A COMPUTATIONAL STUDY ON THE EFFECT OF INJECTION STRATEGY ON EMISSIONS IN A DME FUELED CI ENGINE

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A COMPUTATIONAL STUDY ON THE EFFECT OF INJECTION STRATEGY ON EMISSIONS IN A DME FUELED CI ENGINE

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Thesis

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A computational study is conducted to investigate the effect of fuel injection strategy on emissions in a DME fueled CI engine having displacement of 373.3 cm$^3$ and compression ratio of 17.8 at moderate load. Specifically, the effect of split and pilot injection timing and amount is studied with detailed chemistry using the Converge CFD package. Due to symmetry of the cylinder, the simulations are conducted on a sector of the cylinder, from intake valve closure to exhaust valve opening. In the pilot injection strategy, 10% mass of the total fuel is injected during pilot injection between $40^\circ - 10^\circ$ BTDC and the remaining in the main injection at $5^\circ$ BTDC. Split injection strategy is studied by injecting 20% mass of the fuel during first injection between $40^\circ - 10^\circ$ BTDC and the remaining in the main injection at $5^\circ$ BTDC.

Results show that for advanced first injection, DME shows distinct two-stage ignition characteristics. The pilot injection simulations revealed that NOx emissions are not sensitive to pilot injection timing over the parametric range studied here, whereas, CO emissions increased with advanced pilot injection due to the effect of spray targeting in the squish region as well as over-mixing. With the split injection study, NOx emission increased and CO decreased as the first injection timing was retarded. In both cases, heat release rate of the main injection was not influenced by the variation in the first injection timing.
In addition, the effect of variation in the main injection timing was investigated by injecting 20% of the fuel mass at $20^0$ BTDC and remaining at different times ranging from $10^0$ BTDC to $10^0$ ATDC. As the main injection was retarded, NOx emissions decreased significantly and CO emissions increased. It was also noted that, in contrast to single injection, a split injection strategy allows for moderately retarded main injection with significant reduction in NOx emissions without excessive increase in CO. It is concluded that a split injection strategy with retarded second injection offers potential for optimizing CO and NOx emissions. However, a tradeoff exists between NOx emissions and efficiency. In the present simulations, any reduction in NOx entailed decrease in efficiency. More studies are needed that highlight the effect on efficiency as well as assess the influence of EGR.
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1.1 DME as an Alternative Fuel

Our earth is undergoing tremendous changes and the resources are diminishing. Diminution of fuel reserves and imperiled energy security are important global concerns as the world population continues to grow. It is not possible to provide the amount of energy demanded by the world by only using fossil fuels. What can be done for the future generations of human kind? Development of the usage of renewable energy fuels is one of the strategies. Moreover, recent events such as the rising cost of fuels and the advent of stringent emission regulations have also necessitated the use of renewable energy fuels. There are different kinds of renewable energy fuels like vegetable oil, ethanol, methanol, biodiesel etc. Among them DiMethyl-Ether (typically abbreviated as DME) is also one type of renewable energy fuel which can be derived from many sources, including renewable materials like biomass, industrial waste, agricultural products as well as from fossil fuels (natural gas, coal, residual oil and crude oil).

1.1.1 Why is it Promising?

DME is an organic compound and simplest linear ether, also known as methoxy methane, with formula $\text{CH}_3\text{OCH}_3$, as seen in Figure 1.1. It is a clean, colorless, non-toxic,
slightly narcotic and highly flammable gas under ambient conditions which is easy to liquefy, transport and store when lightly pressurized. It burns with a blue flame which shows that it is suitable for combustion. It has been used in personal care industries (as a benign aerosol propellant) for decades and now it is being exploited for use as a clean burning alternative to gasoline, diesel and liquefied petroleum gas (LPG). Like LPG, DME is gaseous at normal temperature and pressure, but changes to liquid state when subjected to modest pressure or cooling. All these properties, including high oxygen content, lack of sulfur or other noxious compounds, and ultra clean combustion makes DME a promising solution in the list of clean renewable and low-carbon fuels under consideration worldwide.

![Figure 1.1 - Structure of Dimethyl Ether](image)

DME is promising because it is considered as a clean alternative to petroleum derived diesel fuel. Furthermore, with the help of DME there is no particulate matter (PM) formation since there is no carbon to carbon (C-C) direct bond as shown in Figure 1.1. It contains around 35% oxygen by mass and has fewer C-H bonds in comparison to larger hydrocarbons that typically constitute fossil derived transportation fuels. The increasing number of C-H and C-C bonds leads to an increase in PM emissions. In compression ignition engines, DME performance may be superior to diesel and engine operation is less noisy. Its high vapor pressure reduces wall-wetting and allows Premixed
Charge Compression Ignition (PCCI) (Kim et al., 2007). A high cetane rating of 55 – 60 (compared to about 45 for petroleum-derived diesel) and a boiling point of -25 °C provides rapid fuel/air mixing, reduced ignition delay, and excellent cold starting properties, which are additional key advantages of DME. The cetane number of a fuel is used to measure its compression-ignition quality; the higher the value, the better its compression-ignition quality (Teng et al., 2001). The high cetane number of DME indicates that it is suitable for use in diesel engine, because a high cetane number corresponds to a shortened premix burn period. As shown in Table 1.1, low cetane number of propane and butane makes them unsuitable as fuels for CI engines.

<table>
<thead>
<tr>
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<th>DME</th>
<th>Diesel fuel</th>
<th>Butane</th>
<th>Propane</th>
</tr>
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<tbody>
<tr>
<td>Chemical formula</td>
<td>CH₃OCH₃</td>
<td>C₈-C₂₅</td>
<td>C₄H₁₀</td>
<td>C₃H₈</td>
</tr>
<tr>
<td>Molecular weight (g/mol)</td>
<td>46.07</td>
<td>170</td>
<td>58.13</td>
<td>44.11</td>
</tr>
<tr>
<td>Cetane number</td>
<td>&gt;55</td>
<td>40-55</td>
<td>10</td>
<td>5</td>
</tr>
<tr>
<td>Stoich.A/F ratio</td>
<td>9</td>
<td>14.6</td>
<td>14.8</td>
<td>15.7</td>
</tr>
<tr>
<td>Boiling point (K)</td>
<td>248</td>
<td>453-643</td>
<td>272.5</td>
<td>231</td>
</tr>
<tr>
<td>C ratio (wt%)</td>
<td>52.5</td>
<td>86</td>
<td>82.8</td>
<td>81.8</td>
</tr>
<tr>
<td>H ratio (wt%)</td>
<td>13</td>
<td>14</td>
<td>17.2</td>
<td>18.2</td>
</tr>
<tr>
<td></td>
<td>DME</td>
<td>Diesel fuel</td>
<td>Butane</td>
<td>Propane</td>
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<tr>
<td>--------------------------</td>
<td>----------------</td>
<td>-------------</td>
<td>--------</td>
<td>---------</td>
</tr>
<tr>
<td>O ratio (wt%)</td>
<td>34.8</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Modulus of elasticity</td>
<td>$6.37 \times 10^8$</td>
<td>$1.49 \times 10^9$</td>
<td>$3.6 \times 10^8$</td>
<td>$0.22 \times 10^9$</td>
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<tr>
<td>Lower calorific value</td>
<td>28.8</td>
<td>42.7</td>
<td>45.74</td>
<td>46.36</td>
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<tr>
<td>Vapor pressure (kPa @293K)</td>
<td>530</td>
<td>-</td>
<td>210</td>
<td>840</td>
</tr>
<tr>
<td>Autoignition T (K)</td>
<td>508</td>
<td>523</td>
<td>638</td>
<td>743</td>
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<tr>
<td>Liquid viscosity</td>
<td>0.12-0.15</td>
<td>2-4</td>
<td>0.18</td>
<td>0.20</td>
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<tr>
<td>Liquid density</td>
<td>660</td>
<td>800-840</td>
<td>610</td>
<td>490</td>
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<tr>
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<td>1.59</td>
<td>-</td>
<td>2.01</td>
<td>1.52</td>
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<td>3.4-17</td>
<td>0.6-6.5</td>
<td>1.9-8.4</td>
<td>2.1-9.4</td>
</tr>
<tr>
<td>Latent heat of evaporation (kJ/kg)</td>
<td>410</td>
<td>250</td>
<td>390</td>
<td>426</td>
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</table>
One of the advantages of DME is its high latent heat of vaporization with low boiling point. Compared to the diesel combustion process, the higher latent heat of DME reduces the NO\textsubscript{x} concentration, because the injected liquid DME spray absorbs significant heat during the evaporation process, thus the combustion chamber experiences a larger temperature drop. In addition, the low boiling point of DME promotes quick vaporization of liquid DME spray when liquid fuel is injected into the combustion chamber. Fast evaporation of the liquid phase fuel results in temperature drop in premixed combustion in the engine, which decreases the formation of NO\textsubscript{x} during combustion (Arcoumanis et al., 2008).

Formal indication on use of DME as an engine fuel has not been mentioned in literature until 1984 by Majunke and Muller in the form of a patent from Germany. The invention explained the application of DME with a mixture of non-distilled methanol, water and other additives as a fuel in a motorized garden tool. Further in 1986, a U.S. patent described operation of CI engine with 95% to 99.9% of DME fuel (Levine, 1990). However, the use of DME as an alternative fuel started after 1995 only.

In 1995, two technical papers published by Hansen et al. (1995) and Fleisch et al. (1995) showed excellent properties of DME similar to diesel fuel with lower emission level. A large scale manufacturing technology using natural gas was also discussed. They presented DME and its blends as an ultra-clean alternative fuel for diesel. Fuel properties, potential cost, and engine conversion requirements discussed in these papers paved a pathway for further research of DME as an alternative fuel. Significant research has been conducted with the concept of DME used separately or blended to methanol in European
countries. Since 1997, Japan, China and South Korea started working on modification of diesel engines and have done appreciable developments.

In 2006, Ying et al. studied the combustion and engine performance characteristics of DME/diesel blended fuels along with emissions characteristics. They reported that the addition of DME to diesel induced the improvement of fuel and energy consumption at high engine speed and load. In addition, it was revealed by them that the power output at high engine speed at full load in DME blended fuels is lower than that in neat diesel fuel due to its lower calorific value.

