SIMULATING A CONVENTIONAL DIESEL ENGINE FUELED BY DIMETHYL ETHER

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Abstract

Diesel engines are utilized in most of heavy duty vehicles as their good performance. However, fossil fuel is being depleted currently, and emissions from diesel engine contains many toxic substances such as CO, HC, NO_x, PM…which effect adversely on environment and human health. Therefore, research and application of alternative fuels which are renewable and environment friendly are under consideration in countries and as well as Vietnam. Among these fuels, Dimethyl Ether (DME) is considered as the potential fuel for diesel engine. However, DME has some different properties compared to diesel, so that it is needed to modify the engine, especially the fuel system, to be suitable for DME fuel.

This article studies the characteristics of conventional diesel engine fueled by DME. Diesel engine D243 is modeled by using AVL Boost software and the software also simulates engine performance and emissions of DME fueled. In the engine model, DME is injected directly into cylinder as the same way of diesel fuel. Engine power, fuel consumption, cylinder pressure and emissions at various engine speeds are calculated. Two situations are considered: the delivered DME fuel mass per cycle is kept similar to that of diesel fuel, and delivered DME fuel mass per cycle is increased to meet the original engine power. In this case, the CO, Kn_{ox}, and especially soot reduce quite clearly. These preliminary results show the effect of DME fuel and ability to apply DME fuel on in-use conventional diesel engine in Vietnam.

Keywords: Fossil fuel, dimethyl ether, syngas, engine, AVL Boost.

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 an environment friendly fuel, easy to be liquefied 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 is produced either through the dehydration of methanol or a direct synthesis from syngas. However, DME is now attracting great attention as an energy source for the 21st century because of its multiple sources, excellent physical and chemical properties and excellent storage properties. Some experiments were conducted on diesel engine to investigate how DME injection characteristics affect the engine performance and exhaust emissions [1, 2]. Most of the results showed that emissions reduced significantly as being fueled by DME, especially Knox and soot.

2. Model description

2.1. Combustion model

The combustion in diesel engine can be considered by two processes: premixed combustion and mixing controled combustion processes

$$\frac{dQ_{total}}{d\sim} = \frac{dQ_{MCC}}{d\sim} + \frac{dQ_{PMC}}{d\sim}$$

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 [5] model by solving the following differential equation:

$$\frac{dI_{id}}{d\tilde{}} = \frac{T_{UB} - T_{ref}}{Q_{ref}}$$

As soon as the ignition delay integral I_{id} reaches a value of 1.0 (=at α_{id}) at the ignition delay $^{2}{}_{id}$ is caculated from

$^{2}{}_{id} = \tilde{}_{id} - \tilde{}_{SOI}$.

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]
$^{2}{}_{id}$: 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:

$$\frac{\left(\frac{dQ_{PMC}}{Q_{PMC}}\right)}{d\tilde{}} = \frac{a}{\Delta\tilde{}_{c}}.(m+1).y^{m}.e^{-a.y^{(m+1)}} \quad , \quad y = \frac{\tilde{} - \tilde{}_{id}}{\Delta\tilde{}_{c}}$$

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= $^{2}{}_{id}.C_{PMC\text{-}Dur}$
$C_{PMC\text{-}Dur}$: 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):

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

with

$$f_1(m_F, Q) = \left(m_F - \frac{Q_{MCC}}{LCV}\right). \cdot\left(w_{Oxygen,available}\right)^{C_{EGR}}$$

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

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 [-]

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

E_{kin} : kinetic jet energy [J]
C_{turb} : turbulent energy production constant [-]
$\dot{m}_{F,I}$: injection fuel mass (actual) [kg]
${}^{a}_{Diff}$: 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^3s] 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^3s] is caculated as:

$$r_{NO} = C_{PostProcMult}.C_{KineticMult}.2.0.\left(1-\sim^2\right)\frac{r_1}{1+\sim.AK_2}\frac{r_4}{1+AK_4}$$

with

$$\sim = \frac{C_{NO,act}}{C_{NO,equ}}.\frac{1}{C_{PostProcMult}},\ AK_2 = \frac{r_1}{r_2+r_3},\qquad AK_4 = \frac{r_4}{r_5+r_6}$$

