Simulation study on performance and emissions of a Small Direct Injection Diesel Engine fueled by Dimethyl Ether

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Abstract

Recently, Dimethyl ether (DME) has been considered as a potential alternative fuel for diesel engine. This paper presents a simulation study on performance and combustion characteristic of a small direct injection diesel engine fueled by DME. The engine is modeled by AVL Boost and the model is verified by experiment. Due to the difference in fuel properties, the engine power with DME is lower than that with diesel at full load, but emissions are improved. On average with DME, the engine power reduces by 51.55%. To maintain the engine power, the DME fuel mass per cycle must be increased by 39.5%. In this case, smoke, CO, and NO_x of DME engine respectively reduce 75.97%, 70.02% and 75.59% compared with those of diesel engine.

Keywords: engine simulation, alternative fuel, dimethyl ether, exhaust gas emissions.

1. Introduction

Nowadays, research and utilization of renewable fuels in order to ensure energy security and reduce pollution emissions are of interest in many countries. Among these fuels, Dimethyl Ether (DME) is a friendly - environment fuel, easy to liquefy and suitable for use in diesel engines.

DME, chemical formula is CH_3-O-CH_3, is a colorless organic compound. DME is in gaseous form at ambient pressure and temperature. To increase the energy density, DME is usually stored in liquid form under compressed pressure of 7 to 10bar. DME can be produced from a variety of raw materials such as biomass, coal and natural gas and it is considered as a clean alternative fuel in near future. Using DME for diesel engine may reduce not only dependence on fossil fuel but also environmental pollution. DME is not a nature product but a synthetic product which is produced through either dehydration of methanol or a direct synthesis from syngas. DME is now attracting great attention as an energy source for the 21st century because of its available sources, excellent physical and chemical properties and excellent storage properties. Some experimental investigations were conducted on diesel engine to clarify how DME injection characteristics affect the engine performance and exhaust emissions [1, 2]. Most of the results showed that emissions reduced significantly when fueled by DME.

The aim of this paper is to performance and emissions of DME fuelled diesel engine. A Kubota diesel engine is modeled with diesel fuel and DME by using AVL Boost software.

2. Model description

2.1. Combustion model

The combustion in diesel engine can be considered by two processes: premixed combustion and mixing controlled combustion processes[8]

$$\frac{dQ_{total}}{d\alpha}=\frac{dQ_{MCC}}{d\alpha}+\frac{dQ_{PMC}}{d\alpha} \qquad (1)$$

Q_{total}: Total heat release over the combustion process [kJ].

Q_{PMC} : total fuel heat input for the premixed combustion [kJ]

Q_{MCC}: cumulative heat release for the mixture controlled combustion [kJ]

-Ignition delay model:

The ignition delay is calculated using the Andree and Pachernegg [8] model by solving the following differential equation:

$$\frac{dI_{id}}{d\alpha}=\frac{T_{UB}-T_{ref}}{Q_{ref}} \qquad (2)$$

As soon as the ignition delay integral I_{id} reaches a value of 1.0 (=at α_{id}) at the ignition delay τ_{id} is calculated from

$\tau_{id}=\alpha_{id}-\alpha_{SOI}$.

I_{id} : ignition delay integral [-]

T_{ref} : reference temperature = 505.0 [K]

T_{UB} : unburned zone temperature [K]

Q_{ref}: reference activation energy, f(droplet, diameter, oxygen content,…) [K]

τ_{id} : ignition delay

α_{SOI} : start of injection timing [degCA]

α_{id} : ignition delay timing [degCA]

Premixed combustion model:

A Vibe function is used to describe the actual heat release due to the premixed combustion [8]:

$$\frac{\left(\frac{dQ_{PMC}}{Q_{PMC}}\right)}{d\alpha}=\frac{a}{\Delta\alpha_c}.(m+1).y^m.e^{-a.y^{(m+1)}} \qquad (3)$$

$$y=\frac{\alpha-\alpha_{id}}{\Delta\alpha_c}$$

Q_{PMC} : total fuel heat input for the premixed combustion = $m_{fuel,id}$. C_{PMC}

