % resulted in early start of combustion with loss of combustion control, and EGR rates above 55 % resulted in low combustion efficiency with increase in soot, HC and CO emissions, while no significance effect of injection pressure was noted. The combustion event was also sensitive to inlet temperature. The change in inlet temperature increased NOx emissions and high combustion efficiency was achieved because of better oxidation.

In continuation of the work done by (Manente et al, 2013) in developing an advanced injection strategy for gasoline like fuels, (Kaiadi et al, 2013) conducted a study to investigate the best injection strategy for the PPCI combustion fueled with pure ethanol on a single cylinder heavy duty engine from low to medium load. They used two injection strategies, a double injection and single injection, and compared both strategies. For evaluating these strategies numerous experiments were done by first keeping Start of First injection variable between -60 to -20 CAD and Start of Second injection keeping constant
at -5 CAD; secondly, varying second injection and keeping the first injection constant and finally varying the injection duration. The engine performance was analyzed in terms of stability, controllability, emissions and efficiency. Their results showed that double injection is the best strategy for ethanol PPCI as it offers a wide operating range with controllability of combustion and high efficiency by adjusting the injection duration and start of first and second injection.

The use of gasoline type fuels is not limited to ethanol. (Kim et al., 2008) investigated the combustion characteristics and NOx emissions of a dimethyl-ether fueled compression ignition engine using a single cylinder DI engine with use of advanced injection strategies. DME (Dimethyl-Ether) has excellent ignition properties. The absence of soot and the requirement of less air with DME can provide better engine performance and has drawn attention for use in PPCI. The results show that the use of advanced injection strategies with narrow spray cone angle injector, which reduced the wall wetting issues at low load conditions, resulted in low NOx emissions and, at high load, use of dual injection strategy, with first injection at -100 CAD and second injection at 10 CAD, offered low NOx. The use of double injection effectively increased engine load and the emissions were very low when compared with the single injection.

Although PPCI strategies show that NOx and soot levels are very low, still the issues like the combustion phasing control and the rate of heat release control and high levels of peak pressure rise rate at high load limit the use of this strategy. There should be a strategy in which the drawbacks of PPCI can be eliminated without penalizing the thermal efficiency. Therefore it is of interest to investigate dual fuel operation while using the direct injection.
2.4 Dual Fuel PPCI (RCCI) Literature

(Besonette et al, 2007) discuss that in order to increase the HCCI load range, the fuel composition has to be varied. A research study conducted at the University of Wisconsin on HCCI modelling showed that to get high efficiency for a given operating condition, sole use of pure gasoline and diesel cannot be sufficient; different fuel reactivity has to be used at different load conditions. This introduced a new concept that involved port injection of gasoline and direct injection of the diesel fuel. The reactivity of the fuel can be varied by changing the ratio of both fuels.

The initial work on the dual fuel PPCI was conducted by (Ingaki et al, 2006) with in-cylinder blending. In this work they injected isooctane using port fuel injection and diesel fuel using a single direct injection. The isooctane injected using port injection was used to generate a homogenous charge while the diesel injection provided the ignition source. The direct injection of diesel reacts with low temperature reactions, which then ignites the gasoline. The heat release curve appears to be a two stage curve (LTHR, HTHR), which increases the combustion duration and decreases the rapid pressure rise rate. The injection of two fuels gave the advantage of control over fuel stratification and equivalence ratio. The ratio of two fuels controls the combustion phasing. The high temperature heat release (HTHR) phasing depends on the equivalence ratio and the time of direct diesel injection. By using proper injection timings of diesel and isooctane, the operating load range was extended to 12 bar without the use of EGR with low NOx and soot emissions. The thermal efficiency achieved was more than 50 %.

The further expansion of the dual fuel PPCI concept was done by (Kokjohn et al, 2010) using a CFD (Computational Fluid Dynamics) model. A combined Chemical Kinetic
Mechanism of gasoline and diesel was used in the CFD approach. A new injection approach was used which has the capacity to control the heat release rate and combustion phasing. Later, this method was adapted to heavy duty engine and the results showed that the heat release rate can be controlled by stratified fuel reactivity, and the optical investigation showed that the combustion phasing is controlled by overall fuel reactivity and the duration of the combustion is controlled by gradients in the fuel reactivity.

(Kokjohn et al, 2009) call this approach as RCCI (Reactivity Controlled Compression Ignition), which is also a dual fuel PPCI. In this approach, port fuel injection of a low reactivity fuel, like gasoline, is combined with direct injection of a high reactivity fuel, like diesel, resulting in reactivity stratification in the cylinder.

In order to study the functionality (i.e. auto-ignition and mixing) of RCCI concept, (Benajes et al, 2013) conducted an experimental and numerical investigation of RCCI combustion using a heavy duty CI engine with port fuel injection of gasoline as a low reactivity fuel and a direct injection of diesel as a high reactivity fuel. They conducted three parametric studies and studied detailed air-fuel mixing processes using 1-D spray model. Their result showed that auto-ignition of diesel starts the combustion followed by propagation of a flame due to increased temperature and pressure. As the fuel ratio decreases, the ignition delay increases resulting in more mixing time which in turn lowers the first stage combustion while second one is enhanced.

A numerical and experimental study was conducted by (Desantes et al, 2014), using a single cylinder heavy duty engine at light load, to know the effect of oxygen concentration and intake temperature on RCCI combustion efficiency.
(Kokjohn et al, 2011) conducted an experimental and numerical study of RCCI heavy duty test engine over a load range from 4.6 bar to 14.6 bar IMEP. The injection strategy used was port fuel injection of gasoline and direct injection of diesel at 35° BTDC. The results obtained were compared with conventional diesel engine. This study demonstrated that RCCI is a promising strategy which decreased NOx and soot emissions with an increase in efficiency over a wide range of loads. The RCCI results compared with the conventional diesel showed a decrease in three orders of magnitude for NOx and three orders for soot and high gross indicated efficiency. The NOx and soot levels were very low because of low peak temperature and equivalence ratio.

In continuation of the above work and to show that the emissions from RCCI are much below the US tier 2 bin 5 emission levels, (Kokjohn et al, 2013) investigated a light duty RCCI engine from 2.3 bar IMEP to 9 bar IMEP without after treatment devices and compared the results with conventional diesel combustion with the aftertreatment devices. The results showed that RCCI achieved low NOx levels without aftertreatment with 4 and 7.3% improvement in fuel consumption and total fluid consumption (fuel + diesel exhaust fluid) over CDC due to lower heat transfer loss. The obtained RCCI emissions were lower than the US tier 2 standards even without using the aftertreatment devices.

Although RCCI combustion is a promising method which reduces NOx and soot emissions, but CO and UHC are notable. In this regard many researchers conducted various studies by changing the operating conditions and injection strategies to reduce these emissions.
In order to decrease CO and UHC emissions from RCCI engines, a numerical study was conducted by (Lim et al, 2012) by changing the injection strategy of gasoline from port fuel to direct injection and using a common rail injection for diesel. They showed that DI of gasoline for a specific operating conditions reduced CO by 21.7% and UHC by 7.1% while maintaining low NOx and soot emissions in comparison to port injected gasoline RCCI case. A study on a multicylinder (four cylinder) light duty diesel engine was conducted by (Curran et al, 2012) and showed that the efficiency, NOx and soot levels obtained are better than the conventional diesel engine.

An experimental study conducted by (Hendricks et al, 2013) to know the piston heat transfer rate on RCCI and conventional diesel combustion mode using a single cylinder heavy duty engine with the help of Telemetry system and thermocouples fixed on the piston surface found that for the same operating conditions of load, speed, boost pressure and combustion phasing, RCCI combustion showed 24% lower piston heat transfer rate and the surface temperature for RCCI was found to be 25°C less when compared with conventional diesel engine. They suggest that the high reactivity fuel does not affect thermal environment though it controls ignition timing and heat transfer.

Similar to the previous study, (Gingrich et al, 2014) conducted an experimental study to understand the piston heat transfer in a light duty engine under three modes namely conventional diesel, Homogenous charge compression ignition engine (HCCI) and Reactivity Controlled Compression Ignition (RCCI). Their results showed that the integrated heat flux in case of RCCI and HCCI is lower than CDC since these two belong to LTC (Low Temperature Combustion) strategies and allow lower in-cylinder temperature. Soot formation because of the locally rich areas in CDC (Conventional Diesel
Combustion) is also another factor which influences heat flux. The observed HCCI heat flux was similar to the RCCI except when the combustion duration of HCCI was shorter than RCCI.

RCCI has demonstrated high efficiency and high controllability with low NOx and soot emissions. But as with other LTC strategies, the control of combustion at high loads is a major challenge. In order to examine and extend the RCCI operating range to high load (21 bar IMEP), (Lim et al, 2014) conducted a numerical study using Kiva 3v Release 2 code on a 2.44-liter heavy duty engine with 15.1 compression ratio using dual direct injectors. They used a genetic algorithm to identify the optimum injection strategy which simultaneously decreased CO, NOx, UHC, Ringing Intensity (RI), ISFC (Indicated Specific Fuel Consumption) and soot. The results showed that even with high compression ratio it was possible to achieve high load with thermal efficiency of 48.17 %. This is because of the optimum injection strategy used which consisted of two iso-octane injections at -80 CAD and -45 CAD and n-heptane injection at -18 CAD. The first iso-octane injection controls combustion and the second controls the ringing intensity and n-heptane acts as an ignition source for the entire charge.

