Abstract
Homogeneous Charge Compression Ignition (HCCI) combustion is a pioneer method of combustion in which pre-mixed fuel and oxidizer (typically air) are compressed to the point of auto-ignition. HCCI engines can operate with most alternative fuels, especially, dimethyl ether (DME) which has been tested as a possible diesel fuel due to its simultaneously low NOx and PM emissions. In this paper a single zone detailed chemistry combustion model for determining the time evolution of the homogenous reacting gas mixture in the combustion chamber and performance characteristics of the engine has been developed. The aim of this paper is to analyse the effect of intake temperature and EGR on the characteristics of auto-ignition and operating window of the HCCI combustion considering knock and misfire boundaries.

Keywords: Dimethy Ether, Multi Zone Combustion, Emissions, Disel Engine, Modeling
1. Introduction

There is an interest in improving motor vehicle fuel economy while complying with emissions regulations. Naturally diesel engines have improved fuel economy compared to gasoline vehicles, but it is difficult to control NOx and particulate matter according to proposed future emissions standards. As modern spark ignition engines operate at stoichiometric conditions, NOx emissions are controlled by a three-way catalytic converter and particle emissions are low. Since diesel engines operate fuel lean, control of NOx by a catalyst would be difficult. Diesel particulate emissions are higher than from spark ignition engines and can be reduced via traps, fuel additives, or changes in engine operating strategy.

Several recent publications have presented results from diesel engines or diesel vehicles operated on pure DME [1 and 2]. These experiments showed that DME is an excellent alternative to diesel fuel [3-5] which produces very low particulate and soot emissions. Also the amount of NOx formation in DME mode operation is less than current diesel engines under the same engine operating conditions.

This allows the engine operating conditions to be adjusted to further reduction of NOx without an accompanying increase in particulate emissions. DME physical and chemical properties compared with diesel oil are shown in table 1. The properties of DME can be summarized as follows:

- DME has only C-H and C-O bonds without C-C bonds and contains about 34.8% oxygen. Therefore, the combustion produced emissions with DME fuel, such as smoke and PM, are expected to be lower than those using diesel fuels. An engine with DME fuel can tolerate more EGR rate to reduce NOx [7 and 8].
- The lower heating value of DME is only 64.7% of that of diesel fuel; therefore larger amount of fuel supply per cycle is needed to ensure the same engine power.
- The cetane number of DME is higher than that of diesel fuel and other alternative fuels. Therefore, there is no need for an ignition assisted system as used for methanol, ethanol, and LPG and CNG engines.
- DME is in gaseous state even at -20 °C and ambient pressure. Its Reid vapor pressure varies with the temperature. Therefore, DME needs to be pressurized to over 0.5 MPa to keep it in liquid state under ambient temperature (25°C). The fuel delivery pressure should be increased to 1.7-2.0 MPa under engine operating conditions to prevent from vapor lock in fuel system.
- The latent heat of evaporation of DME is much higher than that of diesel, which is beneficial to the NOx reduction due to lower mixture temperature [8].

The objectives of this study are to investigate the performances and combustion characteristics of a heavy duty truck engine operating on DME. So a quasi steady, multi zone model has been used for performance characteristics and emission production analysis of a heavy duty truck engine powered by DME. The effects of combustion system parameters on engine performances have also been studied.

<table>
<thead>
<tr>
<th>Properties</th>
<th>DME</th>
<th>Diesel</th>
</tr>
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<tbody>
<tr>
<td>Chemical formula</td>
<td>CH₃O-CH₃</td>
<td>CH₃</td>
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<tr>
<td>Mole weight, g</td>
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<td>Boiling point, °C</td>
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<td>Explosion limit in air, %</td>
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<td>0.6-6.5</td>
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<td>250</td>
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<td>40-55</td>
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<td>14.6</td>
</tr>
<tr>
<td>%wt of Oxygen</td>
<td>34.6</td>
<td>0</td>
</tr>
<tr>
<td>%wt of Carbon</td>
<td>52.2</td>
<td>86</td>
</tr>
</tbody>
</table>

2. Model descriptions

2.1. Assumption

For injection process simulation, following assumptions have been made:

1- Injection zone modeling was done based on Modified Hiyasu model because of its accuracy and precision. [9]
2- It was assumed that, there is no impingement of the injected fuel into the wall.