$m_{fuel,id}$: total amount of fuel injected during the ignition delay phase

C_{PMC}: premixed combustion parameter

$\Delta\alpha_c$: premixed combustion duration= $\tau_{id}.C_{PMC-Dur}$

$C_{PMC-Dur}$: premixed combustion duration factor

m : shape parameter m=2.0

a : Vibe parameter a= 6.9

-Mixing Controlled Combustion process:

In this regime the heat release is a function of the fuel quantity available (f_1) and the turbulent kinetic energy density (f_2):

$$\frac{dQ_{MCC}}{d\alpha}=C_{Comb}.f_1(m_F,Q_{MCC}).f_2(k,V) \qquad (4)$$

with

$$f_1(m_F,Q)=\left(m_F-\frac{Q_{MCC}}{LCV}\right).$$

$$.\left(w_{Oxygen,available}\right)^{C_{EGR}}$$

$$f_2(k,V)=C_{Rate}.\frac{\sqrt{k}}{\sqrt[3]{V}} \quad (5)$$

C_{Comb} : combustion constant [kJ/kg/deg CA]

C_{Rate}: mixing rate constant [s]

k : local density of turbulent kinetic energy [m^2/s^2]

m_F:vaporized fuel mass (actual) [kg]

LVC: lower heating value [kJ/kg]

V: cylinder volume [m^3]

α : crank angle [deg CA]

$w_{Oxygen,available}$: mass fraction of available Oxygen (aspirated and in EGR) at SOI [-]

C_{EGR} EGR influent constant [-]

$$k=\frac{C_{turb}.E_{kin}}{\dot{m}_{F,I}\left(1+\lambda_{Diff}\,m_{stoich}\right)} \quad (6)$$

E_{kin} : kinetic jet energy [J]

C_{turb} : turbulent energy production constant [-]

$\dot{m}_{F,I}$: injection fuel mass (actual) [kg]

λ_{Diff} : Air Excess Ratio for diffusion burning [-]

m_{stoich} :stoichiometric mass of fresh charge [kg/kg]

2.2. Emission model

2.2.1. NOx Formation Model

6 reactions introduced in Table. 1, which are based on the well-known Zeldovich mechanism are taken into account:

Table. 1 NO_x formation reactions

	Stoichiometry	Rate $k_i=k_{0,i}.T^a.e^{\left(\frac{-TA_i}{T}\right)}$
R_1	N_2+O= NO+N	$r_1=k_1.C_{N2}.C_O$
R_2	O_2+N= NO+O	$r_2=k_2.C_{O2}.C_N$
R_3	N+OH= NO+H	$r_3=k_3.C_{OH}.C_N$
R_4	N_2O+O=NO+ NO	$r_4=k_4.C_{N2O}.C_O$
R_5	$O_2+N_2=N_2O$+ O	$r_5=k_5.C_{O2}.C_{N2}$
R_6	OH+N_2= N_2O+H	$r_6=k_6.C_{OH}.C_{N2}$

All reactions rates r_i have units [mole/cm^{3}s] the concentrations c_i are molar concentrations under equilibrium conditions with units [mole/cm^3]. The concentration of N_2O is calculated according to:

$$C_{N2O}=1.1802.10^{-6}.T^{0.6125}.e^{\left(\frac{9471.6}{T}\right)}.C_{N2}.\sqrt{P_{O2}}$$

The final rate of NO production/ destruction in [mole/cm^{3}s] is calculated as[7]:

$$r_{NO}=C_{PostProcMult}.C_{KineticMult}.2.0.$$

$$.\left(1-\alpha^2\right)\frac{r_1}{1+\alpha.AK_2}\frac{r_4}{1+AK_4} \quad (7)$$

with

$$\alpha=\frac{C_{NO,act}}{C_{NO,equ}}.\frac{1}{C_{PostProcMult}}$$

$$AK_2=\frac{r_1}{r_2+r_3}\ , \qquad AK_4=\frac{r_4}{r_5+r_6} \quad (8)$$

2.2.2. CO Formation Model

CO formations of two following reactions given in Table. 2 are taken into account:

Table. 2 CO formation reactions

	Stoichiometry	Rate
R_1	CO+OH= CO_2+H	$r_1 = 6.76.10^{10}.e^{\left(\frac{T}{1102.0}\right)}.c_{CO}.c_{OH}$
R_2	CO_2+O= CO+O_2	$r_2 = 2.51.10^{12}.e^{\left(\frac{-24055}{T}\right)}.c_{CO}.c_{O_2}$

The final rate of CO production/ destruction in [mole/cm^{3}s] is calculated as [7]:

$$r_{co} = C_{Const}.(r_1 + r_2).(1-\alpha) \tag{9}$$

with $\alpha = \dfrac{C_{CO,act}}{C_{CO,equ}}$

2.2.3. Soot formation model

Soot formation is described by two steps including formation and oxidation. The net rate of change in soot mass m_{soot} is the difference between the rates of soot formed $m_{soot.form}$ and oxidized $m_{soot.ox}$ [7]

$$\frac{dm_{soot}}{d\varphi} = \frac{dm_{soot.form}}{d\varphi} - \frac{dm_{soot.ox}}{d\varphi} \tag{10}$$

with

$$\frac{dm_{soot.form}}{d\varphi} = A_{form}.\left.\frac{dm_{fuel}}{d\varphi}\right|_{diff}.\left(\frac{p_{cyl}}{p_{ref}}\right)^{n_1}.e^{-\frac{T_{a-form}}{T_{ave}}} \tag{11}$$

$$\frac{dm_{soot.ox}}{d\varphi} = A_{ox}.\frac{1}{\tau_{char}}.(m_{soot})^{n_2}.\left(\frac{p_{O_2}}{p_{O_2ref}}\right)^{n_3}.e^{-\frac{T_{a-ox}}{T_{ave}}} \tag{12}$$

- A_{form}: soot formation factor [-]
- A_{ox} : soot oxidation factor [-]
- τ_{char} : characteristic mixing time [^{0}CA]
- m_{fuel}: mass of fuel burned [kg]
- $T_{a\text{-}form}$: activation temp: soot formation [K]
- $T_{a\text{-}ox}$: activation temp: soot oxidation [K]
- T_{ave}: average in-cylinder temperature [K]
- p_{cyl}/p_{ref} : normalized in-cylinder press [-]
- p_{O2}/p_{O2ref} : normalized oxygen partial press [-]
- n_1, n_2, n_3 : model factor [-]

2.3. Fuel description

In this study, Dimethyl ether is defined as gas that includes CO, CO_2, H_2, HC. Properties of DME and Diesel can be specified as follow:

	DME	Diesel
Molar mass:	0.046 kg/ mol	0.17kg/mol
Lower heating value :	27.6 MJ/kg	42.5MJ/kg
Stoichiometric A/F ratio:	8.998	14.7
Carbon/: total mass ratio :	0.521	0.86
Oxygen/ total mass ratio:	0.347	0

2.4. Heat transfer model

The heat transfer to the walls of the combustion chamber, i.e. the cylinder head, the piston, and the cylinder liner, is calculated from equation [9]

$$Q_{wi} = A_i \cdot \alpha_i \cdot (T_c - T_{wi}) \tag{13}$$

Where Q_{wi} - wall heat flow, A_i - surface area, α_i - heat transfer coefficient, T_c - gas temperature in the cylinder, T_{wi} - wall temperature.

Heat transfer coefficient (α_i) is usually calculated by WOSCHNI Model, The Woschni model published in 1978 for the high pressure cycle is summarized as follows [9]:

$$\alpha_w = 130.D^{-0,2}.p_c^{0,8}.T_c^{-0,53}.[C_1.c_m + C_2.\frac{v_D.T_{c1}}{p_{c,1}.V_{c,1}}.(p_c - p_{c,0})]^{0,8} \tag{14}$$

Where C_1 = 2.28 + 0.308.c_u/c_m, C_2 = 0,00324 for DI engines, D - cylinder bore, c_m - mean piston speed, c_u - circumferential velocity, c_u = π.D.nd/60, V_D - displacement per cylinder, $p_{c,o}$ - cylinder pressure of the motored engine (bar), $T_{c,1}$

- temperature in the cylinder at intake valve closing (IVC) , $p_{c,1}$ - pressure in the cylinder at IVC (bar).