An investigation on the drive cycle emissions and fuel economy of the RCCI engine was conducted by (Curran et al, 2014) using E30 and ULSD (Ultra low Sulphur Diesel). The investigated experimental engine map showed that the RCCI operation is not sufficient for some drive cycles and requires a multi-mode operation in which it can operate in RCCI mode when the load is within its range and switch to CDC when the load falls out of the range. The use of E30 as a low reactivity fuel helped to extend the upper load limit but still it doesn’t meet the requirements at all speed and load. At low loads, NOx obtained by RCCI
is similar to the NOx obtained by high EGR diesel combustion. RCCI combustion studies on two stroke engines provided an in-depth understanding of the importance of in-cylinder effects and engine parameters. A computational and experimental study was conducted by (Rocchi et al, 2014) on a direct injected two stroke engine using CFD and zero dimensional modelling. The results showed that thermal stratification was created by the two stroke scavenging process which affected the combustion process. The dual fuel direct injection caused reactivity stratification.

RCCI studies have proven that it is a promising way to achieve high efficiency with low emissions. But these studies also showed that RCCI combustion is difficult to operate at high loads. To operate at high and moderate loads it requires high amount of EGR or ultra-low compression ratio. Both of these methods decrease thermal efficiency. So, to extend the operating range without penalizing the efficiency many research studies have been conducted on RCCI using alternative fuels. In these studies, they replaced the conventional low reactivity gasoline fuel with alternative fuels. (Nieman et al, 2012) conducted a numerical investigation on heavy duty natural gas and diesel RCCI combustion using a multidimensional code called KIVA3V. The results showed that the use of natural gas provide a cleaner combustion. The use of natural gas as a low reactivity fuel produced very low NOx and soot emissions without EGR up to 13.5 bar IMEP. At high loads, 19 bar IMEP was achieved by single direct injection while 22 bar IMEP by using double direction injection of diesel. The results obtained from the natural gas/ diesel RCCI were compared with gasoline/diesel RCCI. These results showed that the natural gas/diesel RCCI has 2 % lower efficiency than gasoline/diesel. Natural gas/diesel RCCI
has high cylinder temperatures which increased heat transfer losses and ultimately decreased efficiency.

(Curran et al, 2012) investigated the effect of E85 on the performance and emissions of RCCI on a single cylinder light duty engine with 17.5 compression ratio. The operating range of RCCI was extended with E85. The HC and CO emissions obtained were higher than the CDC and at certain conditions and NOx after treatment devices were deemed necessary. The usage of after treatment devices in RCCI is a big challenge because of the lower exhaust temperatures.

(Zhou et al, 2014) conducted a numerical and experimental study to know the NOx, soot and CO emissions on RCCI combustion using methanol and biodiesel by introducing methanol at intake and biodiesel directly injected at the end of compression stroke, and found decreased CO emissions at 50 and 100% load while increased CO emissions at 10% load and no effect on NOx.

(Li et al, 2013) numerically studied the combustion and emission characteristics of methanol/diesel RCCI combustion and showed that HC and soot emissions are slightly reduced because of the oxygen atom in methanol. A similar kind of study using 150 proof hydrous ethanol as a low reactivity fuel was conducted by (Fang et al, 2015) on a single cylinder engine using direct injection of diesel and showed that hydrous ethanol can be used as low reactivity fuel till 8.6 bar IMEP as it is able to achieve low NOx levels, and EGR is required with increase in load to lower NOx emissions.

Although the results of the RCCI are promising. This method requires usage of two different fuels, which in turn need two separate fuel tanks and two separate fuel injection
systems. In lab the usage of two separate fuel tanks could be easy, but in practice it is very
difficult to have two fuel tanks in a vehicle which requires regular refueling. So, by keeping
this in mind an alternative strategy was explored by (Hanson et al, 2009), which eliminates
the usage of two different fuel tanks by addition of a small amount of high reactivity
component to the direct injection fuel.

In continuation of the Hanson’s work, (Splitter et al, 2010) explored RCCI
combustion through addition of DTBP (Di-Tert-Butyl Peroxide) cetane improver to the
gasoline to get rid of the usage of two fuels. Adding 1.75 % of DTBP by volume to gasoline
made it to behave like diesel fuel. The operating conditions studied were 6 and 9 bar IMEP
and the results obtained were compared with gasoline/diesel RCCI. At 9 bar IMEP, the
results from the gasoline with DTBP were similar to that of gasoline/diesel. The gross
indicated thermal efficiency increased by 1 %. A decrease in the DTBP % decreased the
combustion duration; as a result, high PPRR (Peak Pressure Rise Rate) was observed. Even
at 6 bar IMEP, gasoline DTBP showed results similar to gasoline/diesel RCCI. These
results demonstrated that single fuel with small amount of addition of cetane improver can
replace the usage of two fuels in RCCI and at the tested operating conditions the DTBP %
was less than 0.2 % which is lower than the urea % in SCR applications. So, similar systems
can be used to store cetane improvers.

In continuation to the previous work, (Hanson et al, 2014) investigated with a
different cetane improver 2-EHN (2-Ethylhexyl nitrate) at 2 and 4.5 bar gross IMEP. The
direct injected gasoline was doped with 3.5 % by volume of 2-EHN. At these loads, the
operating conditions like the inlet temperature, engine speed, and port fuel % were varied
to know their effect on combustion. It showed that the usage of 2-EHN at 4.5 bar IMEP
had results similar to that of gasoline/diesel and the NOx and PM emissions were below the US EPA 2010 HD (Heavy Duty) limits without after treatment for both cases. When compared from the efficiency point of view, the gasoline/2-EHN obtained a maximum of 54% at 4.5 bar IMEP and 44% at 2 bar IMEP. The usage of 2-EHN successfully demonstrated the RCCI operation at selected low loads.

2.5 Focus of this Thesis

As discussed in the literature review above, both single fuel PPCI and dual fuel PPCI (RCCI) are promising concepts that can potentially allow controlled combustion with desired rate of heat release and pressure rise rate. Dual fuel PPCI allows an extra control knob by allowing for a change in the reactivity of in-cylinder mixture, but can be more complicated due to requirement of two fuels. In contrast, single fuel PPCI is relatively simpler.

In this thesis, PPCI using ethanol has been explored. An ethanol fueled PPCI engine is computationally studied to understand the effect of injection strategies on efficiency, emissions, and noise. The CI engine selected for this study is a heavy duty engine having a displacement of 2.123 L and a compression ratio of 17.3. CFD modelling with detailed chemistry is done using converge CFD package. The injection strategy used in this study is a double injection strategy and the start of first and second injection as well as the % mass injected in each injection is varied to get optimum injection strategy.

Subsequently, the sensitivity of engine combustion to change in inlet temperature and inlet pressure is studied. Additionally, the strategies required to recover the optimum performance of the engine are explored. The details of the computational modeling and
validation are presented in Chapter 3. The results are discussed in Chapter 4 followed by conclusions in Chapter 5.
CHAPTER III

COMPUTATIONAL MODELLING AND VALIDATION

In this work, Converge CFD package is used for multidimensional engine simulations. Converge is a multipurpose engine simulation software which eliminates the creation of manual mesh. It has flexibility of generating orthogonal structured mesh based on simple grid generation parameters, which eliminates the laborious work of manually creating the mesh. This computational software can handle any number of species and chemical reactions as well as liquid sprays and laminar and turbulent flows. In this section, a brief description of spray modelling, emissions modelling, turbulent and combustion modelling and grid manipulation are discussed.

3.1 Governing Equations

Converge uses the following compressible mass transport, momentum transport and energy equations (convergent science 2013).

Mass Transport Equation:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = S \]

Momentum Transport Equation:

\[ \frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = - \frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + S_i \]
Where \( u \) is velocity, \( \rho \) is density, \( p \) is Pressure and \( S \) is the source term.

The compressible form of the energy equation is given as

\[
\frac{\partial \rho e}{\partial t} + \frac{\partial \rho u_j e}{\partial x_j} = -p \frac{\partial u_j}{\partial x_j} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j}\left(K \frac{\partial T}{\partial x_j}\right) + \frac{\partial}{\partial x_j}(\rho D \sum m h_m \frac{\partial Y_m}{\partial x_j}) + S
\]

Where \( \rho \) is density, \( Y_m \) is mass fraction of species \( m \), \( D \) is the mass diffusion coefficient, \( S \) is the source term, \( p \) is pressure, \( e \) is the specific internal energy, \( K \) is thermal conductivity, \( h_m \) is the specific enthalpy, \( T \) is temperature and \( \sigma_{ij} \) is the stress tensor.

3.2 Grid Manipulation

Converge has easy and robust grid manipulation and scaling tools which can manipulate the grid before or after the start of the simulation. The features which are provided in Converge to manipulate the grid are Grid Scaling, Fixed Embedding and Adaptive Mesh Refinement (convergent science 2013).

3.2.1 Grid Scaling

Grid Scaling is the feature in which one can easily refine or coarsen the grid according to the need which adjusts the Base grid size. The grid scaling tool is essential because it reduces the run time of the simulation. For example, in a diesel engine simulation, a coarse grid is needed during the compression stroke and a fine grid is needed during the spray and combustion. Therefore grid scaling will help whenever one desires to coarsen or refine the base grid. In Converge the following equation scales the base grid.

\[
scaled\text{-}grid = dx\text{-}base / 2^{grid\_scale}
\]
Where $dx_{\text{base}}$ is the original base cell size, while scaled grid is the new base cell size, and $grid_{\text{scale}}$ is the scaling factor. If a coarse grid is required, then $grid_{\text{scale}}$ value of -1 is taken and if a fine grid is required $grid_{\text{scale}}$ value of 1 is taken.

Figure 3.1 - (a) Coarse grid with $grid_{\text{scale}}$ value -1 and (b) Fine grid with $grid_{\text{scale}}$ value 1

3.2.2 Fixed Embedding

Fixed Embedding is the tool used to refine the grid at particular locations of the domain and the rest of the grid remains unchanged to minimize the simulation time. Fixed Embedding is used where a finer resolution of the grid influences the accuracy and the precision of the solution. Converge allows one to specify the start time and end time for the fixed embedding, which reduces the computational time, since it allows fixed embedding to turn on only during critical simulation times.