As mentioned in the introduction of this paper, the model to be presented is a multi zone one, which means that the resulting jet is divided into discrete volumes, called zones during fuel injection. The number of axial zones is determined by the duration of the fuel injection period and the calculation time step used, while the number of radial zones is determined by making trials and finding the number from which a further increase causes no modification in the model results. In the present study, 80 axial zones and 5 radial zones have been considered for injected spray modeling.

Based on these assumptions, the detailed description of the model is as follows.

2.2. Spray submodel

After the initiation of fuel injection, the zones begin to form and penetrate into the combustion chamber. The Initial conditions at the nozzle exit are obtained from the fuel injection process simulation. The Initial jet velocity is calculated as follows:

\[ u_0(t) = \frac{4 \dot{m}_f(t)}{n_s \pi d_{inj}^2 \rho_1} \]  

(1)

Where \( n_s \) and \( d_{inj} \) are the number and diameter of the nozzle holes and \( \rho_1 \) is the density of the DME.

Similarly to diesel operation, it is supposed that DME fuel initially travels a small distance inside the cylinder before breaking up into droplets. Here, the break up length is computed by the same equation as with diesel operation [9 and 10], but the constant \( C_1 \) is much smaller.

\[ S_h = C_1 \left( \frac{\rho_1}{\rho_0} \right)^{0.5} d_{inj} \]  

(2)
\( \rho_a \) is surrounding air density.

\( C_1 \) is an experimental factor which is related to fuel characteristics.

The velocity along the spray axis is determined by the following equation [9]

\[
\begin{align*}
  u_{ij} &= u_0(t_i) \left\{ \begin{array}{ll}
    S_y \leq S_b & \\
    S_y > S_b & 
  \end{array} \right. \\
  &= u_0(t_i) \left( \frac{S_b}{S_y} \right)^\eta, \quad S_y > S_b
\end{align*}
\]  

(3)

It should be pointed out that \( t_i \) in equation (3) represents the moment at which local zone injects into the cylinder.

Concerning the radial velocity component of the zones, the initial value for all zones formed at a given time step is given by the equation

\[
  u_{ri} = u_a \tan \left( \frac{\alpha r_i}{r_o} \right)
\]

(4)

Where \( r_o \) is the radius of the nozzle hole and \( r_i \) is the radial distance of zone \( i \) from the center line. The initial spray angle of DME, which is used in equation (4), is obtained from the following relation [10]

\[
\alpha = 0.10 \left( \frac{d_{inj}^2 \rho_a \Delta p}{\mu_a} \right)^{0.25}
\]

(5)

Where \( \Delta p \) the pressure difference across the injector hole and \( \mu_a \) the dynamic viscosity of the air.

2.3. Mass entrainment submodel

The mass entrainment of zones is calculated on the basis of the momentum conservation principle

\[
\frac{dm_z}{dt} = -\frac{m_z}{u_z} \frac{du_z}{dt}
\]

(6)

Cui et al. [11] show that the air entrainment process in the cylinder is related not only to the fuel injection process but also to the excess air ratio, which means that the mixing takes place between various zones, not just between fresh air and fuel zones. This view is also verified by the experiments. Therefore, the method for calculating mass entrainment presented in reference [11] is adopted in this study. In this method, zones in a cylinder are classified into three groups: the fresh air group, the pollutant gas group and combustion group. Therefore, the combustion zone \( i \) entrains fresh air and burned gas

\[
\frac{dm_{c_i,a}}{dt} = \frac{dm_{c_i,a}}{dt} + \sum_{j=1}^{f} \frac{dm_{c_i,p_j}}{dt}
\]

(7)

Where \( \frac{dm_{c_i,a}}{dt} \) is derived from equation (6), and

\[
\frac{dm_{c_i,f}}{dt} = \frac{dm_{c_i,f}}{dt} \times \frac{(1-\eta)m_a}{(1-\eta)m_a + \eta m_p}
\]

(8)

Here, \( \eta \) is the coefficient of pollutant entrainment.

The pollutant gas zone \( p_j \) entrains fresh air and is entrained by combustion zones

\[
\frac{dm_{p_j}}{dt} = \sum_{i=1}^{l} \frac{dm_{p_j,c_i}}{dt} + \frac{dm_{p_j,a}}{dt}
\]

(9)

Where \( \frac{dm_{p_j}}{dt} \) is derived from equation (6), and

\[
\frac{dm_{p_j,c_i}}{dt} = -\frac{dm_{p_j,c_i}}{dt}
\]

(10)

The mass change in the fresh air zone can be derived from equations (7) and (11)

\[
\frac{dm_a}{dt} = \sum_{i=1}^{l} \frac{dm_{a,c_i}}{dt} + \sum_{j=1}^{f} \frac{dm_{a,p_j}}{dt}
\]

(11)

The changes in composition and internal energy of each zone that are caused by the mixing between zones can be determined by the same method.

