International Conference on Applied Energy 2020
Dec. 1 - Dec. 10, 2020, Bangkok / Virtual
Paper ID: 234

Numerical study on methanol and formaldehyde emissions of diesel methanol dual fuel engine with different valve overlaps

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ABSTRACT

The diesel methanol dual fuel (DMDF) engine is confronting with the problem of high unregulated emissions of methanol and formaldehyde, although it has better fuel consumption and lower regulated emissions. The previous studies on unregulated emissions of DMDF engine have focused on the measuring methanol and formaldehyde concentrations in the exhaust without distinguishing whether emissions come from leakage during valve overlap or incomplete combustion in the cylinder. In this study, a multi-dimensional computation fluid dynamics (CFD) model coupled with detailed chemical kinetic mechanism was developed to investigate the emissions of methanol and formaldehyde in DMDF engine by using CONVERGE. The model was validated against at 50% load of 1340r/min in a six-cylinder DMDF engine. The results show that the unburned methanol and formaldehyde in the cylinder are the main component of the total methanol and formaldehyde emissions, while the leakage of methanol can be negligible. This is due to the high air fuel ratio in the intake manifold and the low air inflow during the valve overlap period. Then the effects of different intake valve opening (IVO) and exhaust valve closing (EVC) on the unregulated emissions were investigated. It was found that increased valve overlap period can affected the leakage of methanol significantly. However, the increased leaking methanol still was negligible due to the very small mass ratio. Based on the above results, the total methanol and formaldehyde emissions of DMDF engine are hardly affected by the leakage of methanol, but are almost entirely derived from the unburned methanol and formaldehyde in the cylinder.

Keywords: diesel methanol dual fuel engine, methanol emission, valve overlaps, numerical study, formaldehyde emission.

NONMENCLATURE

Abbreviations	
DMDF	diesel methanol dual fuel
CFD	computation fluid dynamics
IVO	intake valve opening
EVC	exhaust valve closing
CI	compression ignition
TDC	top dead center
EVO	exhaust valve opening
MSP	methanol substitution percent

1. INTRODUCTION

The large scale use of high-efficiency internal combustion engines is one of the important reasons for the current shortage of petroleum and environmental pollution. Faced with such a severe energy situation, methanol has become a promising alternative fuel for diesel engines due to its low cost, easy storage, low emissions and renewable [1,2].

However, the application of methanol in the compression ignition (CI) engines is limited due to its low cetane number. Yao et al. [3,4] proposed DMDF combustion, which perfectly solved the application of methanol in CI engines. Now the DMDF engine has been widely used in various fields such as heavy truck, marine, power generation and engineering machinery due to better economy and emissions.

However, an important problem with DMDF engine is the unregulated emissions such as methanol and formaldehyde. Wei et al. [5] carried out the research on reducing unregulated emissions of a DMDF engine with different after-treatment devices. They found that the DMDF engine without any after-treatment device has higher unburned methanol and formaldehyde emissions than those of pure diesel mode. Gong et al. [6] carried out the research on unregulated emissions of a DISI methanol engine during cold start. They found that increasing the intake temperature during cold start can accelerate the combustion and reduce unburned methanol and formaldehyde emissions.

The experimental results can obtain emission values of methanol and formaldehyde, but it is impossible to determine the amount of leakage from the valve overlap period. In order to reveal the effect of valve overlap on emissions, CFD calculation was applied to analyze the leakage. Long et al. [7] investigated the effects of reformed exhaust gas recirculation on the HC and CO emissions of a spark-ignition engine fueled with LNG by using CFD software CONVERGE. Li et al. [8] carried out a numerical investigation on methane combustion and emissions from a natural gas-diesel dual fuel engine using CONVERGE.

However, studies on leaking methanol of DMDF engine are still rare to see in literatures. In this study, the emissions of methanol and formaldehyde were calculated by using CONVERGE to obtain the amount of leakage and unburned methanol. The results determined the source of methanol emissions, thus overturning the traditional view of methanol leakage during valve overlap. In addition, the effects of different IVO and EVC on methanol and formaldehyde emissions were investigated.

2. MODELING METHODOGY

2.1 *Engine model*

The DMDF engine used for this study was a six-cylinder, water cooled, turbo-charged engine, which was produced by Weichai. The detail engine specifications were listed in Table 1. The schematic diagram of experimental system was shown in Fig.1.

Table 1. Specifications of the test engine

Bore × Stroke (mm)	126×130
Compression ratio	17:1
Displacement (L)	9.726
Intake valve opening	−20°CA ATDC
Intake valve closing	214°CA ATDC
Exhaust valve opening	-229°CA ATDC
Exhaust valve closing	21°CA ATDC
Rated power (kW@r/min)	247@1900
Max torque (Nm@r/min)	1550@1200-1400

2.2 *Computational model*

In this study, the intake and exhaust processes were considered in the simulation because the methanol leakage and in-cylinder swirl ratio were significantly affected by the intake and exhaust flows. Therefore, a full computational model with intake and exhaust port was simulated. According to the real structure and specification of the DMDF engine, the computational grid was set up by CONVERGE, as shown in Fig.2.