3.2.3 Adaptive Mesh Refinement:

AMR (Adaptive Mesh Refinement) is the tool which is used to refine the grid automatically based on the fluctuating velocity and temperature conditions. It allows for getting a highly refined grid in the complex situations without slowing down the simulation.
3.3 Emissions Modelling

The Emissions are predicted in Converge by using Emission modelling which incorporates both Soot and NOx modelling. A brief description of these models are given below.

3.3.1 Soot Modelling

Soot formation is modelled using a two-step empirical soot model, named the Hiroyasu Model, which is coupled with Nagle and Strickland-Constable model (NSC) for the simulation of soot oxidation. The production rate of soot mass $M_s$ (g/s) is given by the competition between the soot mass formation rate $M_{sf}$ (g/s) and soot mass oxidation rate $M_{so}$.

$$
\dot{M}_S = M_{sf} - M_{so}
$$

Where the soot formation rate is given by

$$
\dot{M}_{sf} = SF M_{form}
$$

And

$$
SF = A_{sf} P^{0.5} \exp\left(\frac{-E_{sf}}{R_u T}\right)
$$

Where $M_{form}$ is the mass of soot formation in grams, $P$ is the pressure in bar, $T$ is the Temperature in K, $R_u$ is the universal gas constant in cal/(Kg-mol), $A_{sf}$ is the Arrhenius pre exponential factor and $E_{sf}$ is the activation energy in cal/gmol. The soot model used in this study uses acetylene as inception species (convergent science 2013).
3.3.2 NOx Emissions

NOx emissions are predicted using the detailed NO mechanism by (Sivaramakrishnan et al, 2007), which is added to the primary ethanol mechanism, which consists of additional species and reactions.

3.4 Turbulence Modelling

Turbulence modelling is critical to acquire the accurate simulation for the applications like internal combustion engines as it significantly increases the rate of mixing of momentum, energy and species (convergent science 2013).

The turbulence enhanced mixing is a convective process which consists of turbulent eddies at many length scales and if the grid which we selected couldn’t resolve the eddy scales, then the turbulence mixing effects will not be accounted in the CFD simulation. With the current simulation power, it is impractical to resolve these, therefore a turbulence model is highly needed for accurate results.

The turbulence models available in Converge are the Standard k-ε, RNG k-ε and the rapid distortion RNG k-ε models. These models in Converge interact with many other models like the combustion, wall heat transfer, spray etc.

3.5 Combustion Modelling

Converge uses the SAGE detailed chemical kinetics model to include detailed chemistry in combustion applications. This model uses CHEMKIN input files (like thermodynamic and mechanism data files) to use detailed chemical kinetics in combustion simulation.

The chemical kinetic mechanism of a reacting gas mixture is a group of elementary reactions which, in detail, describes the overall chemical reaction. The composition
consists of \( n_r \) reactions involving a total number of \( n_s \) chemical species. The reaction mechanism can be expressed as

\[
\sum_{i=1}^{n_s} \nu'_{k,i} M_i \rightleftharpoons \sum_{i=1}^{n_s} \nu''_{k,i} M_i \quad k = 1, 2, \ldots, n_r
\]

Where \( \nu_{k,i} \) are the stoichiometric coefficients and \( M_i \) are the chemical species in the mechanism. The superscript ' indicates forward stoichiometric coefficients and ' indicates reverse stoichiometric coefficients. The normal elementary reaction consists of only three or four species and the matrix will be large for large set of reactions. To solve these reactions, an analytical Jacobian approach for sparse reaction kinetics is used. To solve these analytical Jacobian reactions, converge has a preinstalled tool named as CVODES (solves initial value problems for ordinary differential equations, ODE systems).

SAGE detailed chemistry solver calculates the reaction rates for each of the elementary reaction while the CFD solver solves the transport equations. The governing equations for mass and energy are solved for a given computational cell at each time step and species are updated appropriately. The SAGE detailed chemistry consists of a multizone model which accelerates the solution of detailed chemical kinetics by solving in zones. Zones are the groups of cells which have same thermodynamic state. In this model at a discrete time \( t \), each cell is at some thermodynamic state and based on this state the cells are grouped in zones. The zoning is basically done with respect to two variables, temperature and equivalence ratio, in 2-D zoning strategy. The average temperature and the composition of each zone is determined to specify thermodynamic state of that zone. Now each zone is allowed to react from time \( t \) to \( t+\Delta t \) and the obtained new compositions are mapped back to their individual cells in the zones (convergent science 2013).
3.6 Spray Modelling

Today’s manufacturers of internal combustion engines are forced continuously to improve the mixture formation and combustion processes to meet the required future emissions, as it is a growing concern. As a result, the optimization of mixture formation and combustion process and numerical simulations are become more important. The use of simulation models in contrast to experiments is that, the results are obtained faster and cheaper although there are many uncertainties in these simulation models when compared with the experiments. These simulation models can give extensive information about the combustion and mixture formation processes in the cylinder, which we can’t get easily from experiments. These simulation models help in calculating the variable of interest inside the computational domain which gives a detailed knowledge of the relevant processes (Baumgarten 2006).

Basically there are three types of models which are being used in simulation processes. First ones are thermodynamic models. These are also called as zero dimensional models and are used only when very less computational time is necessary. These models use very simple submodels without providing any insight of the process and the prediction of pollutants are impossible. The second ones are phenomological models. These models use more detailed submodels for the prediction of combustion process, heat release rate and NO\textsubscript{x} formation. The third ones are CFD models in which detailed submodels are used. These models are most expensive in terms of computational time and power. Though all these models are used in the present numerical simulations, the increase in computational power supports use of more detailed CFD models in modelling in-cylinder processes.
In order to calculate spray in the simulation, converge uses drop parcels. These parcels are identical drops which represent the entire spray field which will have the same radius, temperature and velocity etc. The use of these parcels instead of the liquid spray reduces the computational time. The spray processes used in Converge use many physical droplet processes like the liquid injection, spray breakup, drop drag, collision models, evaporation models etc. from the time of droplet injection to its vaporization. The spray models which are used in the numerical simulation are described briefly in the following sections (convergent science 2013).

3.6.1 Liquid Injection

Converge has two liquid injection mechanisms, one is Injector and the other one is nozzle. Here, in converge an injector can be defined as a group of nozzles which will have some of the characteristics of nozzles and can be having any number of nozzles with its own hole size, cone angle, position and orientation (convergent science 2013).

3.6.2 Spray breakup

The breakup models which are being used in the present CFD simulation include primary breakup, secondary breakup and combined models (Baumgarten 2006).

While modelling the spray and mixture formation, primary breakup is essential as it provides the necessary starting conditions for mixture formation inside the cylinder. The CFD simulation of spray formation always involves drops entering into the combustion chamber and the initial conditions like initial velocity, drop radius etc. for these drops are determined by the primary breakup. Due to the complex nature of experimental investigations, only very few models are present for the primary breakup of the spray.
Today there exist a few primary breakup models depending on various mechanisms like aerodynamic induced, cavitation induced and turbulence induced breakup. The number of inputs required for these models depends on the simplicity of the models. The simpler the model is, the lesser are the inputs required but these models lack in accurate prediction of the structure and starting conditions of the first spray near the nozzle. The detailed models are required for the accurate prediction of the spray breakup process and its influence on the spray and mixture formation but these models require longer computational time.

The secondary breakup is essential in diving the already existing droplets into smaller droplets because of the aerodynamic forces induced by the relative velocity between the droplet and the surrounding gas. There are two type of forces acting on the droplet at this stage. First one is the aerodynamic force which creates formation of unstable waves on droplet surface which finally leads to disintegration and the second one is the surface tension which tries to keep the shape of the droplet spherical and acts opposite to the aerodynamic force. Both these forces counteract each other and they are expressed by a non-dimensional number called Weber number which is the ratio of the aerodynamic force to surface tension force and the equation is given as

\[ We_g = \rho_g U_{rel}^2 d / \sigma \]

Where \( \rho_g \) is the density of the gas, \( U^2 \) is the relative velocity, \( d \) is the diameter of the droplet and \( \sigma \) is the surface tension. Based on the Weber number, different breakup models and breakup mechanisms like Taylor Analogy Breakup model (TAB model), Kelvin-Helmholtz model (K-H model), Droplet deformation model, Rayleigh-Taylor breakup model (R-T model) etc. are available (Baumgarten 2006).
Since it is difficult to predict all the parameters by using an individual model, a combined model is used which consists of two different breakup models (like a primary breakup and a secondary breakup model) in order to increase the accuracy of the solution and to improve the prediction. The combined model which is used in the present numerical simulation using converge is the KH-RT breakup length model.

3.6.3 Blob Injection Model

In Converge the injection drop size is set by Blob Injection Model. This model assumes such that the injected particles drop sizes are equal to the Nozzle diameter or effective diameter. This model is set in converge by the parameter injdist_flag = 0 including with the discharge coefficient model on (convergent science 2013).