2.2.2. CO Formation Model

CO formation following two 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	$CO_2+O= CO+O_2$	$r_2 = 2.51.10^{12}.e^{\left(\frac{-24055.0}{T}\right)}.$ $.c_{CO}.c_{O_2}$

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

$$r_{co} = C_{Const}.\left(r_1 + r_2\right).\left(1-\sim\right)$$

with $\sim = \frac{C_{CO,act}}{C_{CO,equ}}$

2.2.3. Soot fomation model

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

$$\frac{dm_{soot}}{d\ddot{}} = \frac{dm_{soot.form}}{d\ddot{}} - \frac{dm_{soot.ox}}{d\ddot{}}$$

with

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

$$\frac{dm_{soot.ox}}{d\ddot{}} = A_{ox}.\frac{1}{2_{char}}.\left(m_{soot}\right)^{n_2}.\left(\frac{p_{O_2}}{p_{O_2ref}}\right)^{n_3}.e^{-\frac{T_{a-ox}}{T_{ave}}}$$

- 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 can be specified as follow:

Molar mass: 0.046 kg/ mol
Lower heating value : 28860630.89 J/kg
Stoichiometric A/F ratio: 8.998
Carbon/: total mass ratio :0.521
Oxygen/ total mass ratio: 0.347
Nitrogen/ total mass ratio: 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 [3]

$$Q_{wi} = A_i \cdot \sim_i \cdot (T_c - T_{wi})$$

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 [6]:

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

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, $c_u = \pi.D.nd/60$, 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).

3. Modeling engine D243

In this study, AVL Boost software is used to calculate simulated single cylinder engine D243

3.1. The characteristic of engine

This engine is a four-stroke diesel engine, max output 80 hp/2200 rpm. In Vietnam, these models engine are popular. The characteristic of engine is shown in Table 3

Table 3 The characteristic of engine

No	Parameter	Value	Unit
1	Firing order	1-3-4-2	-
2	Displacement volume (V_h)	4,75	dm^3
3	Bore/Stroke (D/S)	110/125	mm/mm
4	Pressure ratio (ε)	16,4	-
5	Power ($N_{e\text{-}dm}$)	80	HP
6	Maximum torque ($M_{e\text{-}max}$)	280	N.m
7	Timing injection (φ_s)	25÷27	BTDC

3.2. Engine model in AVL_BOOST software

The model is built base on the structure of the existing diesel engine and the relative document. Table 4 and 5 show some elements and parameters of model.

Table 4 Some elements of model

No	Element Name	Symbol
1	Intake, Exhaust pipe	-
2	Boundary elements	SB
3	Plenum	PL
4	Cylinder	C
5	Restriction	R
6	Measuring point	MP
7	Air cleaner	CL

8	Turbocharger	TC
9	Wastegate	WG
10	Aircooler	CL
11	Aircleaner	CO

Table 5 The main parameters of model

No	Parameter	Value
1	RPM	1200÷2200
2	Air pressure (bar)	1
3	Air temperature (^{0}C)	25
4	Number cycle	50
5	Fuel per cycle (g/cycle)	0,055÷0,074
7	Low heat value (kJ/kg)	42800
8	Ratio A/F	14,7
9	Combustion Model	AVL MCC
10	Type engine	4 stroke
11	Firing order	1-3-4-2

The engine models in AVL_BOOST is shown in Figure 1:

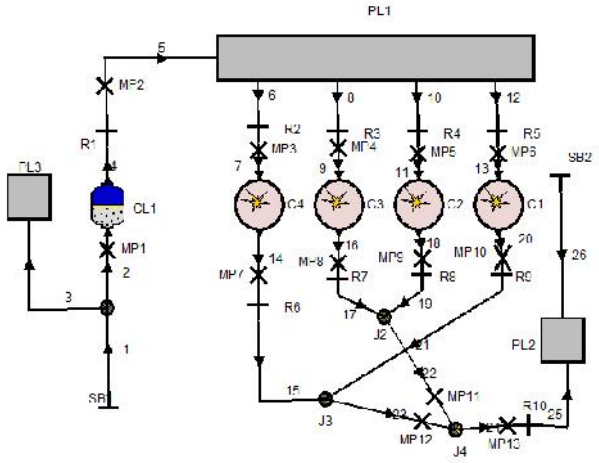

Figure 1 Model engine D243

4. Simulation results and discussion

4.1. Validation of model

Figure 2 and figure 3 show the results of simulation and experiment. The maximum deviation occurs at 2200 rpm at which the difference in fuel consumption is 1,2 % and in power is 4,2 % at 1400rpm. On average over speed range, the difference in power and fuel consumption is about 1,5 % and 0,4 %. It is possible to use the model for further study.