2.4. Heat transfer submodel

Heat transfer to the combustion chamber walls is calculated by Woschni equation

\[
\frac{dQ_w}{d\phi} = \frac{1}{6a} \sum_{i=1}^{3} \alpha A_i (T_{wi} - T)
\]

(14)

\[
\alpha = 265D^{-0.214} (vP)^{0.786} T^{-0.525}
\]

(15)

where \( v \) shows the piston speed, \( P \) is the pressure in the cylinder and the units of \( D, v, P \) and \( T \) are m, m/s, 10^5 Pa and K respectively.

Then, the heat flux is distributed among zones according to the weight factor of each zone

\[
\frac{dQ_{z,w}}{dt} = \frac{dQ_w}{dt} \sum_{z} W_z
\]

(16)
2.5. Combustion submodels

After injection of the liquid fuel, fuel jet atomizes into small-sized droplets to enable rapid evaporation. For better understanding the ignition delay, thermodynamic analysis of the fuel droplets is required. Rate of change in the droplet’s mass is calculated by:

$$\frac{dm_{\text{drop}}}{dt} = - \frac{d}{dt} \left( \frac{\pi}{6} D^3 \rho_{F} \right) = \frac{\pi}{4} \rho_{F} D \beta$$  \hspace{1cm} (17)

where $D$ shows the droplet diameter, $\rho_{F}$ is the droplet density and $\beta = \frac{dD^3}{dt}$ which also can be written as $\beta = \frac{d}{dt} \left( \frac{m_{\text{drop}}}{A_{\text{drop}}} \right)$.

In this equation $A = \pi D^2$ and $\beta$ shows the quick evaporation rate of the droplet. Regarding to the fact that, mass flow rate of the fuel by evaporation process on the droplet area can be written as: $m_{F,S} = \frac{\left( \frac{dm_{\text{drop}}}{dt} \right)}{A_{\text{drop}}}$

the evaporation rate of the droplet can be written as:

$$\beta = 4D \frac{m_{F,S}}{\rho}$$ \hspace{1cm} (18)

Because the critical temperature of DME is only 127 °C, which is lower than the compressed-air temperature at the later stage of the compression stroke, the DME injected into the cylinder may vaporize immediately due to the fact that a liquid phase is thermodynamically unstable above the critical temperature. When the temperature of DME is greater than 127 °C, DME becomes a superheated gas and, therefore, no evaporation is associated during mixing. The combustion delay time of the injected fuel is calculated using modified Hiroyasu-Nishida equation [6]:

$$\tau_z = 0.003 p^{-2.5} \varphi_2^{1.04} \exp \left( \frac{4000}{T_z} \right)$$ \hspace{1cm} (19)

Burned mass gas is calculated via [12]:

$$m_{fb} = \min \left( m_{fb}, \frac{m_{\text{gas}}}{I_0} \right)$$ \hspace{1cm} (20)

The rate of heat release is calculated by:

$$\dot{Q} = H_u m_{fb}$$ \hspace{1cm} (21)

3. Modeling of Nitric Oxide formation

The DME operation is very clean, since almost no soot is produced even under heavy loads. However, there is no complete agreement in the literature for nitric oxide, another main pollutant of CI engines. Sorenson et al. reported much lower NO, with DME [2], whereas Kajitani et al. reported NO emissions approximately the same as for diesel fuel operation [4]. In this study extended Zeldovich [12] model has been used for NO, formation modeling because of its widespread usage and simplicity.

$$N + O_2 \leftrightarrow NO + O$$

$$NO + N \leftrightarrow O + N_2$$

$$OH + N \leftrightarrow NO + H$$

4. Modeling of soot formation

Hiroyasu model has been used for soot formation production [13].

$$\left( \frac{dm_{s,i,j}}{dt} \right)_F = A_f \left( m_{\text{inj,i,j}} - m_{d,i,j} \right) \rho^{0.5} \exp \left( - \frac{E_{sf}}{R_u T_{i,j}} \right)$$ \hspace{1cm} (22)

where $E_{sf} = 1.25 \times 10^4$ kcal/mol

$m_{s,i,j}$ is soot mass in zone [i,j] and $A_f$ is constant that are determined by experimental data.