3.6.4 Kelvin-Helmholtz Break-Up model

Use of this model was proposed by Reitz and is based on the first order linear analysis of Kelvin-Helmholtz instability growing on the surface of a cylindrical jet which is moving with a relative velocity to penetrate into the surrounding incompressible gas. There will be an axisymmetric fluctuating pressure and axial and radial velocity in liquid and gas which are caused by the sinusoidal spectrum of waves covering the jet surface due to turbulence generated in the nozzle hole. The surface waves grow due to relative velocity between liquid and gas which is caused by the aerodynamic forces and the motion of liquid and gas are solved by using Navier-Stokes equation for both phases. The waves move with an axisymmetric displacement of the form

\[ \eta = \eta_0 \cdot e^{\omega t} \quad (\eta << r) \]
This displacement is applied to the initial steady motion to find the relation between the real part of growth \( \omega_{KH} \) to its wave number \( k_{KH} = \frac{2\pi}{\lambda_{KH}} \) and is called a dispersion relation \( \omega_{KH} = \omega_{KH}(k_{KH}) \). The relation between the growth rate \( \omega \) of a perturbation to its wavelength \( \lambda = 2\pi/k \) is given by Reitz and Bracco as

\[
\phi_l = C_1 I_0(k_{KH}r)e^{ik_{KH}z + \omega_{KH}t}
\]

\[
\psi_l = C_2 r I_1(Lr)e^{ik_{KH}z + \omega_{KH}t}
\]

Where \( \phi_l \) and \( \psi_l \) are the velocity potential and stream function, \( C_1 \) and \( C_2 \) are integration constants, \( I_0 \) and \( I_1 \) are modified Bessel functions and \( \nu_l \) is the liquid kinematic viscosity. The numerical solution to this function shows that at \( \omega = \omega(k) \) the wave growth will be maximum and at this point the jet is splitted into small new droplets. The curve fits obtained for the above equation are applied to theory of breakup modelling of liquid droplets and is assumed that the size of the new droplet formed should be proportional to wavelength and is given as

\[ r_{new} = B_0 \Lambda \]

Where \( \Lambda \) is the wavelength and \( B_0 \) is a fixed constant and is taken as 0.6. In this model the parent drop doesn’t undergo complete breakup, instead looses its mass continuously while penetrating into the gas and the rate of reduction is given as the difference between the size of parent droplet and the newly formed droplet. The number of new child droplets can be calculated by the size reduction of the parent droplet and the size of new child droplet. The formed new child droplets become as a parent in the new parcel and are subjected to further breakup. Although this is one of the important mechanisms but the formation of bimodal droplet size distribution is far from the real scenario. Hence
another mechanism which completes the disintegration near the nozzle by breaking the
droplets whose diameter should be greater than KH child droplets in needed. As a result
KH model is combined with RT model (convergent science 2013).

3.6.5 Rayleigh – Taylor Breakup Model

Along with the KH breakup model it is believed that RT instability is also responsible for
breaking the droplets. The rapid deceleration of the drag force induces the unstable RT
waves. The drag force is given as

\[ |F_{D,i}| = M_d |a_i| = M_d \frac{3}{8} C_d \frac{\rho_g |U_i|^2}{\rho_i r_o} \]

Where \( |a_i| \) is the drop deceleration, \( m_d \) is the drop mass and \( C_d \) is the drag coefficient. The
typical RT breakup model neglects viscosity of gas and liquid (Ricart et al, 1997). The
 corresponding wavelength and growth rate if the viscosity is neglected is given by (Xin et
al, 1998).

\[ \Lambda_{RT} = \frac{2 \pi \sqrt{3 \sigma}}{a(\rho_l - \rho_g)} \]

\[ \Omega_{RT} = \frac{2}{3 \sqrt{5 \sigma}} \left[ a(\rho_l - \rho_g) \right]^{3/2} \frac{\rho_l + \rho_g}{\rho_l + \rho_g} \]

Converge spray models makes the standard RT model to include viscosity which
will have a large effect for spray droplets with high decelerations as described by (Senecal
et al, 2007). When viscosity included the RT growth rate can be shown as

\[ \omega_{RT} = -K_{RT}^2 \left( \frac{\mu_l + \mu_g}{\rho_l + \rho_g} \right) + \sqrt{K_{RT} \left( \frac{\rho_l - \rho_g}{\rho_l + \rho_g} \right) a - K_{RT}^3 \frac{\sigma}{\rho_l + \rho_g} + K_{RT}^4 \left( \frac{\mu_l + \mu_g}{\rho_l + \rho_g} \right)^2} \]
Where $K_{RT}$ is the wave number.

Converge uses the bisection method to solve for wave number corresponding to maximum growth rate ($K_{RT} = \frac{2\pi}{\Lambda_{RT}}$). The $K_{RT}$ is then substituted in the above equation to find out the maximum growth rate. If viscosity is neglected the above equation becomes standard RT model (convergent science 2013).

3.6.6 KH-RT break up length model

Converge has the flexibility to run two breakup models concurrently by choosing KH-RT breakup length model. The breakup length in this model is given as

$$L_b = C_{bl} \sqrt{\frac{\rho_l}{\rho_g}} d_0$$

Where $L_b$ is the characteristic breakup length, $\rho_l$ is the density of liquid, $\rho_g$ is the density of gas and $C_{bl}$ is the breakup length constant and $d_0$ is the diameter of the droplet. This model assumes that the instabilities formed by KH is responsible for drop breakup inside the characteristic breakup length and both KH and RT mechanisms are activated beyond the breakup length and Converge first checks whether the drop can breakup by RT mechanism, if not KH mechanism is responsible for the breakup of the droplet. The schematic figure of the KH-RT breakup model is shown in the Figure 3.1. Usually in this model, if Blob method is used to describe the initial drops into the computational grid, then usually two secondary breakup models are used. First one describes the disintegration of spray near the nozzle (part of the primary breakup which is not correctly described by the Blob Method) and the second one describes the remaining spray region. Both models are simultaneously allowed to grow unstable waves and if the RT model predicts breakup length within actual
time, then the disintegration of the drop occurs through this method otherwise it proceeds to the KH mechanism and KH mechanism produces small child droplets. The droplets which leave near the nozzle hole reduce in size very fast using the KH mechanism, and RT mechanism is applied beyond certain distance from the nozzle, the breakup length of dense fragmented core (convergent science 2013).

![Figure 3.2 - schematic figure of KH-RT breakup length model.](image)

Hence only KH breakup is allowed near the nozzle. The schematic diagram of the combined Blob KH-RT mechanism is shown in the Figure 3.2. KH-RT model is the most popular and successful hybrid model which is being used today as this model is extensively validated against experimental data to predict the disintegration of high pressure sprays.

![Figure 3.3 - Combined blob KH-RT model.](image)
3.7 Validation

The computer validation is done by using the engine geometry and conditions from (Kaiadi et al, 2013). A single injection strategy with SOI (start of injection) at -15 CAD is taken to validate the numerical model. The engine used was a modified Scania D13 with bore of 130 mm and stroke of 160 mm. The detailed engine specifications are given in Table 3.1.

Table 3.1 - Specifications of single cylinder engine and injector (Kaiadi et al, 2013).

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displacement Volume</td>
<td>2123 cm$^3$</td>
</tr>
<tr>
<td>Bore</td>
<td>130 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>160 mm</td>
</tr>
<tr>
<td>Connecting Rod length</td>
<td>255 mm</td>
</tr>
<tr>
<td>IVC (inlet valve closing)</td>
<td>40 ABDC (after bottom dead center)</td>
</tr>
<tr>
<td>EVO (exhaust valve opening)</td>
<td>50 BBDC (before bottom dead center)</td>
</tr>
<tr>
<td>CR (compression ratio)</td>
<td>17.3:1</td>
</tr>
<tr>
<td>Fuel System</td>
<td>XPI common rail</td>
</tr>
<tr>
<td>Orifices</td>
<td>8</td>
</tr>
<tr>
<td>Orifice diameter</td>
<td>0.19 mm</td>
</tr>
<tr>
<td>Umbrella angle</td>
<td>148 deg</td>
</tr>
</tbody>
</table>

All simulations were run using ethanol as fuel with specifications presented in the Table 3.2. The computational time taken to run the full geometry engine simulations is too large.
Hence to decrease the computational time, without affecting the accuracy of the output, all the engine simulations were run using sector geometry. The sector geometry is defined based on the number of nozzles or orifices because of the symmetrical location in the combustion chamber. For example, the engine used for the validation has 8 orifices, by using this we get $45^0$ sector mesh ($360^0/8 = 45^0$). The Engine sector geometry along with mesh is shown in Figure 3.2. All CFD calculation are based on the $45^0$ sector mesh.

Table 3.2 - Ethanol Specifications (Kaiadi et al, 2013).

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Ethanol</th>
</tr>
</thead>
<tbody>
<tr>
<td>RON (Research octane Number)</td>
<td>107</td>
</tr>
<tr>
<td>C</td>
<td>2</td>
</tr>
<tr>
<td>H/C</td>
<td>3</td>
</tr>
<tr>
<td>O/C</td>
<td>0.5</td>
</tr>
<tr>
<td>LHV (latent heating value) [MJ/kg]</td>
<td>26.9</td>
</tr>
</tbody>
</table>

The simulations are run from IVC (Intake Valve Closing) to EVO (Exhaust Valve opening) and the initial conditions required were taken from (Kaiadi et al, 2013). The engine used for the CFD simulation was run at a speed of 1300 rpm. The engine operating conditions are given in the Table 3.3.
Figure 3.4 - Engine sector geometry

Table 3.3 - Operating conditions

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine Speed (rpm)</td>
<td>1300</td>
</tr>
<tr>
<td>Injection Pressure (bar)</td>
<td>1500</td>
</tr>
<tr>
<td>Load (bar)</td>
<td>12</td>
</tr>
<tr>
<td>Mass of fuel injected (mg/cycle)</td>
<td>164</td>
</tr>
<tr>
<td>Swirl ratio</td>
<td>2.1</td>
</tr>
</tbody>
</table>

The boundary type used to model the piston, cylinder head and wall is wall boundary type and periodic boundary conditions are used for the front and back face. The wall boundary type can be either moving or fixed. The initial temperature and the initial pressure at the
IVC (Inlet Valve Closing) are taken as 400 K and 2.5 bar and the temperatures taken for the cylinder head, wall and the piston are listed in Table 3.4.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Piston Temperature (K)</td>
<td>600</td>
</tr>
<tr>
<td>Cylinder wall Temperature (K)</td>
<td>490</td>
</tr>
<tr>
<td>Cylinder head Temperature (K)</td>
<td>580</td>
</tr>
<tr>
<td>Pressure at IVC (bar)</td>
<td>2.5</td>
</tr>
<tr>
<td>Temperature at IVC (K)</td>
<td>400</td>
</tr>
</tbody>
</table>

3.7.1 Chemical Kinetic model

In all combustion processes, the rate of combustion is controlled by reaction rates and they also determine pollutant formation and destruction. The study of these elementary reactions and their rates is called as chemical kinetics (Turns, 2000). Converge requires chemical kinetic mechanism and thermodynamic data in order to run the simulation. A chemical kinetic mechanism is a step by step description of the changes occurring on the molecular level in a chemical reaction. A reaction mechanism can be having a number of elementary reactions which are the building blocks of a complex reaction. The detailed chemical kinetic mechanism and the thermodynamic data of the ethanol used in this study is taken from (Mittal et al, 2014). To model NOx emissions, additional NOx formation
species and reactions are taken from (Sivaramakrishan et al, 2007) and added to the primary ethanol mechanism.