2.5. Modelling diesel engine Kubota RT140

Kubota RT140 Engine is a single horizontal cylinder, four-stroke, naturally aspirated, water cooled, DI. The engine specification is shown in Table 3, and the model is built by AVL Boost software (Fig. 1)

Table. 3 Specifications of the engine

Rating output	11kW at 2400 rpm
Maximum torque	42 Nm at 1500 rpm
Bore / Stroke	97/96 mm
Swept volume	709 cm^3
Compression ratio	18:1
Injection pressure	240 bar
Nozzle number x orifice diameter/ mm	4 x 0.30
Static injection timing	25 CA BTDC

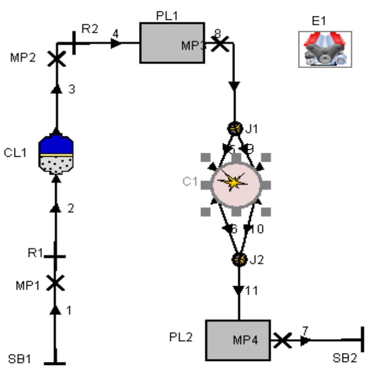

Fig. 1 Diesel engine Kubota RT140 model

3. Experiment for model validation

In order to validate the model, the experiment was carried out on engine test bed (Fig.2). The diesel engine was couple to a dynamometer which can test the engine. The engine was run at full load condition and engine speed varied from 1400 rpm to 2100 rpm [3].

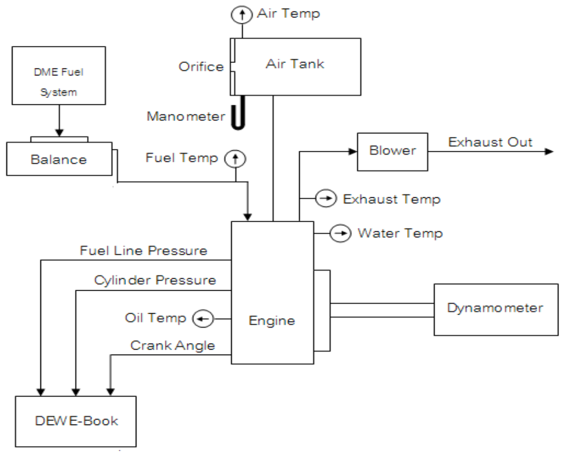

Fig. 2 Experimental lay out

4. Results and discussion

4.1. Model validation

The model has been validated by experiment in case of using conventional diesel and DME. It showed that the torque as well as fuel consumption between simulation and experiment in case of diesel matched quite well: on average the difference in torque and fuel consumption was about 1.7 % and 1.9 %, respectively. Thus, it is possible to use this model to simulate the engine with DME fuel.(Fig.3, Fig.4)

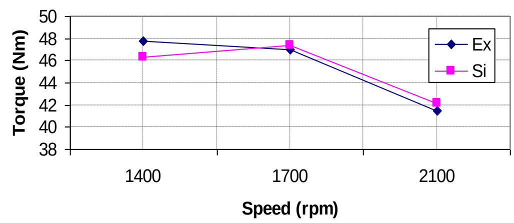

Fig. 3 Torque with diesel

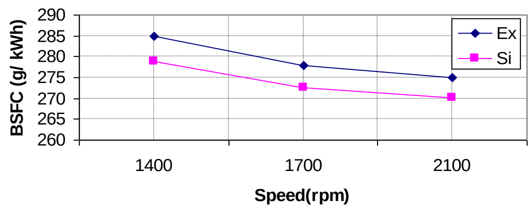

Fig. 4 Fuel consumption with diesel

In case of DME, the torque as well as fuel consumption between simulation and experiment are similar, on average the difference in torque and fuel consumption was about 1.7 % and 3.1 % (Fig.5, Fig.6)

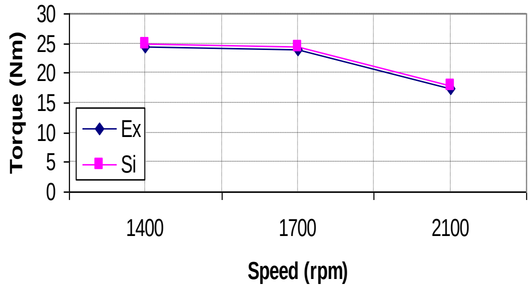

Fig. 5 Torque with DME

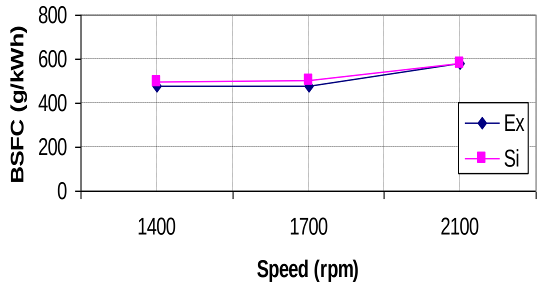

Fig. 6 Fuel consumption with DME

4.2. Simulation results of engine performance and emissions when fueled by DME

4.2.1. Engine performance

With the same fuel mass per cycle of 0.0444 (g/cycle), torque of engine when fueled by DME is smaller than that fueled by diesel (Fig. 7).This is due to the lower heat value of DME as compared to diesel (Q_{H_DME} = 28860 kJ/kg, Q_{H_diesel} = 42800 kJ/kg).

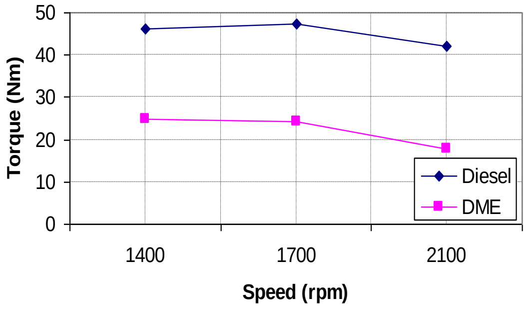

Fig. 7 Engine performance when using diesel and DME (0.0444g/cyc)

To maintain the engine power, it is necessary to increase the DME fuel mass per cycle by 39.5% (Fig. 8) and as a result, the fuel consumption correspondingly increases (Fig. 9)

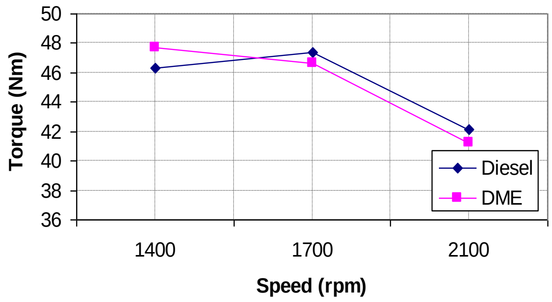

Fig. 8 Engine power with DME (0.0444g/cycle) and diesel(0.0617 g/cycle)

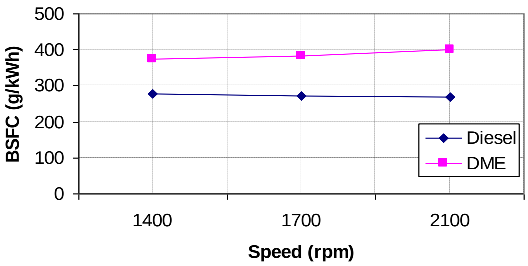

Fig. 9 Fuel consumption with diesel (0.0444g/cycle) and DME (0.0617g/cycle)

4.2.2. Effects of injection timing on engine performance

The torque reduces when increasing injection timing from 21 to 29 crank angle (CA) degree before top dead center (TDC) at 1400 rpm, 1700rpm and 2100rpm (Fig. 10). It is due to earlier injection timing which leads to increase the peak of cylinder pressure and shift it to the left

(Fig. 11).