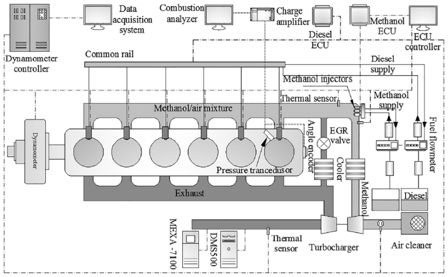

Figure 1. Schematic diagram of experimental system

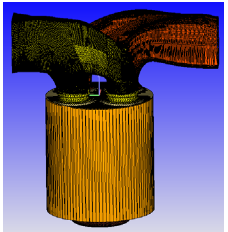

Figure 2. Computational grid

Considering the calculation accuracy and cost, the turbulence model used in this study was the RNG k-ε model [9]. The Kelvin Helmholtz Rayleigh Taylor (KHRT) model was used for the droplet breakup process, and the O'Rourke model was applied for the collision simulation of diesel spray droplets [4] The chiang model was used for diesel evaporation calculation [10]. SAGE, a Multi-zone chemical solver, was used for combustion model [11]. In addition, a reduced n-heptane/methanol mechanism [12], containing 44 species and 65 reactions, was chosen as the DMDF combustion mechanism.

In this study, the intake, compression, expansion and exhaust processes were modeled. Based on the mass and concentration of the in-cylinder and leaking gas, the mass of the methanol and formaldehyde in the exhaust gas were determined, so the total emissions can be calculated. The emissions of methanol and formaldehyde are defined as Eq. (1) and Eq. (2):

$$M_{CH3OH} = M_{CH3OH-1} + M_{CH3OH-2} \quad (1)$$

$$M_{HCHO} = M_{HCHO-1} + M_{HCHO-2} \quad (2)$$

M_{CH3OH}, M_{HCHO}- Mass of methanol and formaldehyde in DMDF mode, g/kW.h.

$M_{CH3OH-1}, M_{HCHO-1}$ -Mass of methanol and formaldehyde in-cylinder at EVO, g/kW.h.

$M_{CH3OH-2}, M_{HCHO-2}$ - Mass of leakage methanol and formaldehyde, g/kW.h.

2.3 *Initial conditions*

In order to obtain the accuracy of the input boundary conditions, the model was validated at A50 (110 kW, 1340 r/min) in the European steady-state cycle test by using GT-Power. 50% methanol substitution percent (MSP) was selected, which can be abbreviated as MSP50. MSP was used to illustrate the rate of the amount of diesel that replaced with the addition of methanol to the amount of diesel in the pure diesel mode, which can be calculated by the formula below:

$$MSP = \frac{M_d - M_{dm}}{M_d} \times 100\% \qquad (3)$$

M_d, M_{dm}- Mass flow rates of diesel in diesel and DMDF modes, kg/h.

Then the temperature, pressure, component and other boundary conditions of the inlet and outlet were calculated by GT-Power. Fig. 3 showed the instantaneous pressure of intake and exhaust port.

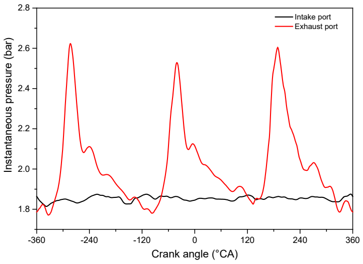

Figure 3. Instantaneous pressure of intake and exhaust

2.4 *Validation of the CFD model*

The cylinder pressure and heat release rate were used to validate the numerical model. Fig. 4 showed the comparisons of the cylinder pressure and heat release rate between experiments and simulations. As can be seen, the predictions of cylinder pressure and heat release rate were in good agreement with the experimental results. And the difference in peak pressure was 0.11MPa, which was lower than ±2% of the peak pressure. The comparison of methanol and formaldehyde in exhaust emissions between simulations and experiments was listed in Table 2.

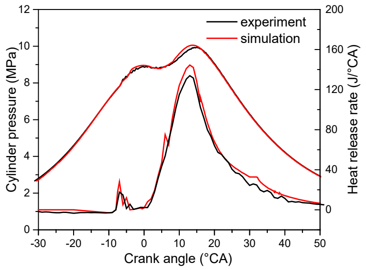

Figure 4. Comparison of the simulated experimental data

As can be seen, the relative deviations of methanol and formaldehyde were 2.6% and 38%, respectively. Considering that methanol produces formaldehyde under high temperature oxidation, they were combined together for calculation in this study [13]. Therefore, the total of methanol and formaldehyde emissions were used for model validation in this study, and the relative deviation is 6.8%. Based on the above comparisons between simulations and experiments, the CFD model was reasonable to predict the gas exchange and combustion process of the DMDF engine.