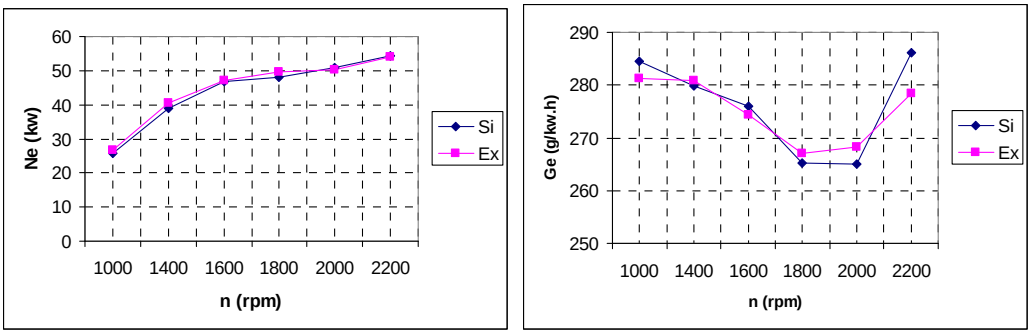

Figure 2, 3 Engine performance of simulation and experiment

4.2. Engine performance of engine D243 use Dimethyl ether fuel

4.2.1. Engine performance

With the same fuel mass per cycle, power of engine when fueled by DME is smaller than that fueled by diesel 18.1% on average (Fig. 4). 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).

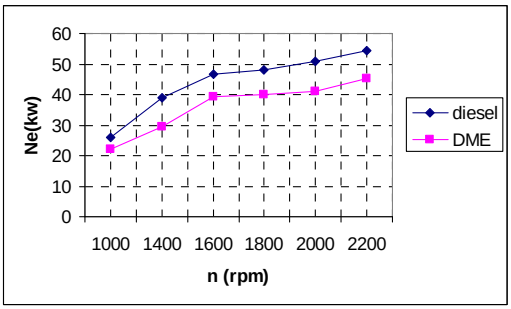

Figure 4 Engine performance when using diesel và DME

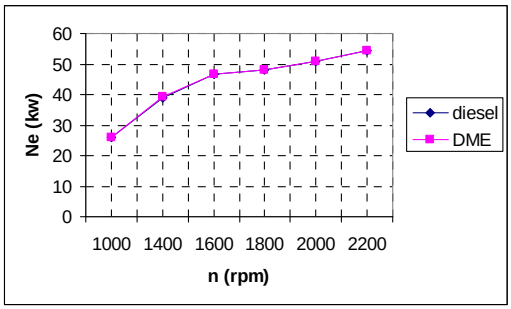

Figure 5 Engine power with DME and diesel

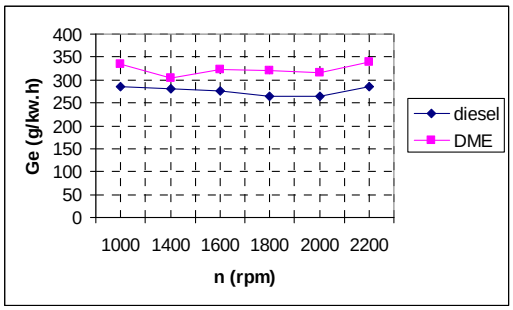

Figure 6 Fuel consumption with DME and diesel

To maintain the engine power, it is necessary to increase the DME fuel mass per cycle by 19.92% on average (Fig. 5), and as a result, the fuel consumption correspondingly increases 14.5% (Fig. 6).

4.2.3. Exhaust emission

Fig. 7, 8, 9 describe the levels of CO, NOx and soot emissions in the case of using DME. And the exhaust emission is significantly reduced in the case of using DME.

The variation of CO emission with respect to speed is depicted in Fig. 7. The CO emission of DME engines is higher than that of Diesel engines. Averagely, the CO emission increases 44.14%.

Fig. 8 shows the reduction of NO_X emission of DME engines. Obviously, NOx emission reduces 67.35 % corresponding to 2200 rpm – speed. Averagely, NOx emission reduces 27.11%.