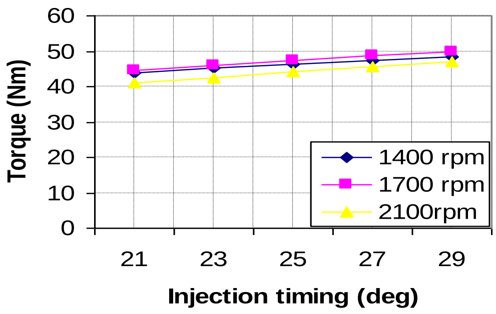

Fig. 10 Engine power versus injection timing at different speed

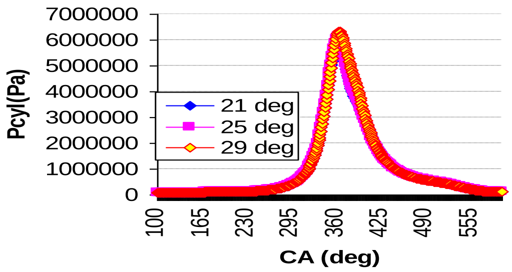

Fig. 11 Cylinder pressure at 1400rpm

When increasing speed, the torque reaches maximum value with earlier injection timing, max torque appears with injection timing of 29 CA degrees before TDC.

Similar to diesel fuel, in case of DME the higher engine speed the shorter evaporation and mixing time. Therefore, the fuel needs to be injected earlier in order to have sufficient time and more complete combustion.

During the combustion process, the peak of rate of heat release in case of DME occurs at 382 CA degree with the value of 46.1J/degree that is about 53.1% higher than that of diesel (Fig. 12). This may be due to the better vaporization of DME that leads to better mixture with air and faster combustion.

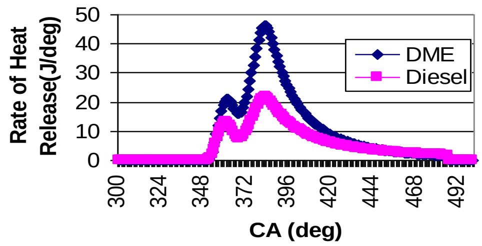

Fig. 12 Rate of heat release at 1400 rpm

4.2.3. Exhaust emission

The results show that the exhaust emission changes when using DME. Fig. 13 shows the significant reduction in smoke when using DME, up to 84.18 % at 2100 rpm. Averagely, smoke reduces by 75.97% over speed range. The variation of CO emission is depicted in Fig. 14. The CO emission with DME is lower than that with diesel. On average, the CO emission reduces by 70.02%. The reduction of NOx emission is shown in Fig. 15 with average value is 75.59%.

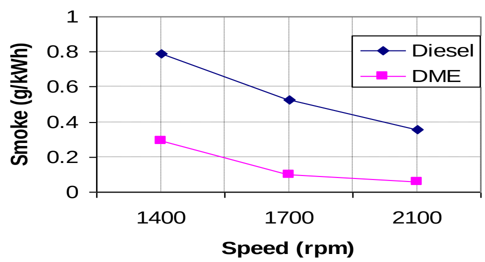

Fig. 13 Smoke emission

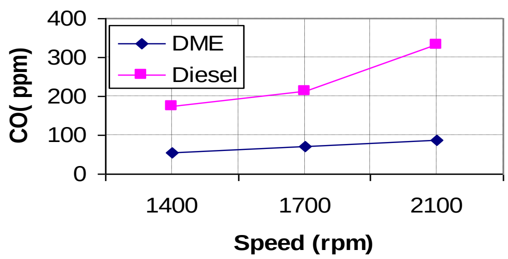

Fig. 14 CO emission

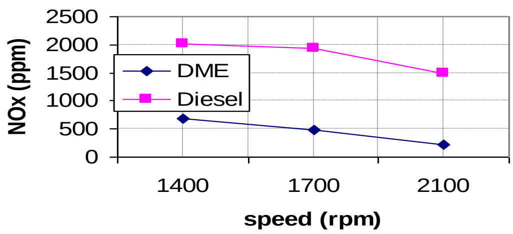

Fig. 15 NOx emission

4. Conclusions

Performance and emissions of DME fueled Kubota diesel engine are simulated by AVL Boost software. The model is verified by experiment.

The results show that: With the same fuel mass per cycle, the engine power with DME is lower as compared to that with diesel. To maintain engine power, it is necessary to increase the DME fuel mass per cycle. Similar to diesel fuel, the DME fuel needs to be injected earlier when increase speed in order to have sufficient time and more complete combustion. Compared to diesel, DME reduces quite clearly smoke, NOx and CO .

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