Table 2. Engine emissions of simulation and experiment

Feature	CH_3OH	HCHO	CH_3OH+ HCHO
Experiment	16.16	2.19	18.35
Simulation	15.74	1.36	17.10
Error (%)	2.6%	38%	6.8%

3. RESULTS AND DISCUSSIONS

3.1 *Characteristics of methanol emission*

The total methanol emissions consist of two parts: methanol from unburned fuel (CH_3OH-1) and methanol from the leakage (CH_3OH-2). Fig. 5 showed the masses of methanol emissions at A50 from -400°CA ATDC to 150°CA ATDC. CH_3OH-1 in cylinder increased rapidly with the valve opening, until the mass reached a maximum value at the -175 °CA ATDC, and then a small amount of methanol returned to the intake port due to the backflow. Then the methanol was ignited by diesel spray in the cylinder near the TDC and the mass of methanol dropped sharply. Finally, the mass of methanol in the cylinder at EVO was 6.87E-6kg, which converted to specific emission of 17.08g/kW.h. CH_3OH-2 was caused by the simultaneous opening of the intake and exhaust valve during the valve overlap. After IVO, the mixture of methanol and air entered the cylinder and then some of the mixture entered the exhaust port directly through the exhaust valve. As can be seen in the Fig 8, the leakage methanol at EVC was 5.80E-9kg, which converted to specific emissions of 0.02g/kW.h.

Simulation results showed that the CH_3OH-2 was almost ignored because it accounted for very small proportion of total methanol emissions, which was inconsistent with general view of people. In order to reveal the cause, a detailed study on methanol leakage was conducted in this study. There were two reasons for this phenomenon. Firstly, although there was a 41°CA valve overlap, the total amount of intake mixture entering the cylinder during valve overlap was very small due to the small valve lift. As can be seen in Fig.5, the mass of CH_3OH-1 at EVC was 3.10E-6kg, which converted to specific emission of 7.71g/kW.h. Considering the whole intake process, the intake mass flow during the valve overlap only accounted for 3.31% of the total intake mass flow. Secondly, Fig. 6 exhibited the variation trend of CH_3OH concentration and velocity at -380°CA, -360°CA and -340°CA ATDC. The CH_3OH concentration cloud charts showed that the intake and exhaust valve lifts were basically the same at -360°CA ATDC. At this time, the methanol in the cylinder was mainly concentrated around the intake valve, and the overall methanol content in the cylinder was low. With the increase of the intake valve lift, the methanol entering the cylinder increased and reached the exhaust valve due to the airflow. However, only a small amount of methanol leaked into the exhaust port because the exhaust valve is nearly closed at -340°CA ATDC.

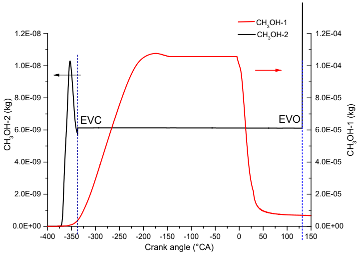

Figure 5. CH_3OH emissions changing with crank angle

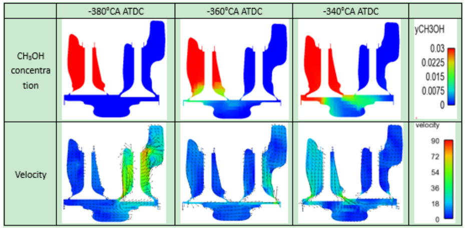

Figure 6. The distribution of CH_3OH and velocity

3.2 *Characteristics of formaldehyde emission*

The total formaldehyde emissions are mainly derived from unburned formaldehyde in the cylinder and the methanol oxidation during the exhaust process. In this study, only unburned formaldehyde in the cylinder was considered.

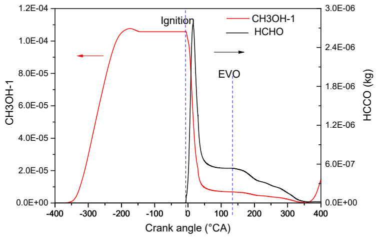

Figure 7. CH_3OH-1 and HCHO emissions changing with crank angle

Fig.7 showed the mass of CH_3OH-1 and HCHO in the cylinder with the changing of crank angle. It was observed that there is no HCHO in the cylinder before the ignition. After the ignition, the CH_3OH-1 in the cylinder decreased rapidly and the HCHO was converted from the CH_3OH in the combustion process, so the mass of the HCHO in the cylinder rose rapidly. After the EVO, unburned methanol and formaldehyde in the cylinder were discharged from the exhaust valve. Some unburned methanol is oxidized to formaldehyde in the exhaust pipe at high temperature. Because this part is beyond the scope of this study, it will not be described in detail.

Based on the above conclusions, only the effects of different IVO and EVC on methanol leakage during the valve overlap were carried out in the subsequent studies.

3.3 *Effects of IVO on methanol emission*

IVO has a significant effect of the valve overlap, which affected the leakage of methanol. Based on the original IVO of -20°CA ATDC, the calculations of IVO delayed 10°CA, 20°CA and advanced 10°CA, 20°CA and 30°CA were carried out, which were labeled as IVO-20, IVO-10, IVO+10, IVO+20 and IVO+30.

The mass of CH_3OH-2 changing with IVO was shown in Fig.8. It was observed that there is no methanol in the exhaust port due to the small valve overlap at IVO delayed 10°CA and 20°CA. When the IVO opened earlier, the valve overlap increased, which caused the mixture of air and methanol to enter the cylinder earlier than the original IVO. Meanwhile, earlier IVO increased the lift of the intake and exhaust valves during the valve overlap. When the IVO advanced 30°CA, the valve overlap reached 71°CA. Adequate valve overlap and intake valve lift resulted in more mixture entering the cylinder before EVC. Therefore, more mixture was discharged into the exhaust port through the exhaust valve.

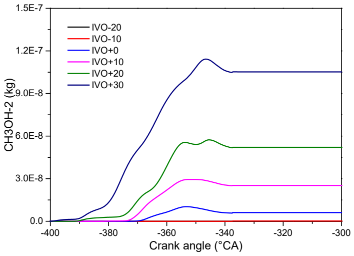

Figure 8. CH_3OH-2 changing with different IVO

The mass of CH_3OH-2 at IVO+30 was about 17 times as much as original IVO as shown in Fig.8. And it was converted into specific emissions about 0.34g/kW.h, which accounted for about 2% of total CH_3OH emissions.

3.4 *Effects of EVC on methanol emission*

EVC has a significant impact on the leakage of methanol due to its effect of valve overlap. Based on the original EVC of 21°CA ATDC, the calculations of EVC advanced 20°CA, 10°CA and delayed 10°CA, 20°CA and 30°CA were carried out. All the cases were labeled as EVC-20, EVC-10, EVC+10, EVC+20 and EVC+30.

Fig.9 showed the mass of CH_3OH-2 changing with EVC. It can be observed that methanol in the exhaust port increased from -373 °CA ATDC and eventually reached equilibrium after the exhaust valve closed. When EVC was 20 °CA advanced, there was no methanol leakage in the exhaust port. This is because the lift of the intake and exhaust valve is very small during the 21°CA valve overlap, and the effective circulation area cannot be formed. With the delay of EVC, the valve overlap and the peak of methanol leakage became larger and larger. At the delay of 30°CA, the valve overlap became 71°CA and the peak of methanol leakage was largest. However, the mass of the final CH_3OH-2 reached its maximum value at the delay of 20°CA. The reason was that with the delay of the EVC, the exhaust process became longer, which resulted in a part of the leaking fresh mixture re-entering the cylinder when the piston moves downward.

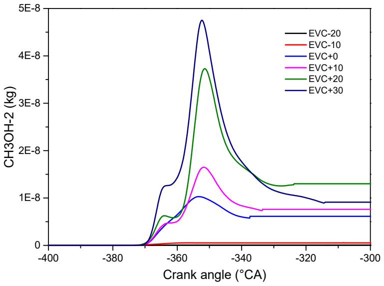

Figure 9. CH_3OH-2 changing with different EVC

As shown in Fig.9, the mass of CH_3OH-2 at EVC+20 was about 2.3 times of original EVC. And it was converted into specific emissions about 0.046g/kW.h, which accounted for about 0.3% of total CH_3OH emissions.

4. CONCLUSIONS

Numerical study was used to carry out the emissions of methanol and formaldehyde based on the GT-Power and experimental results. The influence of different IVO and EVC on methanol emission of DMDF engine was conducted. The main conclusions are as follows:

1) The methanol leakage caused by valve overlap only accounted for a very negligible proportion of the total methanol emission. The emission of formaldehyde mainly derived from the unburned formaldehyde in the cylinder, which has no relationship with the valve overlap.

2) The change of IVO and EVC can lead to the change of valve overlap and affect the leakage of methanol. IVO has a more significant impact on methanol leakage than EVO.

3) The change of valve overlap has a slight effect on methanol leakage, which provides a clear direction for exploring the source of methanol emissions.

ACKNOWLEDGEMENT

The authors wish to thank the Natural Science Foundation of China (No. 51676134) for the financial support.

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