3.7.2 Physical Models

Spray was modelled using modified hybrid KH-RT model. As a single sector simulation was performed, the amount of mass injected is taken for that sector only. The duration of the injection is adjusted based on the injection pressure. The spray is injected based on the rate shape taken from the literature. The spray cone angle is taken as 90° and the umbrella angle as 74°.

SAGE detailed chemistry solver is used to solve the combustion process. A multizone model is incorporated in this solver to solve the detailed chemistry in zones which are group of cells that have the same thermodynamic states. The cells are grouped based on the temperature and equivalence ratio. The temperature and equivalence ratio used in this to group the cells are 5K, 0.05.

Turbulence is modelled by means of RNG k-ε model.

3.7.3 AMR and Embedding

The base grid size used for the simulations is 1.4 mm. AMR is used for the temperature and velocity for a fixed start time and end time from -50 CAD (Crank Angle Degree) to 140 CAD (Crank Angle Degree) i.e. from the start of spray injection to exhaust valve opening. Fixed embedding is used from the start of spray injection to exhaust valve opening for head, wall and piston and also for the nozzle for the duration of injection. This fixed embedding is used for specific locations and for a specific time duration to decrease
the computational time. The change in mesh by using AMR and Fixed Embedding are shown in the Figure 3.3

(a) Mesh before start of AMR and Fixed Embedding at

(b) Change in mesh during injection due to usage of AMR

Figure 3.5 - Mesh change by using AMR and Fixed Embedding.
3.7.4 Validation Results

Based on the inputs taken from (Kaiadi et al, 2013) and with use of above models a simulation is run to obtain the output. The results obtained from the simulation were compared against the experimental data present in the literature. The pressure curve from the literature is taken to compare with the simulated pressure curve. The comparison is shown in Figure 3.3. From the comparison it is clearly evident that an excellent agreement is noted between the two curves in terms of compression, expansion and the peak pressure. Since an adequate match is obtained between the experimental and the numerical simulated curves, it is considered that the mechanism and the models used will give a predictive solution.

![Figure 3.6 - Comparison of pressure curves](image-url)
CHAPTER IV
RESULTS AND DISCUSSIONS

4.1 Introduction

This chapter describes different strategies and conditions used in this study and corresponding results. A double injection strategy is used for this study. The engine geometry and specifications are similar to the one presented in Chapter 3. The boundary conditions used in this study are similar to the validation case and the initial temperature used is 400 K and the initial pressure is 2.5 bar. A medium load point is taken for investigations. The fuel MEP (Mean Effective Pressure) is taken as 23 bar and EGR % (Exhaust Gas Recirculation) is 50. Based on the fuel MEP taken, the amount of fuel mass injected is 164 mg/cycle and the duration of the injection is taken based on the injection pressure of 1500 bar. The models required and the input files needed are similar to the validation case. The calculations begin at IVC (Intake valve Closure) of -140 CAD (Crank Angle Degree) and end at EVO (Exhaust valve opening) of 130 CAD (Crank Angle Degree).

First a series of simulations were run to obtain the best case which will have high thermal efficiency with emissions lower than the EURO VI standards. These simulations were run by changing three parameters, Start of First Injection (SOFI), Start of Second Injection (SOSI) and % mass injected in the first injection. For all these simulations, the initial and boundary conditions and the EGR % is kept constant.
4.2 Start of First Injection (SOFI)

A series of simulations were run to understand the effect of change in the Start of First Injection (SOFI). The SOFI is changed from -60 CAD to -20 CAD with an interval of 10 CAD while the SOSI (Start of Second Injection) is kept constant at -5 CAD. The amount of fuel injected is taken as 20.5 mg/cycle/injector. The injection pressure is taken as 1500 bar. The amount of fuel injected in the first injection is 52% and the remaining is injected in the second injection. The injection duration is obtained based on the injection pressure and the amount of mass injected. The SOFI duration is 9.5 CAD and the SOSI duration is 8.7 CAD. The injection rate shape used is shown in Figure 4.1 and the injection strategy cases are shown in Table 4.1. The results obtained from these simulations are discussed below. The cylinder pressure trace and the heat release rate are shown in Figures 4.2 and 4.3.

From the pressure traces, no correlation is observed between SOFI and the peak pressure. The heat release curve for SOFI of -60 BTDC shows that combustion occurs with high rate of heat release in an HCCI like manner, which is kinetically controlled. The first injected spray targets the wall and the temperature at the center of the bowl is high when compared to the temperature near the walls and this is because of the cold injected spray which decreases the temperature at the walls. Because of an early first injection the fuel air mixture becomes homogenous and the mixture burns rapidly when it reaches its autoignition temperature leading to high temperature and pressure. Because of this high temperature the second injected fuel burns immediately when it is sprayed. As a result the heat release rate is very rapid and high and the combustion duration is shorter.
Table 4.1 - SOFI strategy cases

<table>
<thead>
<tr>
<th>SOFI</th>
<th>FI duration (CAD)</th>
<th>Inj. Mass %</th>
<th>SOSI</th>
<th>SI Duration (CAD)</th>
<th>Inj. Mass %</th>
</tr>
</thead>
<tbody>
<tr>
<td>-60</td>
<td>9.5</td>
<td>52</td>
<td>-5</td>
<td>8.7</td>
<td>48</td>
</tr>
<tr>
<td>-50</td>
<td>9.5</td>
<td>52</td>
<td>-5</td>
<td>8.7</td>
<td>48</td>
</tr>
<tr>
<td>-40</td>
<td>9.5</td>
<td>52</td>
<td>-5</td>
<td>8.7</td>
<td>48</td>
</tr>
<tr>
<td>-30</td>
<td>9.5</td>
<td>52</td>
<td>-5</td>
<td>8.7</td>
<td>48</td>
</tr>
<tr>
<td>-20</td>
<td>9.5</td>
<td>52</td>
<td>-5</td>
<td>8.7</td>
<td>48</td>
</tr>
</tbody>
</table>

Figure 4.1 - Injection Rate Shape
Figure 4.2 - Pressure Trace for change in SOFI

Figure 4.3 - Heat Release rate for SOFI cases
For FI at -50 and -40 CAD we clearly see two peaks. This is due to the fact that after first injection some parts of the combustion chamber is fuel rich and some parts are fuel lean because of insufficient mixing time. The fuel rich portion burns initially leading to the first peak since it has reached its autoignition temperature. This is leads to a rapid increase in temperature which helps in burning the fuel lean zone adjacent to it. As a result the second peak or the plateau is observed. The above explanation is valid for FI at -30 CAD. The only difference is the fuel rich portion of the combustion chamber is large when compared to the previous cases.

For FI at -20 CAD the amount of time for mixing air and fuel is very less. So the mixture burns rapidly leading to high heat release rates similar to -60 CAD even though the fuel is injected early in the combustion chamber. From the above it is clearly understood that the FI injection should be in between -50 to -40 CAD to have a smoother combustion. The too early injection or the injection near to TDC will give high heat release rates.

The combustion phasing, CA50, is defined as the crank angle at which 50 % of the heat release has happened. The CA50 for the SOFI cases is shown in Figure 4.4. From the figure it is evident that CA50 increases as SOFI is advanced from -20 CAD BTDC. The CA50 for FI at -60, -30 and -20 CAD is very less because of the shorter combustion duration and for -50 and -40 CAD is high because of the longer combustion duration.

The maximum pressure rise rate is shown in figure 4.5. From this figure, as expected, for FI at -60,-30 and -20 the maximum pressure rise rate is very high due to the fact that combustion is kinetically controlled like HCCI. The fuel air mixture is more homogenous everywhere leading to rapid burning which increases the pressure rise rate.
For FI at -50 and -40 the peak pressure rise rate is less compared to other cases because of the smoother combustion with long duration.

This indicates that for the parametric study here, SOFI in the range of -50 to -40 provides better charge stratification and moderate rate of heat release, whereas early or late SOFI timings result in HCCI like combustion or rapid combustion near TDC, respectively. The high pressure rise rate also has a disadvantage of reducing the thermal efficiency by breaking the thermal boundary layer which increases heat transfer rate. The thermal efficiency is shown in Figure 4.6. The high thermal efficiency for the advanced injection cases is partly due to the fact that combustion occurs at the center of the bowl as seen by the cut planes colored by temperature in Figure 4.7. It decreases the wall heat transfer losses with an increase in the thermal efficiency. The thermal efficiency can be related with combustion phasing (CA50). Thermal efficiency is low when CA50 is near to TDC and there exists an upper bound value on CA50 (12 CAD) beyond which the thermal efficiency decreases.