As noted in Table 1.1, the vapor pressure of DME falls between those of butane and propane. This means that fuel line and tank pressure designs, that are similar to those used for LPG engine systems, can be used for DME engine system. Gaseous DME is denser than dry air, while the density of liquid DME is 668 kg/m³ at normal temperature and pressure (Mueller et al., 2000). DME differs significantly from conventional diesel in terms of its fuel density and viscosity characteristics. Low density and viscosity of DME results in its leakage from fuel storage tanks, and the fuel supply system from the fuel tank to the injection system in engines. Disadvantages of DME are its low viscosity and low lubricating characteristics, which cause fuel leakage and surface-wear of moving parts in fuel injection system. Addition of proper additives to prevent leakage and surface wear is essential. Therefore, additives need to be formulated to improve the viscosity and lubricity of DME. Another advantage of DME is that it is noncorrosive to the fuel system structure and metal surfaces.

The temperature above which the fuel spontaneously ignition without any external source of ignition is called the auto-ignition temperature. Auto-ignition is the basic
principle in CI engine. One of the most important factors affecting combustion in CI engine is the auto-ignition temperature. Low ignition temperature of DME is important characteristic that is similar to the diesel fuel (Khunaphan et al., 2013; Yeom et al., 2009). The reduction or elimination of particulate emissions, also commonly known as “soot” or black smoke, is an important benefit. Diesel engines running on 100% DME have demonstrated smoke free combustion, while engines using a DME/diesel fuel blend have demonstrated significant reduction of soot. By using EGR, additional NO\textsubscript{x} reduction can be obtained without visible smoke and deterioration in the thermal efficiency (Teng et al., 2006).

1.1.2 Economic Production and use of DME

DME handling is easy and similar to LPG (propane) (Arcoumanis et al., 2008). Also transportation and storage cost is reduced. It can be produced from a variety of abundant sources, including natural gas, coal, waste from pulp and paper mills, forest products, agricultural by-products, municipal waste and dedicated fuel crops. World production today is primarily by means of methanol dehydration, but DME can also be manufactured directly from synthesis gas produced by the gasification of coal or biomass, or through natural gas reforming. Among the various processes for chemical conversion of natural gas, direct synthesis of DME is the most efficient. It is easy to distribute. DME is a gas under ambient conditions with properties similar to those of propane. However, because it can be stored as a liquid under moderate pressure, it eliminates the need for the high-pressure containers used for compressed natural gas (CNG) or cryogenic storage of liquefied natural gas (LNG).
1.1.3 DME use in Present Engines

The liquid density of DME is about 80% of diesel fuel and the specific energy content is about 70% of the diesel fuel. Therefore DME fuel injected should be twice the volume of diesel fuel to obtain the same power output as that of diesel engine. The compressibility of DME is also significantly higher. Its low viscosity and lower lubricity shows that it is not possible to use diesel fuel system without modifications (Sato et al., 2006).

In August 2007, Volvo trucks unveiled seven demonstration trucks, each tailored to run on various bio-fuels. Volvo is the first truck manufacturer to carry out comprehensive customer based field test involving Bio-DME fuel and have intended to install its plant in North America by 2015 (Brandon et al., 2013). Oberon is the first company to announce plans for the production and commercialization of DME in North America with small scale cost effective production facilities.

1.2 Engine Studies using DME

In 2009, Yu et al. conducted numerical studies on spray combustion and characteristics of DME fueled CI engine. DME burns well in combustion system of direct injection (DI) diesel engine at light and medium loads at all speeds. Combustion efficiency of DME with insufficient mixing could be deteriorated at high speed and high load. Compared to n-heptane, DME yields much shorter ignition delay times. DME shows rapid evaporation characteristics during the initial stages. With an increase in pressure, vaporization rate and the droplet surface temperature increases and the droplet
lifetime decreases. Comparisons have been made with conventional hydrocarbon liquid fuels. It has been found that DME has low spray penetration rate due to high evaporation rate, compared to n-heptane (Yu et al., 2009).

In 2009, Park conducted a numerical study on optimal operating conditions for HCCI engine fueled with DME and n-heptane. On the basis of the results for HCCI engines, engine performance and emissions including CO, HC, NOx and soot were shown on peak cycle temperature and equivalence ratio map. The results showed that HC, NOx and soot emissions decreased and CO emissions increased when DME is used in HCCI engine instead of n-heptane. In addition, DME was shown to have a wider optimal operating range than that of n-heptane in HCCI engine.

In 2009, Chen et al. conducted an experimental and numerical study on dual-fuel combustion of methanol/DME. In the experiment, methanol was injected directly and DME was injected in the intake port. At high methanol injection rate and with early injection, the combustion controlled region was narrower and at late injection, smooth combustion occurred along with low NOx formation. For moderate injection rate, higher indicated thermal efficiency was obtained at low methanol concentration. Numerical analysis was done using CFD and CHEMKIN. It was found that the increase in injection pressure is an effective way to shorten the duration of methanol/DME dual-fuel combustion. In the case of injection at 260 BTDC, the high temperature combustion region was concentrated in the combustion chamber, which resulted in higher NO concentration. And for injection timing of 60 BTDC, the high temperature combustion region was dispersed in the clearance volume and near the combustion chamber wall, which leads to a relatively low NO concentration.
In 2007, Yao et al. conducted multidimensional numerical simulations on DME/Methanol dual-fuel HCCI engine combustion and emission process. STAR-CD/KINETICS CFD code was used to simulate the combustion with homogenous charge. With an increase in the total fuel/air equivalence ratio, UHC and CO emissions decreased. However, for too small total fuel/air equivalence ratio or DME proportion, the CO emissions decreased too. Multidimensional CFD models results were better when compared with zero dimensional models.

In 2009, Yeom and Bae studied the knock characteristics of an HCCI Engine fueled with LPG-DME and Gasoline-DME. LPG and Gasoline were injected at the intake port by the port fuel injection equipment and DME, as an ignition promoter, was injected directly into the cylinder during the intake stroke. The ringing intensity analysis was done to find the HCCI combustion characteristics, and the knock intensity of the LPG-DME was noted to be lower than that of the gasoline-DME injected HCCI engine.

In 2009, the concept of LTC of the compound charge with port aspiration and in-cylinder direct injection of DME was used to find the characteristics of HCCI (Junjun et al., 2009). Through experiments it was found that the engine operating range increased with little change in NO\textsubscript{x} emissions and considerable reduction in HC and CO emissions when compared to the HCCI engine fueled with DME. For the fixed port aspiration of DME mass, HC the CO emissions decrease while NO\textsubscript{x} emissions increased as the load increased.

In 2009, Hwang et al. studied, both numerically and experimentally, NO\textsubscript{x} emission characteristics in DME/air non-premixed flames. In the co-axial jet case, experimental DME combustion had the same characteristics as that of a partially premixed flame and a
shorter flame length which caused low NO\textsubscript{x} emissions than that of ethane. Numerical analysis for co-axial jet and counter flow flames was conducted using CHEMKIN-2 and Transport packages. By means of re-burning NO, the DME non-premixed flame has a distinct NO reduction mechanism.

In 2010, Liu et al. studied CI engine fueled with DME to determine the regulated and non-regulated emissions. DME supplied was 1.6 times that of the diesel fuel. In the regulated emissions, it was found that, on average, CO emissions decreased at various speeds, and NO\textsubscript{x} emissions greatly decreased in comparison to the diesel at all load conditions and smoke emissions were almost zero under all engine operation conditions. As the speed increased, NO\textsubscript{x} emissions decreased. The trade off correlation between the NO\textsubscript{x} and smoke emissions breaks for the DME engine. In the case of non-regulated emissions, the formaldehyde emission was little higher than that with the diesel fuel, and the HC emissions were lower than diesel engine.

In 2009, Hyun et al. conducted experiments to determine the effect of multiple injection strategies on spray atomization and reduction of exhaust emissions in a DME fueled CI engine. Low boiling point of DME leads to quick evaporation when liquid phase DME is injected into the engine cylinder and, as a result, it can lead to better mixing with the air inside the cylinder. Multiple injections caused reduction in NO\textsubscript{x} and soot emissions in comparison to single injection. The concentrations of HC and CO emissions for DME were influenced by the first injection timing.

In 2009, Song et al. studied the performance and emission characteristics of a DME engine with high ratio of EGR. Increase of EGR ratio can result in decrease in the maximum rate of pressure rise, which is considered an indication of the reduction in the
combustion noise level. An increase in EGR ratio leads to significant decrease in NO\textsubscript{x} emissions but CO and HC emissions increase. DME engine running with low EGR ratio at high load operating conditions and with high EGR ratio at low load operating condition is better, as the thermal efficiency increases and NO\textsubscript{x} reduction is also obtained. Experiments are needed to realize the reduction of HC and CO emissions by means of an oxidation catalytic convertor.

In 2007, Wang et al. used CI engine fueled with DME and rapeseed oil blend to determine the performance and emission characteristics. Power and torque output increased as the mass fraction of rapeseed oil in the blend was increased. Brake thermal efficiency of the DME/rapeseed oil blend was a little lower than that of the conventional diesel engine. NO\textsubscript{x} emissions at high engine loads were strongly influenced with the addition of rapeseed oil in DME fuel and at low engine loads it had less influence. CO emissions decreased with an increase in rapeseed oil. HC emissions also decreased at high load due to high cylinder temperature, as the blend evaporates quickly and the mixture becomes more homogenous. Smokeless combustion was realized with less than about 6% rapeseed oil mass fraction in the blend because the oxygenate blend and the fast diffusion combustion suppress smoke formation. More studies are required on rapeseed oil and DME blends as fuel in CI engine.

In 2001, Sidu et al. experimentally investigated spray characteristics of DME. Higher injection pressure increased evaporation and dispersion of spray. Compared to diesel engine, the spray penetration was slower in DME i.e. it was 2 times lower penetration than diesel. An increase in the ambient density in the cylinder, leads to a decrease in the penetration of the DME spray, but this kind of difference was much
smaller. At ambient temperature, the evaporating processes of DME were much faster. It was noted that by decreasing the intake swirl ratio and by using injection orifice with a large diameter, fuel engine economy and HC emissions can be increased for the engine fueled with DME.