The reduction of soot emission is shown in Fig. 9. The mean value of soot emission reduces 73.74%.

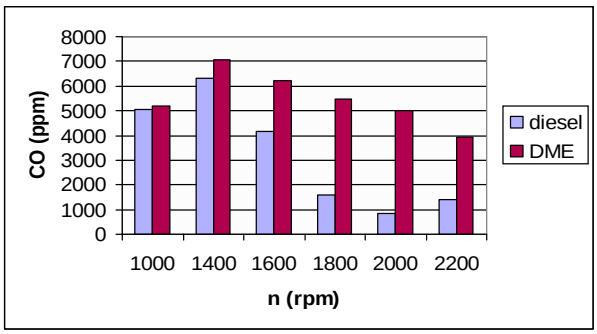

Figure 7 CO emissions

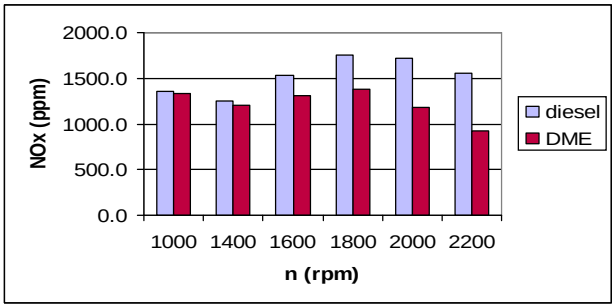

Figure 8 NO_X emissions

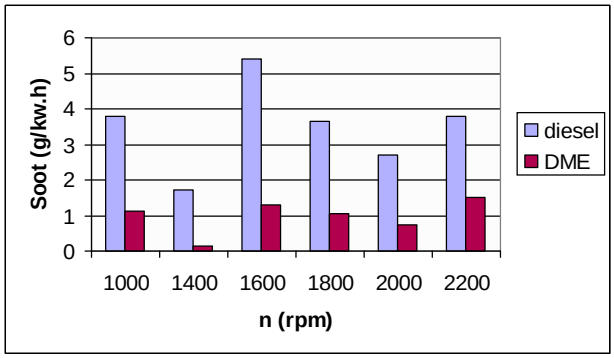

Fig 9 NO_X emissions

5. Conclusions

- Diesel engine D243 is modeled by using AVL Boost software and simulates engine performance and emissions of DME fueled.

The model is verified by experimental results in case of fossil diesel fuelling.

- 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 19.92% on average.

+ The CO increase 44.14% on average,

+ NOx and soot reduce quite clearly.

References

[1] Yoshio Sato, Akira Noda and LiJun, *"Effects of Fuel Injection Characteristics on Heat Release and Emissions in a DI Diesel Engine Operated on DME"*, SAE 2001-01-3634, 2001.

[2] Zhen HUANG, Xinqi QIAO, Wugao ZHANG, Junhua WU, Junjun ZHANG, *Dimethyl ether as alternative fuel for CI engine and vehicle*.

[3] Users guide - AVL Boost version 2011.1.

[4] G. D'Errico, *"Modeling the Pollutant Emissions from a S.I. Engine"*, SAE paper No. 2002-01-0006, et al. (2002)..

[5] Theory - AVL Boost version 2011.1

[6] G. Woschni (1967). *"A Universally Applicable Equation for the Instantaneous Heat Transfer Coefficient in Internal Combustion Engines"*, SAE paper No. 6700931.

[7] DME: An Emerging Global Fuel, *www.methanol.org/Energy/...Fuel/DME-Emerging-Global-Fuel.aspx*.

[8] Nguyen Lan Huong, Luong Cong Nho, Pham Huu Tuyen, *"Dimethyl Ether (DME)- An alternative fuel for diesel engine"*, Journal of Transportation December- 2012.

[9] Nguyen Lan Huong, Luong Cong Nho, Pham Huu Tuyen. *"Investigating Dimethyl ether (DME) fuel systems for Diesel engine"*, Journal of Transportation March- 2013.

[10] Nguyen Lan Huong, Luong Cong Nho, Pham Huu Tuyen, *"Simulation study on diesel engine fueled by Dimethyl Ether (DME)"*, Scientific conference mechanical pneumatic 2013.