![Figure 4.4 - CA50 location for SOFI cases.](image)

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Figure 4.5 - Change in Maximum Pressure Rise Rate for SOFI cases

Figure 4.6 - Efficiency as a function of SOFI
Figure 4.7 - Cut planes colored by Temperature (K) and the grey part represents the Isosurface of the temperature 1250 K
The Emission Index of NO\textsubscript{x} and soot obtained from the simulations of SOFI cases is shown in Figure 4.8. From the Heat release curves, it is noticed that the heat release rate is high for start of first injections at -60, -30 and -20 CAD. The combustion temperature will be high for these cases; as a result, the NO\textsubscript{x} emissions are high. The combustion temperatures are shown in Figure 4.9. The evolution of NO\textsubscript{x} along with the crank angle is shown in Figure 4.10. It is clearly seen that after TDC, as the temperature exceeds 1800 K, the formation of NO\textsubscript{x} increases rapidly with temperature. Soot emissions are lower for the start of injection cases at -50 and -40 and high at -60, -30 and -20 CAD since the fuel burns as it is sprayed into the combustion chamber. The obtained NOx emission are well within the EURO VI limits and the soot emissions for FI at -60, -30 and -20 are beyond the limits.

The simulations are run from IVC to EVO and it is difficult to calculate power and torque from single cycle simulations. So to compare the obtained emissions with EURO VI standards the engine is assumed to run on 50 % efficiency. Based on this assumption and the known LHV (Latent heat Value) of the fuel the EURO VI standard units (g/kWh) are converted to g/Kgf and compared.

Figure 4.8 - NO\textsubscript{x} and soot emissions for different SOFI cases.
Figure 4.9 - Temperature distributions for different start of injections at 6° ATDC
The CO (carbon monoxide) emissions obtained are shown in the Figure 4.11. These emissions are higher than the EURO VI standards. The formation of CO with crank angle is shown in figure 4.12.
Figure 4.12 - CO emissions for different start of first injections
4.3 Start of Second Injection (SOSI)

In the previous section we discussed about the first injection timings while keeping the second injection constant. In this section, the second injection timing is changed while keeping the first injection fixed at some crank angle. From the previous section results, it was noticed that high thermal efficiency with NO\textsubscript{X} and soot within the limits of the EURO VI standards with low pressure rise rate and without penalizing combustion phasing is at start of first injection (SOFI) -50 CAD. The start of first injection is kept constant (i.e. at -50 CAD) and SOSI is varied. The inlet and boundary conditions are similar to the previous section. The injection pressure and mass injected in first and second injection is also kept constant. The parameters taken for the start of second injection simulations are shown in the Table 4.2.

Table 4.2 - Start of second injection (SOSI) parameters

<table>
<thead>
<tr>
<th>SOFI</th>
<th>FI duration (CAD)</th>
<th>FI mass %</th>
<th>SOSI</th>
<th>SI duration (CAD)</th>
<th>SI mass %</th>
</tr>
</thead>
<tbody>
<tr>
<td>-50</td>
<td>9.5</td>
<td>52</td>
<td>-10</td>
<td>8.7</td>
<td>48</td>
</tr>
<tr>
<td>-50</td>
<td>9.5</td>
<td>52</td>
<td>-8</td>
<td>8.7</td>
<td>48</td>
</tr>
<tr>
<td>-50</td>
<td>9.5</td>
<td>52</td>
<td>-6</td>
<td>8.7</td>
<td>48</td>
</tr>
<tr>
<td>-50</td>
<td>9.5</td>
<td>52</td>
<td>-4</td>
<td>8.7</td>
<td>48</td>
</tr>
<tr>
<td>-50</td>
<td>9.5</td>
<td>52</td>
<td>-2</td>
<td>8.7</td>
<td>48</td>
</tr>
</tbody>
</table>

The pressure and heat release rate curves for different SOSI are shown in Figures 4.13 and 4.14.
Figure 4.13 - Pressure trace for different start of second injections

Figure 4.14 - Heat release rate for different start of second injections
From the pressure curves it can be clearly seen that as the start of second injection retards i.e. approaching near to the TDC (Top Dead Center), the peak pressure decreases. This is due to the fact that as SOSI retards, the combustion happens late which results in decrease in peak pressure. From figure 4.14 it can be seen that the heat release curve is clearly divide into two parts. The temperature and the equivalence ratio cut plane figures for the SI at -10 CAD are shown in Figure 4.15. From these Figures it is noticed that the temperature at the piston bowl is low but the equivalence ratio is greater than 1 when compared to the adjacent regions which has high temperatures but low equivalence ratio. The combustion starts at the bowl when the temperature is sufficient to burn the mixture at this region leading to a smooth combustion. As a result, the first peak is noticed. Because of this, the temperature inside the chamber is raised and spread to other regions which burns the remaining mixture leading to the second peak or the plateau. The same explanation is valid for the other cases. The equivalence ratio and temperature figures for SI at -8, -6, -4 and -2 CAD are shown in Figures 4.16-4.19.

The start of combustion moves away from TDC as the SI retards i.e. approaching TDC. It can be seen from the Figures 4.16-4.19 that the sufficient temperature required to burn the mixture at the piston bowl is occurring at the later crank angle degrees (i.e. away from TDC) although equivalence ratio is greater than 1 because of the cold temperature of the second injected spray which decreases the bowl temperature.

If we observe carefully, the second peak in the heat release curve moves forward (later) as SOSI is retarded. Form these curves we can clearly say that the first injection is used to initiate the combustion and the second injection can be used to control combustion duration and phasing. It can be clearly understood that the usage of double injection has
more parameters to control the combustion than the usage of single injection. In double injection, by adjusting the first injection, the occurrence of combustion or the start of combustion (because it initiates the combustion) can be controlled and the duration and phasing can be controlled by adjusting the second injection.

The long combustion duration is achieved because of equivalence ratio and temperature stratification in the combustion chamber. To understand this, ethanol fuel injection and the mass fraction of the ethanol in the combustion chamber are shown in the figure 4.20. The figure clearly depicts that the injected ethanol is targeted on the cylinder walls and we observe an unequal distribution of fuel in the combustion chamber. Hence more amount of fuel is present near the walls and less amount of ethanol is present near the center of the bowl.

The temperature and the equivalence ratio distributions are shown in Figures 4.21 and 4.22. Also refer to Figure 4.7. Before ignition, the region that is rich in ethanol is at lower temperature due to the cooling produced by evaporation of ethanol. The ignition happens in the region where the equivalence ratio/temperature combination allows maximum reactivity and spreads from that region. Therefore, long combustion durations are achieved because of the thermal and equivalence ratio stratification.

The Emission Index of NO\textsubscript{X}, Soot and CO are shown in the figure 4.23. NO\textsubscript{X} emissions are very low and are within the EURO VI limits. The NO\textsubscript{X} emissions decrease slightly as the start of second injection is retarded because of the lower peak combustion temperature. This decrease in temperature increases CO emissions. The Soot remains constant for all the SI cases and well within the EURO VI limits.
Figure – 4.15 (a) Temperature distribution for SI at -10 CAD. (b) Equivalence ratio distribution for SI at -10 CAD.
Figure – 4.16 (a) Equivalence ratio distribution for SI at -8 CAD. (b) Temperature distribution for SI at -8 CAD.
Figure 4.17 (a) Equivalence ratio distribution for SI at -6 CAD. (b) Temperature distribution for SI at -6 CAD.
Figure 4.18 (a) Equivalence ratio distribution for SI at -4 CAD. (b) Temperature distribution for SI at -4 CAD
Figure - 4.19 (a) Equivalence ratio distribution for SI at -2 CAD. (b) Temperature distribution for SI at -2 CAD
At -45.9 Crank Angle degrees

At -43.9 Crank Angle degrees

At -5.9 Crank Angle degrees

Figure 4.20 - Spray Penetration and ethanol massfraction for SI -8 CAD
At -1.9 Crank Angle degrees

Figure 4.20 - Spray Penetration and ethanol mass fraction for SI -8 CAD

At -4 crank Angle Degree

At -6.5 crank Angle Degree

Figure 4.21 - Temperature distributions for SI -8 CAD
Figure 4.22 - Equivalence Ratio distributions for SI -8 CAD

Figure 4.23 - Emission Index of NO\textsubscript{x}, Soot and CO
The maximum temperature for different start of second injections with crank angle is shown in the figure 4.24. The maximum peak temperature decreases as the start of second injection (SOSI) moves from -10 to -2 CAD. This is the reason for decrease in NO$_x$ emissions. The soot emissions obtained are well below the EURO VI standards.

The combustion phasing is shown in Figure 4.25. CA50 increases as the SI retards. The start of combustion occurs away from TDC as the SI retards which is the reason for the increase in CA50.

The maximum pressure rise rate is shown in Figure 4.26. It increases with the second injection moving towards TDC (Top Dead Center). This is because of the high combustion temperature obtained as the SI retards.
The obtained thermal efficiency is shown in the Figure 4.27. The thermal efficiency remains constant for all the cases. From this it can be said that CA50 should lie within 5 to 12 CAD (Crank Angle Degree) to provide maximum thermal efficiency.

![Graph showing CA50 vs Second Injection Deg](image)

**Figure 4.25 -** Combustion phasing for different start of second injections.

![Graph showing Max. Pressure rise rate vs Second Injection Deg](image)

**Figure 4.26 -** Maximum pressure rise rate for different start of second injections.
Figure 4.27 - Thermal Efficiency for different start of second injections
4.4 Change in Injection Mass percentage

The previous sections describe the effect of variation in SOFI and SOSI. In this section, both the SOFI and SOSI are kept constant and the amount of fuel injected in the first and second injection is varied. For this study, the optimum SOFI and SOSI times, where the engine will have high efficiency with low NO\textsubscript{X} and soot emissions and low peak pressure rise rate are obtained from the previous sections. SOFI is taken as -50 CAD and the SOSI as -10 CAD. The amount of fuel injected in the first injection is increased from 50 % to 90 % while the amount of fuel injected in second injection is reduced from 50 % to 10 %. The duration of the injection changes for each case since the injection pressure has to keep constant at 1500 bar. The parameters considered for the simulations are shown in the following Table 4.3.