In 2002, Yu et al. experimentally studied DME and conventional diesel sprays by employing a common-rail high pressure injection system. At atmospheric pressure conditions, intrinsic spray characteristics of the DME were obtained, characterized by forming mushroom like shape at the spray tip and flash boiling. The evaporation characteristics were evaluated in terms of apparent vapor phase area. In the regions of the spray edge and downstream, the vapor phase of the DME spray appeared more, which implied that there is a more chance of ignition there. Compared to diesel in a cylinder, the DME spray provides better chance to contact with surrounding oxidant but more investigations are needed in more realistic way considering the temperature effect.

In 2004, Yao et al. simulated HCCI process using a detailed kinetic model of DME and methane dual fuel. Simulations were carried out using a single-zone thermodynamic model. Experimental study was performed using single-cylinder, water cooled, direct injection, diesel engine. The calculated pressure-increase ratio was larger than actually measured because in-cylinder distribution of pressure, temperature and chemical species are not taken into account in a zero-dimensional model. The heat release shape of the dual-fuel is that of the typical two-stage auto-ignition, and DME oxidation precedes methane. DME oxidation causes heat release in the first stage and methane oxidation causes the heat release in the second stage. LTR (Low Temperature Reaction) of DME is inhibited by methane but it promotes HTR (High Temperature Reaction) of DME.
oxidation. DME also helps to promote methane oxidation. This includes both thermal and chemical effects. In the first stage of the heat release, OH is mainly generated from the oxidation DME. The CO, generated from DME, and methane are oxidized at the same time.

In 1999, Longbao et al. studied the performance and combustion characteristics of DME by experimenting water cooled, single cylinder, four stroke, naturally aspirated, direct injection diesel engine. DME usage reduced NO\textsubscript{x} emissions significantly and achieved zero-smoke combustion. The injection delay was longer, ignition delay was shorter and the peak pressure, maximum rate of pressure rise and the combustion noise were lower with DME fuel when compared to the diesel fuel. Compressed nitrogen was used to keep DME in liquid state in the tank and flow meters. DME is an excellent alternative fuel for compression ignition engines.

In 1995, Sorenson studied performance and emission characteristics of a 0.273 liter DI diesel engine fueled with neat DME. An experimental study was presented in a small non-turbocharged diesel engine. By making minor modifications in the fuel system of DME, it gave good results in combustion, emissions and performance. The thermal efficiency of DME was almost equivalent to diesel engine with much lower NO\textsubscript{x} emissions, very low smoke emissions and low engine noise. EGR was used for additional reduction of NO\textsubscript{x} without visible smoke and decrease in thermal efficiency.

In 2007, Park et al. studied CI engine fueled with DME to determine the combustion performance and emission reduction characteristics. Compared to diesel or biodiesel fueled CI engine, ignition in the combustion chamber for DME started early. Multiple injection and premixed combustion helped reduce NO\textsubscript{x} emissions from the DME fueled
engine. A single-cylinder or four-cylinder diesel engine equipped with an electronically controlled common rail injection system was used for the study. DME fuel has a higher discharge coefficient than that of the diesel fuel and even the period of cavitation was longer than that of the diesel engine. The DME fuel supplied to the engine was more than diesel because of lower energy density. In addition, due to lower bulk modulus, DME required higher compression energy compared to conventional diesel fuel.

Heavy-Duty truck has been developed with DME fueled CI engine by Sato et al. (2006). EGR and NO\textsubscript{x} reduction catalyst helped in reduction of NO\textsubscript{x} emissions. Power and performance of the DME fueled engine and the truck was higher than that of the diesel engine. More research is needed to include the investigation of user-friendliness, reliability and durability of the DME truck at different environmental conditions by extensive testing.

In 2013, Khunaphan et al. studied the characterization and potential of Dimethyl ether (DME) for dual fuel combustion in a compression ignition engine. The results of DME and LPG dual fuel were compared to that of the diesel fuel and dual fuel diesel + DME. Brake thermal efficiency increased for DME and LPG dual fuel at high engine load compared to that of the neat diesel fuel and diesel + DME. The presence of DME and LPG helped reduce CO, HC concentration, smoke emission and also the fuel consumption when compared to diesel.

In 2007, Crookes et al. studied rapeseed methyl ester (RME) and DME as fuels for diesel engine to determine the performance and combustion characteristics. Due to the lower density and specific combustion enthalpy of DME, it required twice the injected volume of diesel. For both single and dual-fuel diesel engine applications, DME gave
lower NO$_x$ emissions than that of both RME and diesel fuel. A gradual reduction of specific NO$_x$, CO and HC was observed in engine operating with dual-fuel.

In 2011, Ji et al. investigated combustion and emission characteristics of a four-cylinder SI engine fueled with DME/gasoline mixture. Modifications to the SI engine were made for the injection of both gasoline and DME. As the DME blending level increased, the HC and NO$_x$ emissions decreased. But the CO emissions first decreased and later on increased with the addition of DME, due to the reduced reaction time for oxidation. At DME energy fraction larger than 15%, CO emissions increased. Fuel energy flow rate dropped with the addition of DME, but thermal efficiency increased. Addition of DME in gasoline engine improved the emission performance and economy, especially when DME energy fraction was less than 10%.

In 2014, Thomas et al. investigated CI engine experimentally to determine if the emissions from combustion of DME in engine would meet the future emission norms. With the use of promising techniques to control emissions and by taking the advantage of combustion and emission properties of the fuel, it is expected that DME engines are able to achieve future emission norms with less aftertreatment when compared to diesel engines. Optimized EGR ratios can significantly reduce NO$_x$. The benefits of normal EGR system has been improved by the use of multi-stage cooled EGR system. With the increasing EGR ratio, there is no effect on PM and therefore, CO and HC emissions can be controlled by the use of oxidation catalysts downstream of the exhaust manifolds. Future research is needed to determine the capabilities of injection strategies like multiple injection, injection and spray angles, injection pressure etc. to achieve control over engine operating parameters and complete combustion with lesser emissions.
1.3 Focus of this Thesis

The major focus of the present work is to computationally investigate the effect of various fuel injection strategies on emission characteristics of a DME fueled engine. The soot-NOx tradeoff that is characteristic of diesel combustion is absent for DME and therefore, NOx and soot can be simultaneously decreased by using EGR. However, it can lead to increased emissions of CO, HC and other unregulated species. Optimization of injection strategy offers another control to tackle this issue.

In this work, multidimensional CFD simulations are conducted to understand the effect of various injection strategies, such as pilot and split injection and injection timing, on in-cylinder processes and emissions. Despite of few studies at low and high load conditions for split injection, there is limited data for medium load condition and this study aims to address that.

1.4 Thesis Organization

The organization of the thesis is as follows. Chapter two describes in detail about the computation model and the simulation software used.

Chapter three describes computational specifications and results of numerical validation using available engine data.

Chapter four describes the details of the injection strategies, and the results of the injection strategy investigation are presented in Chapter five.

Finally, Chapter six presents the summary of the work, and provides recommendations for further study.
CHAPTER II

COMPUTATIONAL MODEL DESCRIPTION

2.1 Introduction

The computational model was built by means of the Converge CFD code. The details of various models, specifically the liquid injection, spray, combustion and, turbulence are provided in the following.

2.2 Computational Model

In this work, the Converge CFD software package is used as the computational framework for running the spray and combustion simulations. Converge is a general purpose CFD code for the calculation of three-dimensional, incompressible or compressible, chemically-reacting fluid flows in complex geometries with stationary or moving boundaries. Converge can handle an arbitrary number of species and chemical reactions, as well as transient liquid sprays, and laminar or turbulent flows. Converge uses an innovative modified cut-cell Cartesian method that eliminates the need for the computational grid to be morphed with the geometry of interest while still precisely representing the true boundary shape. This approach allows for the use of simple orthogonal grids and completely automates the mesh generation process. This section
presents a brief overview of the governing equations, spray modelling, liquid injection, combustion model and the turbulence model used in the current work.

2.2.1 Governing Equations

Converge uses the following compressible continuity, momentum transport and energy equations

Continuity Equation,
\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = S
\] (2.1)

Momentum Transport Equation,
\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + S_i
\] (2.2)

Where \( u \) is velocity, \( \rho \) is density, \( P \) is Pressure, \( \sigma_{ij} \) is the stress tensor and \( S \) is the source term.

The compressible form of the energy equation is given as
\[
\frac{\partial \rho e}{\partial t} + \frac{\partial u_j \rho e}{\partial x_j} = -P \frac{\partial u_j}{\partial x_j} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left( K \frac{\partial T}{\partial x_j} \right) + \frac{\partial}{\partial x_j} (\rho D \sum_m h_m \frac{\partial Y_m}{\partial x_j}) + S
\] (2.3)

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 the pressure, \( e \) is the specific internal energy, \( K \) is conductivity, \( h_m \) is the specific enthalpy, \( T \) is temperature and \( \sigma_{ij} \) is the stress tensor.

Along with these, equations for the turbulent kinetic energy and dissipation rate are solved.
2.2.2 Liquid Injection

Converge offers two categories of liquid injection mechanisms: injectors and nozzles. An injector is a group of nozzles that have some of the same characteristics, as described below. Each injector can have any number of nozzles, each with its own hole size, cone angle, position, and orientation.

The polar coordinate system option is selected to specify the nozzle locations, even the location and orientation of each injector is specified. As shown in Figure 2.1, the variables $x_{cen}$, $y_{cen}$, and $z_{cen}$ are used to set the $x$, $y$ and $z$ coordinates of the injector center. The two angles $angle_{xy\_inj}$ and $angle_{xz\_inj}$ are used to determine the orientation of the injector.

2.2.2.1 Blob Injection Model

The blob injection method of Reitz and Diwakar (1987) is used to initialize drop size with injection drop distribution flag ($injdist\_flag$). By setting the parameter $injdist\_flag=0$, injected drop sizes are equal to the nozzle diameter or effective diameter when the discharge coefficient model is on ($discharge\_switch=1$ or 2).

2.2.3 Spray Modelling

Converge includes several spray breakup mechanisms, including models based on the Kelvin-Helmholtz (KH) and Rayleigh-Taylor (RT) instability mechanisms, the LISA sheet breakup model, and the Taylor Analogy Breakup (TAB) drop breakup model.
2.2.3.1 Kelvin-Helmholtz Breakup Model

The Kelvin-Helmholtz instability is based on a liquid jet stability analysis that is described in detail by Reitz and Bracco (1986). This analysis considers the stability of a cylindrical, viscous, liquid jet of radius $r_0$ issuing from a circular orifice at a velocity $U$ into a stagnant, incompressible and inviscid gas of density $\rho_g$. The liquid has a density $\rho_l$
and viscosity \( \mu \) and a cylindrical polar coordinate system is used which moves with the jet.

In the KH model, the initial parcel diameters are set equal to the nozzle hole diameter \( d_0 \) and the atomization process of the relatively large injected blobs is modeled using the stability analysis for liquid jets. The breakup of the parcels and resulting drops of radius \( r_0 \) is calculated by assuming that the breakup drop radius \( r \) is proportional to the wavelength of the fastest growing unstable surface wave. In other words

\[
    r = B_0 \Lambda_{KH},
\]

where \( B_0 \) is a model constant typically set to 0.61 based on the work of Reitz (1987) and \( \Lambda_{KH} \) is the wavelength of the fastest growing unstable surface wave. Although \( B_0 \) in Equation (2.4) is typically set to 0.61, it has been included in the input files to allow adjustment if necessary. A smaller value of \( B_0 \) will result in smaller drops from breakup, while a larger value will result in larger drops.

On the other hand, in the limit of very high gas Weber numbers and an inviscid liquid, Equation (2.4) reduces to

\[
    r = 9.8B_0 \frac{\sigma}{\rho_g U}
\]

which is equivalent to the bag regime breakup criterion

\[
    We_g > 6.0,
\]

for a \( B_0 \) value of approximately 0.61. It has been noted by Reitz (1987) that very similar drop sizes are obtained if equation (2.5) is always used to determine the breakup drop
size. As a result, running the present KH model without the addition of new child parcels is consistent with the Reitz and Diwakar (1987) model for high-speed, inviscid sprays.

2.2.3.2 Rayleigh-Taylor Breakup Model

In addition to the KH breakup mechanism, the Rayleigh-Taylor (RT) instability is also believed to be responsible for droplet breakup. The unstable RT waves are thought to occur due to the rapid deceleration of the drops from the magnitude of the drag force, $|F_D|$ , which is given as

$$|F_D| = M_d |a| = M_d \frac{3}{8} C_D \frac{\rho d |U|^2}{\rho i r_0}$$  \hspace{1cm} (2.7)$$

where $|a|$ is the deceleration of the drop, $M_d$ is the mass of the drop, $r_0$ is the drop radius and $C_D$ is the drag coefficient. Typical implementations of the RT breakup model ignores both gas and liquid viscosity (Ricart et al., 1997).

In Converge, the wavenumber corresponding to the maximum growth rate ($K_{RT} = 2\pi / \Lambda_{RT}$) is solved numerically using bisection method. As in the study of Xin et al. (1998), if the scaled wavelength given by $C_{RT} \Lambda_{RT}$ is calculated to be smaller than the droplet diameter, RT waves are assumed to be growing on the surface of the drop. When the RT waves have been growing for a sufficient time (i.e., $C I / \Omega_{RT}$ where $C_I$ is a constant and $\Omega_{RT}$ is the corresponding growth rate), the drop is broken up according to the RT mechanism. The RT size constant $C_{RT}$ can be increased or decreased to change the size of the predicted RT breakup radius. Similarly, the RT time constant $C_I$ can be increased to delay RT breakup, or decreased to promote faster RT breakup.
2.2.3.3 KH-RT Breakup Length Model

Converge allows us to run KH and RT model. One option for running them together is to use the so called KH-RT breakup length model. By activating the KH-RT breakup length model, an intact core or breakup length $L_b$ can be specified as

$$L_b = C_{bl} \sqrt{\frac{\mu_1}{\rho_g}} d_0$$

(2.8)

![Figure 2.2 - Schematic of the KH-RT spray breakup model.](image)

The liquid blobs are injected with a diameter equal to that of the injector nozzle. In addition, the KH breakup mechanism is applied to a droplet throughout its lifetime, while the RT mechanism is only initiated once the drop reaches a characteristic breakup distance, $L_b$, from the injector. As shown in Figure 2.2, this model assumes that only KH instabilities are responsible for drop breakup inside of the $L_b$, while both KH and RT
mechanisms are activated beyond the breakup length. In this case, Converge first checks if the RT mechanism can break up the droplet. If not, the KH mechanism is responsible for breakup. The breakup time $\tau_{KH}$ is given by

$$\tau_{KH} = \frac{3.726 B_1 r_0}{\Lambda_{KH} \Omega_{KH}}$$  \hspace{1cm} (2.9)

The KH breakup time constant $B_1$ has been found to vary from one injector to another. The value of $B_1$ has been taken as 40. In addition, the breakup length constant $C_{bl}$ in equation above can be tuned to increase or decrease spray breakup. A methodology for tuning $C_{bl}$ has been described by Senecal (2000), which showed that for very high gas Weber numbers (typical of Diesel sprays) and $\mu_l = 0$ ($\mu_l$ is the drop viscosity), the KH model breakup time (i.e., equation $2.9$) reduces to

$$\tau_{KH} = \frac{B_1}{U \sqrt{\rho_l/\rho_g} r_0}$$  \hspace{1cm} (2.10)

Which results in a breakup length $L_{KH} = U \tau_{KH}$ or

$$L_{KH} = B_1 \sqrt{\rho_l/\rho_g} r_0$$  \hspace{1cm} (2.11)

Equation 2.11 is compared with equation 2.8, it is clear that $C_{bl}$ must equal $B_1/2$ in order for $L_b$ and $L_{KH}$ to be consistent. Tuning the two spray constants together as described above has been shown to result in accurate predictions of vaporizing spray penetration when compared to experiments (Beale, 1999). The breakup length can be removed from the model by setting $C_{bl} = 0$ in equation 2.8. This results in both the KH and RT mechanisms acting on droplets as they exit the nozzle (Patterson, 1997).
2.2.4 SAGE Detailed Chemical Kinetics Model

In order to include detailed chemistry in combustion applications, the SAGE model (Senecal et al., 2003) has been incorporated into Converge. This approach allows us to use detailed chemical kinetics in combustion simulations with a set of CHEMKIN formatted input files, which here become the standard format for defining chemical mechanisms. The SAGE model uses the CVODES solver (solves initial value problems for ordinary differential equation, ODE systems) which is part of the SUNDIALS (SUite of Nonlinear and DIfferential/ALgebraic equation Solvers) package. The necessary routines have been incorporated into Converge and so it is not needed to have the SUNDIALS package installed on the computer systems.

A chemical reaction mechanism is a set of elementary reactions that describe, in detail, an overall chemical reaction. The combustion of different fuels can be modeled by changing the mechanism (e.g., there are mechanisms for iso-octane, gasoline, n-heptane, natural gas, etc.). The detailed chemistry solver, SAGE, calculates the reaction rates for each elementary reaction while the CFD solves the transport equations. SAGE, along with Adaptive Mesh Refinement (AMR), and an accurate mechanism can be used for modeling many combustion regimes (ignition, premixed, mixing-controlled).

2.2.5 Turbulence Modeling

Turbulence significantly increases the rate of mixing of momentum, energy, and species. For many applications, such as an internal combustion engine, the turbulence is critical for an accurate simulation.
The turbulence-enhanced mixing is a convective process that results from the presence of turbulent eddies in the flow. These turbulent eddies occur at many length scales. If the discretized domain (grid) does not resolve the smallest eddy length scales present in the flow, then the enhanced mixing effects of the turbulence will not be entirely accounted in the CFD simulation. With the current computational power, it is not practical to resolve all of the turbulent scales in typical CFD simulations; therefore, a turbulence model may be needed to account for the additional mixing.

The turbulence model interacts with many of the other models in Converge (e.g., spray, combustion, and wall heat transfer). The Reynolds Averaged Navier-Stokes (RANS) turbulence models available in Converge are the Standard $k$-$\varepsilon$, the RNG (Renormalization Group) $k$-$\varepsilon$, and the Rapid Distortion RNG $k$-$\varepsilon$ (Han and Reitz, 1995) models. Rapid Distortion RNG $k$-$\varepsilon$ is used in the present simulations.

2.2.5.1 RANS Models

Traditionally, in RANS models, an effective turbulent viscosity is used to model the Reynolds stress term. For $k$-$\varepsilon$ and the RNG $k$-$\varepsilon$ models, two additional transport equations are needed in order to obtain the turbulent viscosity; one equation for turbulent kinetic energy, $k$, and one for the dissipation of turbulent kinetic energy, $\varepsilon$.

The transport equation for turbulent kinetic energy is given by

$$ \frac{\partial \rho k}{\partial t} + \frac{\partial \rho u_i k}{\partial x_i} = \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \mu + \frac{\mu}{\Pr_{\text{tke}}} \frac{\partial k}{\partial x_j} \right) - \rho \varepsilon + S $$  \hspace{1cm} (2.12)
where $\rho$ is density, $u$ is velocity, $\mu$ is viscosity, $k$ is the turbulent kinetic energy, $Pr_{tke}$ is turbulent kinetic energy Prandtl number, $\varepsilon$ is the turbulent dissipation, $S$ is the source term, the stress tensor is given by

$$
\sigma_{ij} = 2\mu_t S_{ij} - \frac{2}{3} \delta_{ij} \left( \rho \frac{\partial u_i}{\partial x_j} + \mu \frac{\partial u_j}{\partial x_i} \right)
$$

(2.13)

And the turbulent viscosity is given by

$$
\mu_t = C_{\mu} \rho \frac{k^2}{\varepsilon}
$$

(2.14)

where $\delta_{ij}$ is the so-called Kronecker delta and $C_{\mu}$ is the turbulence model constant.

The transport equation for turbulent dissipation is given by

$$
\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial (\rho u_i \varepsilon)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \mu \frac{\partial \varepsilon}{\partial x_i} \right) - \rho c_{\varepsilon 3} \varepsilon^2 - \rho \frac{c_{\varepsilon 1}}{\varepsilon} \frac{\partial u_i}{\partial x_i} \frac{\partial \varepsilon}{\partial x_i} + \left( \frac{c_{\varepsilon 1} \partial u_i}{\partial x_i} \sigma_{ij} - \frac{c_{\varepsilon 2}}{\varepsilon} \rho \varepsilon + c_s S_S \right) \frac{\varepsilon}{k} - \rho R,
$$

(2.15)

where $R$ is dependent on the turbulence model, $c_{\varepsilon 1}$, $c_{\varepsilon 2}$ and $c_{\varepsilon 3}$ are model constants, and $S$ is a source term.

The Rapid Distortion RNG k-\varepsilon model uses the transport equation for $\varepsilon$ given by

$$
\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial (\rho u_i \varepsilon)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \mu \frac{\partial \varepsilon}{\partial x_i} \right) - \frac{2}{3} c_{\varepsilon 1} - c_{\varepsilon 3} + \frac{2}{3} c_\mu c_{\varepsilon} \frac{k}{\varepsilon} \frac{\partial u_k}{\partial x_i} \frac{\partial \varepsilon}{\partial x_i} \rho \varepsilon \frac{\partial u_i}{\partial x_i} \frac{\partial \varepsilon}{\partial x_i} + \left( \frac{c_{\varepsilon 1} - c_{\varepsilon}}{\varepsilon} \frac{\partial u_i}{\partial x_i} \sigma_{ij} - \frac{c_{\varepsilon 2}}{\varepsilon} \rho \varepsilon + c_s S_S \right) \frac{\varepsilon}{k}
$$

(2.16)

where

$$
c_{\varepsilon} = \frac{\eta (1 - \eta)}{1 + \beta \eta^2}
$$

(2.17)
where $S_{ij}$ is the mean stress rate tensor.
3.1 Literature Data for Computational Validation

Based on the literature review (Chapter 1), the experimental and numerical studies of Kim et al. (2010) were selected for computational validation. The comparison between the experimental and numerical data at injection timing of 20\(^0\) BTDC was selected to validate the numerical model. A single cylinder and four valve DME fueled test engine with a common-rail fuel injection system was used by Kim et al. (2010). The bore and stroke of the engine are 75 mm and 84.5 mm, respectively. It has a re-entrant type of piston with a compression ratio of 17.8, and a high pressure diesel injector with 156\(^0\) of injection angle and six holes of 0.128 mm diameter each. The detailed engine specifications are listed in Table 3.1.

Spray inclination angle is taken as the half of the injection angle as shown in Figure 3.1. As there are six injection nozzles or holes, the engine can be divided into six sectors, each of 60\(^0\). Because of the symmetrical location of the injector at the center of the combustion chamber, the CFD calculations are performed on a 60\(^0\) sector mesh.
Table 3.1 Specifications of the DME Fueled Engine

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore (mm)</td>
<td>75</td>
</tr>
<tr>
<td>Stroke (mm)</td>
<td>84.5</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>17.8</td>
</tr>
<tr>
<td>Displacement volume (cm³)</td>
<td>373.3</td>
</tr>
<tr>
<td>Intake valve close timing (IVC)</td>
<td>BTDC 128°</td>
</tr>
<tr>
<td>Exhaust valve open timing (EVO)</td>
<td>ATDC 172°</td>
</tr>
<tr>
<td>Injection nozzles</td>
<td>6</td>
</tr>
<tr>
<td>Injector hole diameter (mm)</td>
<td>0.128</td>
</tr>
</tbody>
</table>

![Image of injection and spray angle of spray](image)

Figure 3.1 - Injection and spray angle of spray

Simulations were run from intake valve closing (IVC) to exhaust valve opening (EVO) with initial thermodynamic conditions as well as wall temperatures estimated from the experimental data (Kim et al., 2010). Thus, closed-cycle computations on sector grids with periodic boundaries were carried out due to computational efficiency. In these
calculations $1/n_{th}$ of the combustion chamber, where $n$ the number of nozzle orifices, is modeled. The CFD code uses a structured Cartesian grid with base cell size of 1.0 mm. Two additional types of grid refinements were performed by means of an adaptive mesh refinement (AMR) as well as a fixed refinement (embedding) within the spray region.

The engine running at a speed of 1500 rpm and swirl ratio of 1.63 is modeled. The DME fuel is injected into the cylinder at a temperature and pressure listed in Table 3.2. Mass of the fuel injected into each injector per cycle is 1.33 mg.

<table>
<thead>
<tr>
<th>Engine speed (rpm)</th>
<th>1500</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spray inclination angle (deg)</td>
<td>78</td>
</tr>
<tr>
<td>Swirl ratio</td>
<td>1.63</td>
</tr>
<tr>
<td>Fuel Injection pressure (MPa)</td>
<td>50</td>
</tr>
<tr>
<td>Mass of fuel injected(mg/cycle)</td>
<td>8</td>
</tr>
<tr>
<td>Fuel Injection temperature (K)</td>
<td>300</td>
</tr>
</tbody>
</table>

3.2 Chemical Kinetic Model

In order to improve the efficiency and to reduce emissions, an in depth understanding of the fundamental chemical processes involved in combustion is necessary. Chemical kinetics is a study of the rates of reactions; it involves how various physical conditions attribute to the rate of a chemical reaction.
Chemical kinetic modeling helps understand and predict the behavior of a hydrocarbon fuel under various physical conditions. It generally involves a set of elementary reactions; a mechanism for a single fuel component can contain a very large number of reactions pertaining to various physical conditions. The primary purpose of a chemical kinetic mechanism is to reproduce the experimental data and for use in computational modeling of combustion systems. In order to use these mechanisms in computations and combustion modeling, a rigorous validation against experimental data is highly important for accurate predictions.

In kinetic research, several detailed chemical models for low and high temperature DME oxidation (Curran et al., 1998; Fischer et al., 2000; Curran et al., 2000; Zhao et al., 2008) have been developed and validated against multiple experimental observations. Of particular importance to the present study is the ability of the available chemical kinetic models to accurately reproduce DME autoignition properties at engine-like conditions. DME displays the classical two-stage, negative temperature coefficient (NTC) ignition behavior similar to that observed with linear alkanes (Iida et al., 2000; Pfahl et al., 1996; Fieweger et al., 1997; Curran et al., 1998). This behavior stems from low temperature reactions involving hydrocarbon radicals and molecular oxygen (Curran et al., 1998). Therefore, a comprehensive, detailed DME kinetic model for gas turbine and engine applications should correctly predict these low-temperature auto-ignition features. The original kinetic model for DME oxidation and pyrolysis (Zhao et al., 2008), is used for the present study. It consists of 55 species undergoing 290 reversible reactions and has been validated for a wide range of physical conditions, which includes flow reactor species-time history profiles at pressures up to 18 atm and temperatures near 1000 K.
(Fischer et al., 2000; Curran et al., 2000), flow reactor reactivity profiles at 12.5 atm and initial reaction temperatures from 550 K–900 K (Curran et al 2000), jet-stirred reactor species profiles up to 10 atm over the temperature range of 550 K–1100 K (Bowman et al., 2006; Dagaut et al., 1996), pyrolysis in a flow reactor up to 10 atm (Fischer et al 2000; Zhao et al., 2008), shock tube ignition delay measurements at low and high pressures (Pfahl et al., 1996; Dagaut et al., 1998; Bowman et al., 2006), species profiles in low pressure and atmospheric burner stabilized flames (Kaiser et al., 2000; McIlroy et al., 2000; Cool et al., 2007), and also laminar flame speeds up to 10 atm (Daly et al., 2001; Zhao et al., 2004; Qin et al., 2005). Additional 7 species (i.e., NO, NO\textsubscript{2}, NO\textsubscript{3}, N\textsubscript{2}O, HONO, HNO, and CH\textsubscript{3}O\textsubscript{2}) are added to account for NO\textsubscript{x} formation. The NO\textsubscript{x} chemistry model assembled by Mueller et al. (2000) is used here. The final augmented chemistry model involves 62 species and 320 reactions (Hossam et al., 2014).

3.3 Model Formulation for the DME Fueled Engine

The engine sector along with the mesh is shown in Figure 3.2. The wall temperatures of piston, cylinder head, and cylinder are also listed in Table 3.3. In the simulations, pressure and species concentration gradient at wall are specified as zero along with no slip boundary condition for velocity. The initial gas temperature inside the cylinder at intake valve closure (IVC) is 320 K and initial pressure is 1.07825 atm.

Spray atomization and break-up are modeled using the hybrid KH-RT (Kelvin-Helmholtz Rayleigh-Taylor) model. Turbulent flow is modeled by means of the RNG (re-normalization group) k-ε model with wall-functions in order to account for wall heat transfer. The base grid size is taken as 0.001m. Concerning combustion modeling, a
direct integration of detailed chemistry approach was used by means of the Converge code and the SAGE (SAIC adaptive grid Eulerian) solver. A multi-zone model from Babajimopoulos et al. (2005) is used to solve the detailed chemistry in zones, i.e., groups of cells that have similar thermodynamic state, in order to speed-up chemistry calculations. Cells are grouped based on two variables, temperature and equivalence ratio. The calculations performed in this project use a 5K bin size for temperature and 0.05 bin size for equivalence ratio zones.

![Computational mesh for analysis of a DME fueled CI engine](image)

Figure 3.2 – Computational mesh for analysis of a DME fueled CI engine
The initial axial velocity ($z$ direction) is calculated using the equation,

$$w(z) = w_{piston} \left( \frac{z_{\text{head}} - z}{z_{\text{head}} - z_{\text{piston}}} \right)$$

Where $z_{\text{head}}$ and $z_{\text{piston}}$ are the $z$-coordinates of the head and piston, respectively, and $w_{\text{piston}}$ is the speed of the piston. Along with this, the initial velocity in the circumferential direction is specified based on the swirl number.

Table 3.3 - Initial and boundary conditions for of the DME fueled engine

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Piston temperature (K)</td>
<td>550</td>
</tr>
<tr>
<td>Head temperature (K)</td>
<td>520</td>
</tr>
<tr>
<td>Cylinder wall temperature (K)</td>
<td>430</td>
</tr>
<tr>
<td>Initial gas temperature (K)</td>
<td>320</td>
</tr>
<tr>
<td>Initial pressure (atm)</td>
<td>1.07825</td>
</tr>
</tbody>
</table>

3.4 AMR Mesh Details/ Grid Manipulation

Grid can be coarsened or refined by using grid scaling feature in Converge which adjusts the base grid size. Secondly, fixed or time-dependent refinements (embedding) in the grid can be made when and wherever it is needed. Lastly, Adaptive Mesh Refinement (AMR) can be used to automatically add grid refinement in critical areas of the domain.

During spray and combustion, a higher resolution of grid is needed to ensure the accuracy. But for compression and expansion stroke, lower resolution grid may be sufficient. So the grid needs to be coarsened during compression and expansion stroke.
a. Mesh before AMR and embedding or before spray injection

b. Change in mesh during pilot injection due to AMR and embedding

c. Change in mesh during main injection due to AMR and embedding

d. Change in mesh after main injection due to AMR

Figure 3.3 – Change in mesh due to AMR and embedding
and it needs to be refined during spray and combustion to improve the accuracy and precision during the simulation.

Fixed embedding is used to refine the grid in specific locations in the domain where finest grid is required to obtain both precision and accuracy for the solution. It allows the rest of the grid to remain coarse for reducing the simulation time. The simulation timing for fixed embedding has been set as $25^0 \text{BTDC}$ to $172^0 \text{ATDC}$.

AMR is used to refine the grid automatically, whenever it is required, based on temperature, velocity field calculation. It allows for obtaining a highly refined mesh in complex simulations. For velocity AMR is taken from $45^0 \text{BTDC}$ to $30^0 \text{ATDC}$ and for temperature it is taken from $45^0 \text{BTDC}$ to $172^0 \text{ATDC}$. Fixed embedding has been used from $45^0 \text{BTDC}$ to $172^0 \text{ATDC}$ for piston head, cylinder wall and cylinder head, and $45^0 \text{BTDC}$ to $30^0 \text{ATDC}$ is used for nozzle and injector. By using AMR and fixed embedding, the mesh is changed as shown in Figure 3.3.

3.5 Model Validation Simulation

Computation are performed for a $60^0$ sector of the combustion chamber. According to experiments (Kim et al., 2010), the start of injection timing has been selected as $20^0 \text{BTDC}$. In the present numerical study for model validation, the injection time or the duration of injection used as the input is estimated from the spray penetration curve or injection rate curve (Kim et al., 2007).

The results from the validation study are compared against the experimental data (Kim et al., 2010) in Figure 3.4. An excellent agreement is noted between the experiment
and simulation during the compression and expansion stroke as well as in the peak pressure and combustion phasing. Since the chemical kinetic mechanism used here was already comprehensively validated, the agreement in the engine pressure traces may be taken as a sufficient evidence of the suitability of the present engine model for predictive simulations.

Figure 3.4 - Pressure comparison curve for validation
CHAPTER IV
PILOT AND SPLIT INJECTION STRATEGY

4.1 Introduction

Multiple injections have been shown to be an effective means for reduction of pollutants emissions in diesel engines. Multiple injections divide the total quantity of fuel into two or more injections per combustion event. Pilot injection is also usually defined as an injection where 10% or less of the total mass of fuel is injected in the first injection. Many researchers are now investigating pilot and split injection as an effective means to simultaneously reduce soot and NO\textsubscript{x} formation. By using DME as a fuel in diesel engine there is no soot formation, and by using multiple injection strategy, NO\textsubscript{x} formation can potentially be reduced.

The benefits of multiple injections have been found to be highly dependent on the specification of the quantity of fuel in each injection and the dwell between injections. Shundoh et al. (1992) reported that NO\textsubscript{x} could be reduced by 35\%, and smoke by 60 to 80\%, without a penalty in fuel economy if pilot injection was used in conjunction with high pressure injection. Nehmer et al. (1994) studied the effect of split injection in a heavy-duty diesel engine by varying the amount of fuel in the first injection from 10\% to 75\% of the total amount of fuel. They found that split injection utilized the air charge
better and allowed combustion to continue later into the power stroke than a single injection case, without increased levels of soot production. Tow et al. (1994) found that using a double injection with a relatively long dwell on a heavy duty engine resulted in a reduction of particulate emissions by a factor of three with no increase in NO\textsubscript{x} and only a slight increase in BSFC compared to a single injection. Zhang (1999) used a single cylinder HSDI diesel engine to investigate the effect of pilot injection with EGR on soot, NO\textsubscript{x} and combustion noise, and found that pilot injection increased soot emissions. The author also showed that reducing the amount of fuel in the pilot injection and increasing the interval between pilot and main injections could reduce the pilot flame area when the main injection starts, resulting in lower soot emissions.

4.2 Injection Strategies

Following the validation with single injection, presented in chapter 3, several cases for split and pilot injection strategy were simulated. In these simulations, the amount of fuel injected in each pulse as well as the timing of the first injection and the dwell between pulses was varied. The injection strategies are described in the following.

4.2.1 Pilot Injection

Table 4.1 shows the injection strategies by changing the time of the first injection used in pilot injection. In the pilot injection cases, only 10% of the mass of the fuel is injected during the first pulse of injection or during pilot injection and remaining 90% of the mass of the fuel is injected during the main injection timing at 5\textdegree BTDC as shown in
Figure 4.1. The time between the pilot injection and the main injection is called the dwell time. The total amount of the fuel injected in all the cases was maintained the same. The dwell time was changed throughout the simulations.

![Figure 4.1 - Pilot injection](image)

**Table 4.1 - Various pilot injection cases**

<table>
<thead>
<tr>
<th>Pilot injection</th>
<th>Main injection</th>
</tr>
</thead>
<tbody>
<tr>
<td>10°BTDC</td>
<td>5°BTDC</td>
</tr>
<tr>
<td>20°BTDC</td>
<td>5°BTDC</td>
</tr>
<tr>
<td>30°BTDC</td>
<td>5°BTDC</td>
</tr>
<tr>
<td>40°BTDC</td>
<td>5°BTDC</td>
</tr>
</tbody>
</table>

4.2.2 Split Injection

Table 4.2 and 4.3 show the injection strategies by changing the time of first injection and main injection in split injection cases. In split injection, 20% of the mass of the fuel
is injected during the first injection and remaining 80% during the second/main injection. Initially, the main injection is fixed and four different cases at different first injection timing are simulated. And later by selecting best case among the first 4 cases, more cases are simulated by fixing the first injection timing and changing the main injection timings. Figure 4.2 shows the injection strategy for the split injection.

Figure 4.2 - Split injection

<table>
<thead>
<tr>
<th>Split injection</th>
<th>Main injection</th>
</tr>
</thead>
<tbody>
<tr>
<td>10°BTDC</td>
<td>5°BTDC</td>
</tr>
<tr>
<td>20°BTDC</td>
<td>5°BTDC</td>
</tr>
<tr>
<td>30°BTDC</td>
<td>5°BTDC</td>
</tr>
<tr>
<td>40°BTDC</td>
<td>5°BTDC</td>
</tr>
</tbody>
</table>
Table 4.3 - Split injection cases with 20% mass injected during first injection and fixed first injection timing

<table>
<thead>
<tr>
<th>Split injection</th>
<th>Main injection</th>
</tr>
</thead>
<tbody>
<tr>
<td>20°BTDC</td>
<td>10°BTDC</td>
</tr>
<tr>
<td>20°BTDC</td>
<td>0°BTDC</td>
</tr>
<tr>
<td>20°BTDC</td>
<td>5°ATDC</td>
</tr>
<tr>
<td>20°BTDC</td>
<td>10°ATDC</td>
</tr>
</tbody>
</table>

4.3 Operating Conditions

While section 4.2 outlined the various injection strategies used in this study. The engine specifications are same as mentioned earlier in Table 3.2. The initial temperature in the cylinder is taken as 320K and pressure as 1.74atm. Mass of the fuel injected per cycle, injection temperature and pressure are listed in the Table 4.4. Mass of the fuel injected into each injector per cycle is 4.33 mg. All the remaining conditions are similar as mentioned earlier in chapter 3.

Because of the symmetrical location of the injector at the center of the combustion chamber, the CFD calculations are performed on a 60° sector. Exhaust and intake ports are not included in the computational mesh by concentrating this simulation on in-cylinder flow and combustion processes. Calculations begin at Intake Valve Closure (IVC) and end at Exhaust Valve Opening (EVO). The same initial and boundary conditions are used for all the computations.
Table 4.4 - Numerical conditions of DME fueled engine

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine speed (rpm)</td>
<td>1500</td>
</tr>
<tr>
<td>Initial temperature (K)</td>
<td>320</td>
</tr>
<tr>
<td>Initial pressure (atm)</td>
<td>1.74</td>
</tr>
<tr>
<td>Injection pressure (MPa)</td>
<td>60</td>
</tr>
<tr>
<td>Mass of fuel injected(mg/cycle)</td>
<td>26</td>
</tr>
<tr>
<td>Injection temperature (K)</td>
<td>300</td>
</tr>
</tbody>
</table>

4.4 Example Case

This section explains, in depth, one of the simulations mentioned in section 4.2. The case with the pilot injection at $40^0$ BTDC and main injection at $5^0$ BTDC, as shown in Figure 4.3, is explained in detail here. The operating conditions were similar throughout the simulations as mentioned in section 4.3.

![Figure 4.3 - Pilot injection at $40^0$ BTDC and main injection at $5^0$ BTDC](image)
Figure 4.4 illustrates the injection rate of the DME spray for pilot injection at $40^\circ$ BTDC and main injection at $5^\circ$ BTDC. 10% of the total mass is injected during pilot injection and remaining 90% during main injection. The duration of injection for DME is longer due to its low heating value compared to diesel, which necessitates increased volume of liquid. Figure 4.5 shows the in-cylinder pressure trace for a firing cycle and the motored pressure trace collected at the same engine operating conditions. The difference between the two pressure traces indicates the extent of energy release from combustion. From the pressure traces, it is evident that there is significant heat release from the pilot injection even before the onset of main injection.

The heat release rate curve is shown in Figure 4.6. The initial peak in heat release is around $15^\circ$ BTDC, followed by a lower peak before the main injection. Both of these peaks are due to combustion of the pilot injection. Combustion of the main injection is noted only after TDC. An important aspect is to understand the manner in which the combustion of the pilot charge modifies the in-cylinder temperature and concentration fields at the time of main injection. Two types of modifications take place, namely an
Figure 4.4 - Injection rate for pilot injection at 40° BTDC and main injection at 5° BTDC

Figure 4.5 - Pressure curve for pilot injection at 40° BTDC and main injection at 5° BTDC
increase in temperature and change in concentration, which includes products, such as 
CO₂, H₂O and other intermediate species, which might have an effect similar to EGR. 
Both of these modifications can influence the combustion of the main injection.

![Figure 4.6 – Heat release rate for pilot injection at 40° BTDC and main injection at 5° BTDC](image)

The reason for two distinct heat release curves for pilot injection is temporal 
separation of the first and second stage heat release. This is discussed in the following. 
The maximum temperature in the cycle and the concentrations of formaldehyde, DME, 
and CO are shown in Figure 4.7 and 4.8. The concentrations in Figure 4.8 are scaled for 
clarity. From these plots, it is clear that the first peak in heat release at 15° BTDC is due 
to the first stage ignition of the pilot injection. During this phase, significant amount of 
formaldehyde is produced due to low temperature reactions involving peroxidation. 
Furthermore, the rise in maximum temperature is small as the peak temperature remains 
less than 1000 K even after the first peak in heat release. Following the first stage
ignition, the peak temperature reaches 2500 K at around 11° BTDC, which is followed by a second, smaller peak in the heat release. This indicates that the second peak in heat release is due to the second stage or hot ignition during which combustion in the part of the domain goes to completion.

![Diagram](image)

**Figure 4.7 - Maximum temperature curve for pilot injection at 40° BTDC and main injection at 5° BTDC**

The second stage ignition is, however, highly non-uniform and occurs only in part of the domain. This is based on the observation that the concentration of CO remains significant as well as formaldehyde persists. Persistence of these species is a clear indication that some regions in the domain are over-mixed and do not allow for the second stage ignition to occur. It has important implications for emissions as the CO and HC in the over-mixed region, which did not undergo hot ignition, might not burn even during the main injection and lead to engine out CO and HC emissions. The heat release
following main injection, Figure 4.6, is typical of diesel combustion where a premixed burning phase is followed by the mixing controlled combustion as spray continues. The premixed burning phase here, however, has only peak as the cylinder temperature is high and the first stage and hot ignition are not temporally separated.

![Graph showing maximum temperature, formaldehyde (CH₂O), CO, and DME concentration on heat release rate (HRR) with crank angle.]

Figure 4.8 - Effect of maximum temperature, Formaldehyde (CH₂O), DME and CO on Heat Release Rate (HRR)

Spray penetration and DME vapor mass fraction following pilot and main injection is shown in Figure 4.9 and 4.10, respectively. The pilot injection is targeted in the squish region. The larger and colder droplets are closer to the injector. As they travel away from the injector, they are broken down and evaporated, due to the rise in the temperature by absorption of heat from the surrounding gases and finally fuel is converted from liquid state to gaseous state. Once it is gasified, it keeps mixing with the gases that are already present in the cylinder.
Figure 4.9 - Spray penetration and spray vaporization in the cylinder after the pilot injection at 40° BTDC and before main injection at 5° BTDC
Crank angle 2.01738° ATDC

Crank angle 6.00365° ATDC

Crank angle 22.0162° ATDC

Figure 4.10 - Spray penetration and vaporization inside the cylinder after the main injection at 5° BTDC
Figure 4.11 – Temperature distribution (K) inside the cylinder after pilot injection
In Figure 4.9, DME vapors are observed only close to the wall. This is, however, misleading because the mass fraction shown is only in the plane of injection, whereas, DME vapors are convected in the direction of swirl. Before the main injection, all the fuel injected during pilot injection mixes completely with the gas/air present in the cylinder. Main injection starts at 5\(^0\) BTDC.

The main injection is targeted in the bowl where it burns as also noted by temperature fields shown in Figure 4.11. Since the first injection is targeted in squish, which may not be ideal, additional studies could be conducted by changing the spray umbrella angle.

![Graph of CO production vs Crank angle](image.png)

**Figure 4.12 – CO production for pilot injection at 40\(^0\) BTDC and main injection at 5\(^0\) BTDC**

Production of CO and NO\(_x\) with crank angle in the case of pilot injection at 40\(^0\) BTDC and main injection at 5\(^0\) BTDC is shown in Figures 4.12–4.13. Significant CO
concentration is noted before the main injection and is attributed to incomplete pilot combustion due to over-mixing. During the main combustion, CO increases as fuel is progressively broken down and then decreases as it is oxidized. Significant NO\textsubscript{x} formation starts after the TDC where maximum temperature above 2500 K is attained. NO\textsubscript{x} concentration increases rapidly and later remains stable as shown in Figure 4.13.

![Figure 4.13 – NO\textsubscript{x} production for pilot injection at 40\textdegree{} BTDC and main injection at 5\textdegree{} BTDC](image)

CHAPTER V

RESULTS AND ANALYSIS

This research has been carried out taking into account two main constraints: NO\textsubscript{x} and CO emissions (for example, under EURO VI limits for HD diesel engines; NO\textsubscript{x} < 0.4g/KWh and CO < 1.5g/KWh). In order to fulfill the above constraints, injection strategy can be optimized. As discussed earlier in chapters 3 and 4, the engine operating conditions and setting were kept constant except for the fuel injection timings and ratios.

NO\textsubscript{x} is a combination of nitrogen monoxide and nitrogen dioxide. Formation of oxides of nitrogen is a side effect of combustion. Being strongly bonded, molecular nitrogen requires high temperature and oxygen for the formation of NO\textsubscript{x}. In direct-injection CI engines, NO\textsubscript{x} primarily forms outside the sprays, where the temperature is high and where the hydrocarbons competing with nitrogen for oxygen are lower (Teng, et al., 2006).

5.1 Influence of Change in Pilot Injection Timing

The influence of change in pilot injection timing is discussed in the following. Fuel is injected in two stages, namely a pilot injection (10% of total mass of the fuel) and a main injection (90% of total mass of the fuel) at 5\textdegree BTDC. Figure 5.1 shows the effect on combustion with and without pilot injection. It can be observed that the pressure rise in
the case of pilot injection is more than that with single injection. It occurs due to the heat release attributed to the pilot injection.

Figure 5.1 – Pressure profiles with pilot injection at $40^0$ BTDC, single injection and motored curve

Figures 5.2-5.4 show the effect of pilot injection timing on the combustion and emission characteristics at the main injection timing of $5^0$ BTDC. Specifically, the pressure traces, heat release rate, peak temperature, and CO and NOx emissions are shown here. There is not much difference in the peak pressure and temperature for different pilot injection timings, however, the rate of heat release for pilot combustion increases and the separation between the first-stage and hot ignition of pilot fuel decreases as pilot injection is delayed, as noted in Figure 5.3 (a). On the other hand, the heat release profiles during the combustion of main injection (after TDC) are virtually
identical. It may be inferred that for the main injection timing of $5^\circ$ BTDC, there is no significant effect of pilot injection timing on combustion.

![Pressure profiles at various pilot injection timings](image)

Figure 5.2 - Pressure profiles at various pilot injection timings

Regarding emissions, there is significant effect of pilot injection timing on CO emissions as is evident from Figure 5.4 (a), even though the peak temperatures in all cases are similar. Generally, the injected fuel at an advanced injection timing leads to piston wall wetting due to the low ambient temperature and pressure in conventional diesel engines. However, the DME spray evaporates rapidly after the start of injection due to the volatile properties of the DME fuel and then fuel and air in the cylinder are mixed until autoignition. The difference in CO emissions here is attributed to spray targeting in the squish region as well as longer ignition delay for advanced pilot injection, which can lead to over-mixing and consequent incomplete combustion and higher CO emissions. Ignition delay is the duration between the start of injection and discernible
heat release, which can be deduced from Figure 5.3 (a) and is noted to decrease as pilot injection is delayed. In contrast, NO\textsubscript{x} emissions from all cases are similar due to similar peak temperature.

(a) Heat release rate (HRR) profiles for various pilot injection timings

(b) Maximum temperature curves for pilot injection

Figure 5.3 – Heat release and peak temperature at various pilot injection timings.
(a) Comparison of CO formation for various pilot injection timings

(b) Comparison of NO\textsubscript{x} emission for various pilot injection timings

Figure 5.4 - Emissions at various pilot injection timings.
Figure 5.5 - Comparison of temperature, CO mass fraction and O₂ mass fraction distribution at 6° BTDC with respect to various pilot injection timings
Pilot injection at 40° BTDC

Pilot injection at 30° BTDC

Pilot injection at 20° BTDC

Pilot injection at 10° BTDC

Figure 5.6 - Comparison of temperature, mass fraction of CO and mass fraction of O₂ distribution at 12° ATDC
Figures 5.5-5.6 show a comparison of temperature, mass fraction of CO and O\textsubscript{2} inside the cylinder after pilot injection and main injection, respectively, for all the four cases. Figure 5.7 shows the distribution of NO\textsubscript{x} after the main injection for all the four pilot injection cases. Similar features are seen in all cases.

NO\textsubscript{x} and CO emissions are summarized in Figures 5.8-5.9. It has been noted that the low boiling point of DME can have positive effects on the CO emissions, because evaporation of fuel drops in DME spray is much faster than in diesel spray for the same cylinder pressure and temperature (Paolo et al., 2001; Lim, 2014). With an appropriate pilot-main injection strategy, the pilot injection timing must be adjusted carefully because an advanced pilot injection can lead to increased CO emissions resulting from over-
mixing. From the present study, it is unclear if the increase in CO emissions for advanced pilot injection is solely due to over-mixing or also due to spray in the squish region. More simulations with different injection angle are necessary to confirm this.

Figure 5.8 - NO$_x$ emission index with pilot injection timing

Figure 5.9 - CO emission index with pilot injection timing
5.2 Effect of Changing Split Injection Timing

As discussed in chapter 4, for the spilt injection cases, 20% of the fuel mass is injected into the cylinder before the main injection and remaining at 5\(^{0}\) BTDC. The effect of variation in the first injection timing on the pressure, maximum temperature, heat release rate, NO\(_x\) formation and CO formation is shown in Figures 5.10 -5.12. The peak pressures in Figure 5.10 are same for all cases.