Soot oxidation model investigated in this study is the Nagle and Strickland-Constable oxidation model. The NSC oxidation model is based on oxidation experiments of carbon graphite in an O$_2$ environment over a range of partial pressure. In this model, carbon oxidation occurs by two mechanisms whose rates oxidation occurs by two mechanisms whose rates A sites and less reactive B sites [14]. The chemical reactions are:

$$A + O_2 \leftrightarrow A + 2CO$$

$$B + O_2 \leftrightarrow A + 2CO$$

$$A \leftrightarrow B$$

The soot oxidation rate will be calculated from:

$$\left( \frac{dm_{s,i,j}}{dt} \right)_O = \frac{MW_C}{\rho_s d_s} m_{s,i,j} w$$ \hspace{1cm} (23)

Therefore

$$\frac{dm_{s,i,j}}{dt} = \left( \frac{dm_{s,i,j}}{dt} \right)_F - \left( \frac{dm_{s,i,j}}{dt} \right)_O$$ \hspace{1cm} (24)

where $MW_C$, is molecular weight of carbon, $\rho_s$, is soot density (2.0 g/cm$^3$), $d_s$, is soot diameter (4.5 $\times$ 10$^{-6}$ m) and $w$ is net reaction rate of proposed reactions mentioned above. This factor is calculated from the method mentioned in [14] and is not presented here.
5. Experimental analysis

In this study the simulation results were validated with experimental results presented in SAE paper [6]. Since in the engine test the indicatory diagram wasn’t achieved, the results of another experiment were used to validate the simulated pressure diagram.

The test engine used in this analysis was a water cooled, four cylinder, four stroke naturally aspirated, direct injection diesel engine (Daimler Chrysler motor type, OM314) which is locally produced in I.D.E.M. Co and installed on different models of trucks and buses. The specifications of the engine are shown in table 2. Significant effort was directed at overcoming difficulties with DME leakage in the fuel injection system and at modifying the fuel system to provide the appropriate injection characteristics.

DME is kept in liquid state in the tank in the pressure range of 5-10 bar. Then the fuel pressure is increased up to 300 bar by a geared pump.

<table>
<thead>
<tr>
<th>TABLE 2: Specifications of the test engine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cylinder number</td>
</tr>
<tr>
<td>Piston Bore (mm)</td>
</tr>
<tr>
<td>Stroke (mm)</td>
</tr>
<tr>
<td>Compression ratio</td>
</tr>
<tr>
<td>Injection pressure (bar)</td>
</tr>
<tr>
<td>Nozzle hole diameter, mm</td>
</tr>
<tr>
<td>IVO, IVC</td>
</tr>
<tr>
<td>EVO, EVC</td>
</tr>
<tr>
<td>Start of injection</td>
</tr>
</tbody>
</table>

6. Results and discussion

Fig. 1 presents a comparison of measured cylinder pressure in reference No. 6, table 3, with calculated ones. As shown, the calculated pressure traces accurately match the measured ones for load examined.

The engine speed is 1600 RPM and for this case only closed cycle, from IVC to EVO, is simulated.

<table>
<thead>
<tr>
<th>TABLE 3: Specification of engine used in Reference 6</th>
</tr>
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<tbody>
<tr>
<td>Bore</td>
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<tr>
<td>Stroke</td>
</tr>
<tr>
<td>Compression Ratio</td>
</tr>
<tr>
<td>Con-Rod length</td>
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<tr>
<td>Pressure @IJC</td>
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<tr>
<td>Injection start</td>
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<tr>
<td>Start of injection</td>
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<tr>
<td>Fuel amount per cycle</td>
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<tr>
<td>Injection shape</td>
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<tr>
<td>Injection Pressure</td>
</tr>
<tr>
<td>Temperature @ IVC</td>
</tr>
<tr>
<td>Injection duration</td>
</tr>
</tbody>
</table>

Fig. 2 shows the results of simulation and engine test. It can be seen that the calculated power error in low speed operation is less than 5% and in high engine speed is approximately 2%.

Fig. 3 shows both the calculated and experimental torque values. Results show that the highest torque in middle range speed can be predicted with less than 4% error. Table 4 shows a summary of the results.

Fig. 4 shows the results of volumetric efficiency in different engine speed at WOT. According to the simulation results, maximum value is achieved in middle speed range which consequently gives higher torque values in this operating region. It is worthwhile to mention that reduction in volumetric efficiency in high speed range will cause a proportional reduction in torque values (Figs. 3 and 4).