<table>
<thead>
<tr>
<th>SOFI</th>
<th>FI duration</th>
<th>FI Mass %</th>
<th>SOSI</th>
<th>SI duration</th>
<th>SI mass %</th>
</tr>
</thead>
<tbody>
<tr>
<td>-50</td>
<td>10.9 CAD</td>
<td>60</td>
<td>-10</td>
<td>7.3 CAD</td>
<td>40</td>
</tr>
<tr>
<td>-50</td>
<td>12.8 CAD</td>
<td>70</td>
<td>-10</td>
<td>5.5 CAD</td>
<td>30</td>
</tr>
<tr>
<td>-50</td>
<td>14.6 CAD</td>
<td>80</td>
<td>-10</td>
<td>3.5 CAD</td>
<td>20</td>
</tr>
<tr>
<td>-50</td>
<td>16.5 CAD</td>
<td>90</td>
<td>-10</td>
<td>1.82 CAD</td>
<td>10</td>
</tr>
</tbody>
</table>

The pressure and the heat release rate curve for the four different cases considered are shown in the Figures 4.28 and 4.29.
Figure 4.28 - Pressure Traces for different Mass Injection

Figure 4.29 - Heat release rate curves for different Mass Injection
When the mass injected is 60 % in the first injection and 40 % in second injection, two distinct peaks in the heat release rate are clearly seen. From the Figure 4.30 it can be seen that at 4 CAD the equivalence ratio in the bowl is greater than 1 but it doesn’t have the sufficient temperature to burn. The center of the bowl and few other parts has high temperature but the mixture is very lean. So mixture doesn’t burn until it has sufficient temperature. At 6 CAD it can be seen that combustion occurs in the bowl which gives the first peak in the heat release curve and it also noticed that mixture is burning smoothly leading to a smoother combustion. After first peak the temperature in the combustion chamber is increased which spreads to other regions leading to the second peak.

As first injection mass % increases the portion in the combustion chamber having sufficient temperature and equivalence ratio is decreasing as a result the first peak decreases and the second peak increases.

For the FI with 90 % mass we see a longer combustion duration than the others. This is because 90 % of the fuel mass is injected into combustion chamber at an early stage which will have the sufficient mixing time and the mixture becomes homogenous and fuel lean everywhere. As a result, even though the temperature is high but the mixture is fuel lean everywhere so it doesn’t burn. At some point where the temperature is high the combustion triggers and it spreads to other regions. The cut plane temperature distribution for the FI with 90 % mass is shown in the Figure 4.31.
Figure – 4.30 (a) Equivalence ratio distribution for FI with 60 % mass. (b) Temperature distribution for FI with 60 % mass.
Figure – 4.30 (a) Equivalence ratio distribution for FI with 60 % mass. (b) Temperature distribution for FI with 60 % mass.
Figure – 4.31 Temperature distribution for FI with 90 % mass.
The combustion phasing for different injection mass cases is shown in figure 4.32. From heat release rate it is seen that as the FI mass % increases the combustion duration increases because of this the CA50 increases.

The maximum pressure rise rate decreases as the mass injected in the second injection is decreased as shown in figure 4.33. This is due to long combustion duration because of the insufficient temperature to burn the mixture which results in low peak pressures.

The NO\textsubscript{x}, soot and CO emissions and thermal efficiency are shown in the figures 4.34 and 4.35. NO\textsubscript{x} decreases with increase in mass of first injection because of the obtained lower combustion temperature. Soot emissions remains constant. The obtained NO\textsubscript{x} and Soot emissions are well below the EURO VI limits.

Thermal efficiency remains constant till the mass injected in the second injection is reduced to 20 %. But for the 10 % mass injected, the combustion duration is very long which ultimately decreases the efficiency.
Figure 4.33 - Maximum pressure rise rate

Figure 4.34 - NO\textsubscript{X} and Soot emissions for different mass injected cases.
From all the above cases, we can also get a base case for sensitivity studies which has high thermal efficiency with low NO\textsubscript{X} and soot emissions (below EURO VI standards) and also with low peak pressure rise rate. It is found out from the above cases that SOFI at -50 CAD and SOSI at -10 CAD with 70 % of the fuel injected in first injection and 30 % of the fuel injected in the second injection has all the features in terms of efficiency, emissions and peak pressure rise rate so as to be considered as the base case. For this case, the thermal efficiency is in the range of 45 % and emissions are well below EURO VI standards and the peak pressure rise rate is 10.3 bar/CAD. The considered base case parameters along with obtained emissions, efficiency, and CA50 and pressure rise rate are shown in the following table 4.4. The inlet and boundary conditions are similar to the previous cases.
Table 4.4 - Base condition parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Start of first Injection (SOFI)</td>
<td>-50 BTDC</td>
</tr>
<tr>
<td>Start of second Injection (SOSI)</td>
<td>-10 BTDC</td>
</tr>
<tr>
<td>Injected mass in First Injection</td>
<td>70%</td>
</tr>
<tr>
<td>Injected mass in Second Injection</td>
<td>30%</td>
</tr>
<tr>
<td>First Injection duration</td>
<td>12.8 CAD</td>
</tr>
<tr>
<td>Second injection duration</td>
<td>5.5 CAD</td>
</tr>
<tr>
<td>Injection Pressure</td>
<td>1500 bar</td>
</tr>
<tr>
<td>Efficiency obtained</td>
<td>45%</td>
</tr>
<tr>
<td>Emissions (NOx, Soot)</td>
<td>0.1 g/kgf, 0.001 g/kgf</td>
</tr>
<tr>
<td>Peak Pressure Rise rate (bar/CAD)</td>
<td>10.3</td>
</tr>
<tr>
<td>CA50</td>
<td>7.9</td>
</tr>
</tbody>
</table>
4.5  Sensitivity Analysis

This section describes the sensitivity analysis performed on the base case. The parameters selected are temperature and pressure. The main aim of this section is to understand the dependence of the base case selected on change in inlet temperature and pressure. The sensitivity analysis is performed by changing the temperature and pressure while keeping all other parameters constant. The operating parameters considered for the temperature and pressure sensitivity cases are shown in Tables 4.5 and 4.6.

Table 4.5 - Operating parameters for temperature sensitivity cases

<table>
<thead>
<tr>
<th></th>
<th>Base Case</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
<th>Case 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet Temperature</td>
<td>400 K</td>
<td>390 K</td>
<td>395 K</td>
<td>405 K</td>
<td>410 K</td>
</tr>
<tr>
<td>Inlet Pressure</td>
<td>2.5 bar</td>
<td>2.5 bar</td>
<td>2.5 bar</td>
<td>2.5 bar</td>
<td>2.5 bar</td>
</tr>
</tbody>
</table>

Table 4.6 - Operating parameters for pressure sensitivity cases

<table>
<thead>
<tr>
<th></th>
<th>Base Case</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
<th>Case 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet Temperature</td>
<td>400 K</td>
<td>390 K</td>
<td>395 K</td>
<td>405 K</td>
<td>410 K</td>
</tr>
<tr>
<td>Inlet Pressure</td>
<td>2.5 bar</td>
<td>2.4 bar</td>
<td>2.45 bar</td>
<td>2.55 bar</td>
<td>2.6 bar</td>
</tr>
</tbody>
</table>
4.5.1 Change in inlet Temperature

The pressure and the heat release rate curves for change in temperatures are shown in figures 4.36 and 4.37.

Figure 4.36 - Pressure trace for Different Inlet Temperatures

Figure 4.37 - Heat release rate curve for different Inlet temperatures
For the inlet temperature 390 K, the pressure curve is similar to the motored curve which clearly shows that combustion didn’t pick up even though there is some heat release as seen in the heat release curve. This is because of the cooling effect of the Ethanol and the higher autoignition temperature of ethanol. For the inlet temperature of 395 K, combustion is late and possibly only partial burning is there. With these two cases, it is clearly understood that for the test conditions taken the minimum required temperature for the ethanol to burn satisfactorily is 400 K. For the inlet temperatures case 405 K and 410 K, the peak pressures are higher because of higher inlet temperature. The heat release curve shows two peaks. This can be explained by the equivalence ratio and temperature distribution from Figures 4.38 and 4.39. As it is known that combustion starts in the bowl and the portion in the bowl which is fuel rich and having high temperature is small compared to other portions in the chamber. As a result a small first peak is observed. Then the high temperature produced by the initial combustion spreads to the entire region which gives the second-high peak.

As the inlet temperature increases the start of combustion shifts towards TDC and combustion duration will be low because of the high temperature in the combustion chamber which makes the fuel air mixture to burn fast.

The maximum pressure rise rate is shown in the figure 4.40. The peak pressure rise rates are very high for the inlet temperature cases of 405 K and 410 K. This is because of the formation of high combustion temperatures in the cylinder due to high inlet temperature. For the other two cases, the pressure rise rate is very low because of misfire and incomplete combustion.
Figure – 4.38 (a) equivalence ratio distribution for Initial temperature 405 K.

(b) Temperature distribution for inlet temperature 405 K
Figure – 4.39 (a) equivalence ratio distribution for Initial temperature 410 K.

(b) Temperature distribution for inlet temperature 410 K
Figure 4.40 - Maximum pressure rise rate for different inlet temperatures

The combustion phasing is shown in the figure 4.41. For inlet temperature 395 K and 390 K the CA 50 is very high because of the partial combustion and misfire. For inlet temperature 405 K and 410 K we see that CA 50 decreases as the inlet temperature increases because of the shorter combustion duration. From this it is clearly understood that the phasing is very sensitive to inlet temperature.

The emission index of NO\textsubscript{X}, CO and soot are shown in figure 4.42. NO\textsubscript{X} emission increases as the inlet temperature increases because of the higher incylinder temperatures. Even though the NO\textsubscript{X} emissions increase, they are well below the EURO VI standards. Soot emissions remains constant. As temperature increases CO emissions decrease because the formed CO is converted to CO\textsubscript{2}.

Figure 4.43 shows the efficiency obtained for change in different inlet temperatures. As expected, for the inlet temperatures 405 K and 410 K the efficiency is equal and high compared to the other two cases. Because of the misfire and the partial burn, the efficiencies for the inlet temperatures of 390 K and 395 K are low.
Figure 4.41 - CA50 for different inlet temperatures

Figure 4.42 - Emission Index of NO\textsubscript{X} and Soot for different inlet temperatures
Figure 4.43 - Efficiency obtained for different inlet temperatures
4.5.2 Change in Inlet Pressure

The pressure and the heat release rate curves are shown in figures 4.44 and 4.45 for different intake pressures. As the inlet pressure increases, the peak pressure increases as expected. From the heat release rate curve, it is understood that the increase in inlet pressure increases the maximum heat release rate and the start of combustion happens closer to the TDC (Top Dead Center) because of the higher inlet pressure which increases the temperature inside the cylinder. The formation of two peaks in the heat release curve is explained in the similar manner of FI with 70 % mass. The combustion duration remains same for all the cases.

![Pressure trace for different inlet pressures.](image-url)

Figure 4.44 - Pressure trace for different inlet pressures.
The maximum pressure rise rate is shown in the figure 4.37. The peak pressure rise rate increases moderately with increase in the inlet pressure because of the increase in the incylinder temperature.

Figure 4.38 shows combustion phasing with change in inlet pressure. As inlet pressure increases, the combustion event shifts towards the TDC because of the fast burning of the mixture due to higher temperature in the cylinder as a result the CA50 decreases moderately with increase in pressure.

The emission index of NOX, CO and soot are shown in figure 4.39. NOx emissions increases slightly while the Soot remains constant. The obtained NOx and soot emissions are much below the EURO VI standards and insensitive to inlet pressure. The obtained efficiencies are shown in the figure 4.40. As expected the efficiency is same for all the cases.
Figure 4.46 - Peak Pressure Rise rate for different inlet pressures.

Figure 4.47 - Combustion phasing for different inlet pressures
Figure 4.48 - Emission Index of NOx, CO and Soot for different inlet pressures.

Figure 4.49 - Efficiencies for different inlet pressures
From the sensitivity analysis, it is clearly understood that the base case is not very sensitive to change in inlet pressure but it is very sensitive to change in inlet temperature. It is observed that a decrease in the inlet pressure shifts combustion away from TDC but there is no effect on efficiency.

A decrease in inlet temperature has a great effect on combustion. The use of inlet temperature of 390 K doesn’t ignite the charge and only partial combustion happens at 395 K. An increase in the inlet temperature resulted in rapid combustion causing the combustion phasing to shift accordingly. Form these it can be understood that inlet temperature has a greater effect on the combustion event than inlet pressure for the chosen base case and the minimum required temperature for ethanol with the chosen test conditions is 400 K. This work can be extended in future by exploring sensitivity at other conditions of SOFI, SOSI, mass injection distribution and inlet temperature and identifying the conditions at which high efficiency and low emissions are obtained along with low sensitivity to change in inlet temperature. Ideally, the engine should be operated at conditions at which sensitivity to inlet temperature is small as this will ensure stable operation even when outside condition of temperature may change.

Since, for the base case explored here, combustion is very sensitive to intake temperature, in the following we further explore if it is possible to recover combustion phasing and obtain acceptable pressure rise rate when inlet temperature is increased to 410 K. From the sensitivity cases presented above, not that the temperature of 410 K gave unacceptably high peak pressure rise rate.
4.6 Recovering combustion phasing

This section explores a strategy for recovering the combustion phasing to its normal position. The strategy used should be such that it can get back the combustion phasing without penalizing the efficiency, emissions and pressure rise rate. It was realized from the previous cases, that advancing the first injection makes the mixture to burn in HCCI like mode and results in higher pressure rise rate and a change in second injection and injection mass % makes the combustion to occur away from TDC. Here we explore the option to increase the EGR %. In the new strategy used, the EGR is increased by 10 %. From the previous sections it is clearly understood that the combustion phasing is not very sensitive to the inlet pressure hence this strategy is not applied for the inlet pressure cases. This strategy is applied to the inlet temperature case at 410 K while all the other parameters taken are similar to the base case.

4.6.1 Inlet temperature 410 K with 60 % EGR.

Figures 4.50 and 4.51 show the pressure and heat release rate curves for the inlet temperature 410 K with 60 % EGR. From the pressure trace and heat release rate curves, it is noted that even though the inlet temperature is increased by 10 K but the usage of 60 % EGR is effective in recovering combustion phasing. The formation of two peaks and the combustion duration is explained similar to the base case. Because of the usage of high EGR the ignition delay increases as a result the usage of high EGR with high inlet temperature gives the same start of combustion and duration similar to the base case.
Figure 4.50 - Pressure trace of inlet temperature 410 K with 60 % EGR in comparison with the base case

Figure 4.51 - Heat Release rate curve of inlet temperature 410 K with 60 % EGR in comparison with the base case
The peak pressure rise rate in comparison with the base is shown in the following table 4.7. Because of the use of high EGR, the peak pressure rise rate decreases. The long ignition delay is also a reason for the decrease in pressure rise rate. The use of high EGR makes the combustion event to occur away from the TDC which helps to get back the combustion phasing back to its original position even with the use of high inlet temperature. The comparison of combustion phasing, efficiency and the emissions are shown in the Table 4.7. The efficiency obtained is same as the efficiency of the base case. The NOx emissions obtained are very low and the soot emissions increased but are below EURO VI standards.

Table 4.7 - Comparison of base case with Inlet temperature 410 K with 60 % EGR

<table>
<thead>
<tr>
<th></th>
<th>Base Case</th>
<th>Inlet temperature 410 K with 60 % EGR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak Pressure rise rate (bar/CAD)</td>
<td>10.34</td>
<td>8.97</td>
</tr>
<tr>
<td>CA50 (CAD)</td>
<td>8.14</td>
<td>8.19</td>
</tr>
<tr>
<td>Efficiency (%)</td>
<td>43</td>
<td>43</td>
</tr>
<tr>
<td>NOx (g/kgf)</td>
<td>0.07</td>
<td>0.023</td>
</tr>
<tr>
<td>Soot (g/kgf)</td>
<td>0.004</td>
<td>0.024</td>
</tr>
<tr>
<td>CO (g/kgf)/10</td>
<td>8.0487</td>
<td>4.0121</td>
</tr>
</tbody>
</table>
CHAPTER V

CONCLUSIONS AND FUTURE WORK

5.1 Conclusions

This thesis focuses on understanding the effect of injection strategies on ethanol PPCI and sensitivity of ethanol PPCI to change in inlet conditions. Multidimensional CFD simulations were performed using Converge CFD package. The engine selected for these simulations was a single cylinder heavy duty engine operating at medium load (approximately 12 bar IMEP) with 50% EGR. A double injection strategy was used for these simulations. The goal was to find out the optimum injection parameters which will have high thermal efficiency with low noise and emissions lower than the EURO VI standards. Initially, a validation of the simulation strategy was done and then the simulations were conducted to explore the abovementioned conditions.

A series of simulations were performed in order to obtain the optimum injection parameters which will give high efficiency with reduction in noise and emissions. The simulations were conducted by varying the start of first injection (SOFI) time, start of second injection (SOSI) time and changing the mass injected in each injection. In the SOFI simulations, the start of first injection was varied from -60 to -20 CAD (Crank angle degree) while keeping the SOSI constant at -5 CAD. The study found that SOFI timing cannot be used to control combustion. The peak pressure rise rates were high for SOFI at -60 CAD and also for SOFI that was retarded to more than -40 CAD.
The efficiency remained same for SOFI at -60 to -40 CAD and decreased as SOFI was further retarded. The NOx emissions obtained were within the EURO VI limits because of high EGR %. The optimum SOFI obtained for this load was -50 CAD and will be different for different loads.

In start of second injection simulations, the SOSI was varied from -10 CAD to -2 CAD while keeping the SOFI constant at -50 CAD. The results show that as SOSI is retarded, combustion phasing (CA50) is delayed and peak pressure rise rate increases moderately. The CA50 increases almost linearly as SOSI is retarded. There was no change in efficiency with change in SOSI. The optimum SOSI obtained for this load is -10 CAD. Lastly, the amount of fuel injected in the first and second injection was changed from 60-40 to 90-10 % while keeping the SOFI and SOSI at their optimum conditions. The results show that as the amount of fuel injected in the first injection is increased, combustion duration increases significantly even though the start of combustion remains unchanged. The effect is an increase in CA50, and decrease in peak pressure rise rate. The optimum fuel injected in first and second injection was obtained as 70% and 30%, respectively. The efficiency decreased rapidly as the fuel injected in the first injection was increased beyond 80%.

A sensitivity study was subsequently conducted in which the sensitivity of engine combustion to inlet conditions, i.e. inlet temperature and inlet pressure, was explored. The results showed that the engine combustion is not very sensitive to change in inlet pressure but highly sensitive to change in inlet temperatures. Simulations were performed to investigate the strategy to recover combustion phasing. The results showed that the optimum performance of the engine can be recovered with increase in EGR to 60%.
5.2 Future work

1. This study was performed at a medium load 12 bar IMEP. Investigations at higher load can be conducted as operation becomes more challenging at higher loads.

2. The efficiencies showed in this study are based on simulation from IVC to EVO. Work should be done to assess efficiency for the whole cycle.

3. This study was performed by keeping SOSI constant while changing SOFI and SOFI constant while changing SOSI. For future study, design of experiments (DOE) method is recommended.
REFERENCES


Dempsey. 2013. "Dual-Fuel Reactivity Controlled Compression Ignition (RCCI) with Alternative Fuels."