![Pressure traces for various split injection cases](image)

Figure 5.10 –Pressure traces for various split injection cases

The heat release rate profiles, Figure 5.11 (a), show distinct two stage ignition of the first injection for 40\(^{0}\) and 30\(^{0}\) BTDC injection. In contrast, the distinction is not clear for the 10\(^{0}\) BTDC case due to higher cylinder temperature at injection. In addition, for the 10\(^{0}\) BTDC case, the ignition dwell (duration between the end of first injection and the start of combustion) is negative which leads to more diffusive combustion of the first injected
charge. The heat release profiles after the TDC are identical for all cases, indicating that the first injection timing does not influence the main heat release.

![Heat release rate and maximum temperature for split injection cases](image)

(a) Heat Release Rate (HRR)

(b) Maximum temperature traces

Figure 5.11 – Heat release rate and maximum temperature for split injection cases
Figure 5.12 – NO\textsubscript{x} and CO formation for split injection cases
The maximum temperature, in Figure 5.11 (b), for the $10^0$ BTDC injection case is higher than other cases and it also manifests as increased NOx emissions as noted in Figure 5.12 (a). It is known that NOx is formed in the region of high temperatures. The NOx level freezes at a near-maximum value at about $40^0$ ATDC as the piston expansion lowers the charge temperature. Therefore, the high temperature zones during the early combustion period have important effect on the NOx formation rate. Similar to the pilot injection case, increased CO emissions are noted for advanced first injection in Figure 5.12 (b).

Figure 5.13 shows the comparison of temperature, mass fraction of CO and NOx for all the split injection cases at $12^0$ ATDC. Consistent with the results presented in Figures 5.11-12, maximum temperature in the piston bowl and higher NOx concentrations are observed with split injection at $10^0$ BTDC. Emissions of CO and NOx vs the split injection timing, Figures 5.14-15, show a trade-off relation between the two, where in delayed first injection leads to a decrease in CO at the expense of increase in NOx.
Figure 5.13 – Comparison of temperature, mass fraction of CO and NO\textsubscript{x} distribution inside the cylinder after main injection at 12\textdegree\ ATDC
Figure 5.14 - NO\textsubscript{x} emission index vs split injection timing

Figure 5.15 - CO emission index vs split injection timing
5.3 Influence of Changing Main Injection Timing

Split-main injection of DME has the potential to reduce NO\(_x\) emissions with combustion phasing retardation regardless of the dwell time between the split injection and main injection timing. The main injection timing has to be retarded after TDC for the pilot and split injection technique to be effective for the reduction of NO\(_x\) (Jeong et al., 2014). To evaluate the effect of main injection timing on the emissions, several cases were simulated in which 20% of the total mass was injected at 20\(^\circ\) BTDC and remaining during main injection as discussed previously in chapter 4.

Figure 5.16 shows a comparison of pressure traces for motored curve, single injection cases and split injection cases for various main injection timings. It is noted that as the main injection timing is retarded, the combustion for the case of single injection occurs later during the expansion stroke. This will lead to large cycle to cycle variability and unstable combustion with high HC and CO emissions for single injection. On the other hand, with split injection, the combustion of the main charge is expected to be stable even with moderately retarded main injection. This is because the temperature and pressure rise due to the first injection boosts the reactivity of the main injection. The difference between single and split injection becomes more pronounced as the main injection is retarded. For instance, for main injection at 10\(^\circ\) ATDC (although unrealistic for actual engine operation), the single injection does not manifest any heat release and misfire occurs.

Pressure curves for different main injection timing, while keeping the first injection at 20\(^\circ\) BTDC, are shown in Figure 5.17. For main injection at 5\(^\circ\) BTDC and later, the
pressure profiles up to TDC are identical. The difference in profiles after TDC implies that retarded injection will entail an efficiency penalty.

![Graphs showing pressure profiles for different injection timings](image)

Figure 5.16 - Comparison of single and split injection at various main injection timings

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Figure 5.17 - Pressure curves for main injection at $-10^0$, $-5^0$, $0^0$, $5^0$, $10^0$ ATDC

The maximum temperature and heat release curves are shown in Figure 5.18. For too retarded main injection, heat release rises at a slower rate. An interesting observation in temperature profiles is the cooling of the cylinder charge between two injections. This is evident for main injection at TDC and later. It has significant implications for CO and NO$_x$ emissions as discussed in the following.

CO and NO$_x$ emissions are plotted in Figure 5.19, showing that the main injection timing has significant influence on NO$_x$. In the case of split injection, combustion and NO$_x$ formation is influenced by the main injection. During the pause period between the first and second injection, the combustion gas cools, and the reaction of the DME-air mixture is controlled. Also, the division of injection into two installments suppresses the potential for high pressure and high temperature conditions under which NO$_x$ is actively formed. The effective charge temperature in the split injection is low when main injection
is retarded because more fuel is burned at a retarded crank angle and there is cooling of charge between two injections.

Figure 5.18 – Maximum temperature and Heat Release Rate (HRR) for various main injection timings
Figure 5.19 – NOx and CO formation for various main injection timings
High temperature is produced as shown in Figure 5.18, when main injection is at \(10^\circ\) BTDC which results in increased production of NO\(_x\). These results are in general agreement with experimental work of Jeong et al. (2014).

Retardation of the main injection timing, with fixed split injection timing, results in an increase in CO emissions as shown in Figure 5.19. This is due to late burning during the expansion stroke which results in rapid drop in temperature and freezing of CO oxidation. Temperature and mass fraction of CO and NO\(_x\) at \(22^\circ\) ATDC are shown in Figure 5.20 for various main injection timing. Most significant in this Figure is the reduction in temperature and NO\(_x\) concentration with increased retardation of main injection. NO\(_x\) and CO emission indices are summarized in Figures 5.21-22. There is a trade-off relation between the two. However, it is clear that, in contrast to a single injection strategy, split injection offers potential for moderately retarded main injection with significant reduction in NO\(_x\) without excessive increase in CO. Kim et al. (2008) also reported that in the case of split injection, main injection at later timings produces negligibly low level of NO\(_x\) emission.
Figure 5.20 - Temperature, mass fraction of CO and NOx at 22° ATDC
Figure 5.21 - NOx emission vs main injection timing

Figure 5.22 - CO emissions vs main injection timing
5.4 Comparison of Specific Emissions

As shown in Figure 5.23 NO\textsubscript{x} were high in the case of split injection case in comparison to pilot injection. CO emissions are almost similar in pilot and split injection cases. By retarding the main injection timing NO\textsubscript{x} emissions decreases but CO emissions increased; there is a tradeoff between NO\textsubscript{x} and CO emissions.

Figure 5.23 - Comparison of specific NOx and CO emissions for pilot and split injection
5.5 Indicated Efficiency

As shown in Figure 5.24, the indicated efficiency was slightly higher for split injection than with the pilot injection. Further, the efficiency decreased as the main injection was retarded. In addition, the efficiency for split injection was higher than single injection.

(a) Comparison of indicated efficiency for pilot and split injection timings

(b) Comparison of indicated efficiency for single injection and change in main injection timing

Figure 5.24 - Indicated efficiency for change in first and main injection timing
CHAPTER VI
CONCLUSIONS AND FUTURE WORK

6.1 Conclusions

In this work, a computational investigation is conducted to understand the influence of injection strategy on pollutant formation in a DME fueled CI engine. DME is a potential alternative and renewable fuel for CI engines and offers several advantages such as high cetane number, soot-free combustion due to absence of C-C bond and it is liquid at moderate pressure.

Computational Fluid Dynamic (CFD) simulations of a DME fueled CI engine sector were conducted with detailed chemistry by using the Converge CFD package. The simulations provided temporal and spatial evolution of various species and temperature as well as pressure and heat release rates. Specifically, after the validation of the engine model, effect of pilot and split injection strategy on pollutant formation was assessed.

In the pilot injection strategy, 10% mass of the total fuel was injected during pilot injection at 40°, 30°, 20° and 10° BTDC and the remaining in the main injection at 5° BTDC. These simulations revealed that the NOx emissions are not sensitive to pilot injection timing over the parametric range studied here, whereas, CO emissions increased with advanced pilot injection. This was due to the combined effect of spray targeting in the squish region for advanced pilot injection as well as over-mixing resulting from
increased ignition delay for advanced injection. The combustion phasing as well as the heat release rate of the main injection charge, however, was not influenced by the variation in the pilot injection timing.

Split injection strategy was studied by injecting 20% mass of the fuel during first injection at 40\(^0\), 30\(^0\), 20\(^0\) and 10\(^0\) BTDC and the remaining in the main injection at 5\(^0\) BTDC. It was noted that, for advanced first injection, DME showed a distinct two-stage ignition characteristics. The heat release rate of the main injection, however, was not influenced by the variation in the first injection timing. NOx emission increased and CO decreased as the first injection timing was retarded.

Following the above study, the effect of variation in the main injection timing was investigated by injecting 20% of the fuel mass at 20\(^0\) BTDC and remaining at different times ranging from 10\(^0\) BTDC to 10\(^0\) ATDC. These simulations were also compared with corresponding single injection cases. As the main injection was retarded, NOx emissions decreased significantly and CO emissions increased. It was also noted that, in contrast to single injection, a split injection strategy allows for moderately retarded main injection with significant reduction in NOx emissions without excessive increase in CO. This is because the temperature and pressure rise due to the first injection boosts the reactivity of the retarded main injection and, at the same time, the duration between the two injections allows for cooling of the cylinder gas and lower maximum temperature, thereby reducing NOx.
6.2 Recommendations for Future Work

The following computational investigations are recommended in the near future.

1. Present investigation was conducted without any EGR. At moderate load, EGR can be used to reduce NOx with increase soot with DME. Investigations are recommended with EGR.

2. Investigations were conducted at moderate fuel MEP of around 19 bar. Investigations at higher load are recommended.

3. The NOx formation mechanism in the present study was not validated and led to unrealistically low NOx levels. Study with more realistic and adequately validated NOx chemistry is warranted.
REFERENCES


Yao, M., and Qin, J. (2004) Simulating the Homogeneous Charge Compression Ignition Process Using a Detailed Kinetic Model for Dimethyl Ether (DME) and Methane Dual Fuel. SAE Paper, 01-2951.