Considering the accuracy of the simulated results, we have calculated the in-cylinder pressure, rate of heat released and incylinder temperature in full load and also high torque operations. Figs. 5, 6 and 7 show the pressure, temperature and heat release trajectory respectively for full load and maximum torque operations. Results show 13% pressure rise in the case of full load operation.

| TABLE 4: Results of engine torque in different speed range in two cases at WOT |
|-----------------------------|-----------------------------|-----------------------------|
| Engine speed | Engine torque (experiment) | Engine torque (simulation) |
| 1300 | 45.12 | 47.37 |
| 1500 | 46.55 | 47.89 |
| 1800 | 47.28 | 48.39 |
| 2200 | 46.55 | 47.36 |
| 2400 | 45.35 | 46.06 |
| 2800 | 40.1 | 40.854 |

Fig. 1. Comparison of simulation results with experiment

Fig. 2. Comparison of the results of brake power in experiment and simulation

Fig. 3. Comparison of the results of brake power in experiment and simulation
Theoretical and Experimental Analysis of OM314 Diesel Engine Combustion and Performance Characteristics Fueled with DME

In-cylinder pressure in the case of maximum torque has occurred 2 CA earlier respect to full load operation and maximum in-cylinder temperature has decreased up to 53 °K which shows approximately 5% reduction in this case. As shown in Fig. 7, in full load operation, the portion of premixed heat released is up to 40% higher than maximum torque case which causes higher rate of pressure rise. Figs. 8 and 9 show a comparison between simulated results of power and torque diagrams for Diesel and DME operation mode in different speed conditions respectively.

It can be clearly seen that in diesel mode operation and in higher speed range (more than 2500 rpm) significant reduction of engine power occurs while in DME mode it is not remarkable. It is also predicted that, in engine speed less than 1900 rpm, maximum power and torque in diesel mode is higher, while in higher speed range (more than 1900 rpm) this would be in the contrary.

Figs. 10 and 11 show the simulated results of brake specific NOx and Soot in different speed conditions. Results show that in the worst condition, the maximum value of NOx reaches to 3.2 g/kWh and soot production in the worst case would be less than 0.45 g/kWh which indicates that, DME appears to be a promising alternative fuel for CI engine operation regarding to future exhaust emissions regulations. Significant reductions in many regulated and unregulated exhaust emissions were observed for DME operation without performing additional engine modifications directed at lowering emissions.

It should be noted that because no experimental emission data was available, exhaust emission with DME and DIESEL fuel are compared relatively based on model simulation.
7. Conclusion

Results can be summarized as follows:

• Performances and combustion characteristics of a water cooled, 4 stroke naturally aspirated, direct injection diesel engine (Daimler Chrysler motor type, OM314) operating on DME have been experimentally investigated.

• Simulation results show respectively less than 5% and 3% deviation with experimental results in predicting brake power in low engine speed and high engine speed ranges.

• Considering the accuracy of the simulated results, in-cylinder pressure and temperature diagram have been compared in the case of maximum brake torque and maximum brake power.

• In the case of maximum torque, in-cylinder pressure was occurred earlier respect to full load operation and maximum in-cylinder temperature also decreased in this case.

• In full load operation, the portion of premixed heat released was up to 40% higher than maximum torque case which caused higher rate of pressure rise.

• Results of brake power and related torque in different engine speed have been compared for DME and diesel mode operation. In diesel mode operation, a significant reduction of engine power was occurred in high speed range while in DME mode operation it was not remarkable.

Acknowledgement

The authors would like to thank National Petrochemical Company and the Research and Technology Council of National Petrochemical Company for their kind contributions and support of this project
Theoretical and Experimental Analysis of OM314 Diesel Engine Combustion and Performance Characteristics Fueled with DME

Notation

<table>
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<th>Symbol</th>
<th>Description</th>
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<td>C1</td>
<td>Constant</td>
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<tr>
<td>S_b</td>
<td>Break up length</td>
</tr>
<tr>
<td>d_inj</td>
<td>Diameter of nozzle holes</td>
</tr>
<tr>
<td>u_a</td>
<td>Local swirl velocity</td>
</tr>
<tr>
<td>m_f(t)</td>
<td>Rate of fuel injection</td>
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<tr>
<td>u_i,j</td>
<td>Axial velocity of zone [i,j]</td>
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<td>u_r,i</td>
<td>Initial value of radial velocity</td>
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<td>S_i,j</td>
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REFERENCES: