Preliminary Numerical Study on Exhaust Emission Characteristics of Particulate Matters and Nitrogen Oxide in a Marine Engine for Marine Diesel Oil and Dimethyl Ether Fuel

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Abstract: As concerns regarding environmental pollution, energy security and future oil supply continue to grow, communities around the world are looking for non-petroleum-based alternative fuels along with advanced energy technologies (e.g., fuel cells) to increase energy use efficiency. Compared with the main alternative fuel candidates (e.g., methane, methanol, ethanol and Fischer–Tropsch fuels), dimethyl ether (DME) seems to have a significant potential to solve the aforementioned problems and can be used as a clean, high-efficiency compressed ignition fuel with reduced nitrogen oxide, sulphur oxide and particulate matter (PM) emissions. In this study, the results of experiments using a ship engine and numerical analysis were verified using AVL BOOST software. Based on these verifications, nitrogen oxide and PM reduction characteristics were numerically analysed by controlling the diameter and spraying time of the fuel nozzle, which is the fuel injection system of a marine engine. When DME fuel was used, nitrogen oxide and PM emissions were reduced by 40% and 90%, respectively, compared with marine diesel oil fuel. To prove the viability of DME as an alternative fuel, combustion and exhaust characteristics were analysed in accordance with injection timing and the variation of nozzle hole.

Keywords: nitrogen oxide emission; black carbon emission; dimethyl ether (DME) fuel; marine diesel oil (MDO); numerical methods

1. Introduction

In automobiles and ships, nitrogen oxides and particulate matter in a large amount of exhaust gases are strongly restricted by strong exhaust regulations worldwide. In response to this situation, major developed countries (e.g., the USA, Japan, and European countries) have set targets for reducing carbon dioxide (CO2) emissions through the Intergovernmental Panel on Climate Change (IPCC) climate change agreement. In the transportation sector, global energy-consumption-related greenhouse gas emissions account for about 23%, and the Japan Automobile Manufacturers Association (JAMA) has projected an increase of greenhouse gas emissions in the transportation sector by more than 60% from 2008. Therefore, major developed countries are planning to divert from existing fossil fuels to effectively respond to fuel consumption and CO2 greenhouse gas emission restrictions in the transportation sector, and diversify energy policies promoting the use of renewable fuels such as biodiesel and dimethyl-ether (DME) [1–3]. Moreover, governments decided that these changes must be implemented urgently. Accordingly, in response to the problems faced worldwide,
the low-carbon fuel market in the transportation sector is expected to gradually expand. In addition to fuel economy and CO2 greenhouse gas emission limit regulations in the transportation sector, which have recently been strengthened, efforts to develop technologies in the automobile industry are being intensely made, and alternative fuels such as biodiesel, bioethanol, dimethyl ether and low-carbon fuels are being supplied. Investment in technology development and securing competitiveness are also actively underway [4–7].

DME is the simplest ether; its molecular structure is CH₃OCH₃. This substance is in the gaseous state at room temperature (293 K) and normal pressure at 101.3 kPa and in the liquid state at the condition of 253 K temperature and 1MPa pressure. DME has an ether structure and is soluble in organic compounds but is not corrosive to metals and is harmless to humans. Moreover, there is little concern about environmental damage, such as greenhouse effect promotion and destruction of the ozone layer, owing to DME use. In particular, DME is a good fuel because it presents a large volume change due to pressure owing to its low volume and elastic modulus in the liquid state. As a characteristic of DME combustion, since the DME molecular formula contains oxygen molecules, the possibility of generating particulate matter during combustion is extremely small [8–10]. The main characteristic of diesel engine fuel is its low self-ignition temperature, and DME ignites at almost the same temperature as diesel. DME is injected into the engine above its critical pressure (53.7 bar) and vaporised at the same time as injection at a high vapour pressure. In addition to the low ignition temperature, DME has a particularly high cetane number (above 55). Moreover, as DME has a high oxygen content and no carbon–carbon bonds, it does not generate fumes, which are a problem in diesel engines [2]. The calorific value per weight of DME is 6900 kcal/kg, which is lower than those of propane, butane and methane, but higher than that of methanol. Gaseous DME provides 14,200 kcal/Nm³, which is a higher calorific value than that of methane. The heat of evaporation of DME is less than half of that of methanol, and its lower explosion limit, which is the most important characteristic for safety management, is about two times those of propane and butane, rendering it relatively safe upon leakage. Existing synthetic fuels are limited to replacing liquid fuels for transportation such as gasoline and diesel, but DME can be widely used for household, transportation and power generation such as LPG [3,4].

Industrially mass-produced DME is a very promising alternative to diesel fuel for application in diesel engines [11–13]. Its simple molecular structure confers this substance a very high cetane number (>55), which resembles that of diesel fuel; DME presents a high oxygen content (34.8 mass%) and therefore exhibits better atomisation, combustion and fuel economy than diesel [14,15]. Moreover, DME is an oxygen-containing fuel with small post-combustion; therefore, it emits very little smoke and is a potentially clean fuel that can be burned with a much-reduced release of particulate matter (PM) from combustion. In addition, high exhaust gas recirculation (EGR) can be used to meet increasingly stringent regulatory standards by reducing nitrogen oxide emissions [16]. However, some of the physical properties of DME fuels are very unfavourable compared with those of ordinary diesel fuels. The characteristics of both fuels include bulk modulus, low calorific value, density and viscosity. DME’s bulk modulus and viscosity values (6.37E + 08 N/m² and 0.1 cSt) are significantly lower than those of diesel (14.86E + 08 N/m², 3 cSt), leading to high pressure and strong pressure fluctuations as well as gas vapour leakage in fuel supply systems (e.g., high pressure pumps, common rails and injectors). To solve this problem, it is not possible to use a fuel supply system for regular diesel; therefore, a DME-specific fuel supply system should be used and elements with rubber components should be avoided because of the risk of corrosion [17,18]. A realistic alternative to DME [19–22] is biodiesel, an alternative oxygen-containing fuel for diesel engines that is gaining significant importance owing to its sustainability, good exhaust quality and biodegradability [23–26]. In DME engines, good lubricity and high-calorie biodiesel can be tailored to complement the properties of DME and thus achieve biofuel-like properties by employing lubricant additives.

Since 1995, many studies have been conducted with emphasis on the combustion characteristics and exhaust characteristics according to the nozzle shape of the DME engine and on the spraying characteristics and spray visualisation of DME fuel [27–31]. This study required a modification of the
injection system (longer injection period or larger nozzle hole) to achieve the same power as that of the diesel engine owing to the lower density, viscosity and calorific value of the DME supplied by the inline pump. In Gill et al. [32] and Zhang et al. [33], the study of the spray properties of DME was conducted on the overall behaviour of the spray and piston and the collision in the actual combustion chamber. The aforementioned authors suggested that the forward angle of the fuel supply should be larger for engines running on DME than for engines using diesel fuel, owing to the low viscosity and density of DME fuel; with DME, fluctuations in line pressure, nozzle needle lift, opening time and closing time are greater than those in diesel engines. Yu and Bae [34] compared the spray characteristics of DME and diesel at injection pressures of 25 MPa, 40 MPa and 60 MPa, atmospheric pressure and a chamber pressure of 3 MPa in a common rail fuel injection system; it was stable and the maximum value was low. Considering the atomisation characteristics of DME and diesel fuel, it was found that the fuel injection speed and fuel injection delay were shorter than those of diesel fuel. As DME is an oxygen-containing fuel, burns faster than diesel and presents a higher combustion pressure, lower peak heat emission and shorter post-combustion compared with diesel, resulting in low emissions of particulate matter. Moreover, DME fuel engines feature lead-free combustion, low hydrocarbon (HC) and CO emissions, and slightly higher NOx emissions, and can use EGR to mitigate NOx emissions [35]. Wu et al. [36] investigated the combustion and emission characteristics of DME-powered turbocharged diesel engines; they reported that the injection timing of DME engines should be improved by considering engine speed and engine load. This DME engine presented the advantage of significantly reducing NOx emissions compared with diesel engines. DME fuel was used to control the injection system and injection timing and thus significantly reduced nitrogen oxide emissions and PM as the engine load increased.

When using DME, biodiesel and DME-biodiesel blends, nitrogen oxide emissions are much higher than those of diesel engines owing to faster combustion. Song et al. [37] studied the effect of EGR on DME engine performance and emissions; owing to DME’s lead-free combustion, the engine operated at high EGR speeds and was not limited by NOx emission trade-offs. Zhao et al. [38] studied the effect of EGR on combustion and emissions of naturally aspirated DME engines; NOx emissions meeting the requirements of Euro IV and V specifications were achieved under electronic stability control operating conditions after using the EGR strategy. Zhao et al. [38] also used the EGR rate to investigate the effect of the diesel ratio on combustion and emissions of naturally aspirated DME-diesel engines and obtained an optimum intake air to DME fuel ratio. Their results showed that, as the EGR rate increased, the ignition delay increased and the NOx emissions rapidly decreased; particulate matter was reduced owing to the decrease in the heat release rate (HRR) and the pressure increase rate. The higher the premix ratio of DME fuel, the smaller the particulate matter and NOx emissions, but the higher the HC and CO emissions. Yang and Lee [39] researched a comparison of the soot concentration with the injection pressure for operating speed of DME and diesel engines at the engine operating speed of 1800 rpm, light load condition, and injection timing of 14 CA BTDC. In the case of an engine using DME fuel, compared with diesel combustion, it showed a characteristic of emitting less particulate matter and nitrogen oxides [40–42].

Based on the aforementioned studies, we conducted an optimisation study to significantly reduce HC, CO and NOx emissions in DME engines by controlling the EGR ratio. More specifically, in this study, experimental data from an existing marine diesel engine and numerical analysis results obtained using AVL BOOST software were analysed and compared for the cases of the engine being fuelled with DME and with marine diesel oil (MDO). As mentioned earlier, the fuel pump system needs to be improved owing to the characteristics of diesel fuel and DME fuel. Because of DME’s low density compared with diesel fuel, numerical analysis methods were used to assess the nitrogen oxide and the PM characteristics according to the hole diameter and injection timing of the engine’s fuel nozzle in consideration of these problems. In practice, there are many cases applied to automobile engines; herein, this approach is applied to marine engines to perform numerical analysis and conduct research using experimental variables.
2. Materials and Research Methods

2.1. Experiment Methods

Regarding the engine used in this study, a 600 kW-class generator engine was constructed as shown in Figure 1. An encoder was installed on the crankshaft of the experimental apparatus to measure the number of revolutions of the engine and a pressure sensor (model 6056 A, Kistler, Winterthur, Switzerland) was installed on cylinder 1 to measure the pressure in the combustion chamber and the combustion pressure. In addition, to measure the flow rate of the incoming fuel, a flow meter, a load regulator, and a system capable of measuring nitrogen oxides and particulate matter were installed at the outlet of the exhaust pipe. In addition to the advantages mentioned in Section 1, DME has a low carbon-to-hydrogen ratio (C:H).

![Figure 1. Schematic of the four-stroke marine engine.](image)

Table 1. Specifications of the test engine.

| Item                              | Specifications                                      |
|-----------------------------------|----------------------------------------------------|
| Engine type                       | Four-stoke turbocharged DI marine generator engine  |
| Number of cylinders               | 6                                                  |
| Compression ratio                 | 15.9                                               |
| Bore × stroke (mm)                | 165 × 265                                          |
| Displacement (cc)                 | 20,000                                             |
| Fuel injection system             | Mechanical pumping system (Max. 1400 bar)          |
| Engine’s maximum continuous rating (MCR) (kW/rpm) | 600 kW/900 rpm                                    |
Table 2. Exhaust gas instruments.

| Items                          | Specifications                  |
|-------------------------------|--------------------------------|
| Dynamometer                   | Load controller (in a marine ship) |
| Exhaust gas analyser          | SWG 300                        |
| Smoke meter                   | Diesel opacimeter (OP 130D)     |

Table 3. Experimental conditions.

| Items               | Specifications       |
|---------------------|----------------------|
| Fuel                | Marine diesel oil    |
| Engine speed (rpm)  | 900                  |
| Load (kW)           | 150, 300, 450, 600   |

Table 4. Properties of dimethyl ether (DME) and diesel fuel [27,39].

| Properties (unit/condition) | Units | DME | Diesel fuel |
|-----------------------------|-------|-----|-------------|
| Chemical structure          | CH₃–O–CH₃ | –   |             |
| Molar mass                  | g/mol  | 46  | 170         |
| Carbon content              | mass%  | 52.2| 86          |
| Hydrogen content            | mass%  | 13  | 14          |
| Oxygen content              | mass%  | 34.8| 0           |
| Carbon-to-hydrogen ratio    |        | 0.337| 0.516     |
| Critical temperature        | K      | 400 | 708         |
| Critical pressure           | MPa    | 5.37| 3.00a       |
| Critical density            | kg/m³  | 259 | –           |
| Liquid density              | kg/m³  | 667 | 831         |
| Relative gas density (air = 1) |       | 1.59 | –           |
| Cetane number               |        | >55 | 40–50       |
| Auto-ignition temperature   | K      | 508 | 523         |
| Stoichiometric air/fuel mass ratio |       | 9.0 | 14.6        |
| Boiling point at 1 atm       | K      | 248.1| 450–643   |
| Enthalpy of vapourisation    | kJ/kg  | 467.13| 300       |
| Lower heating value          | MJ/kg  | 27.6| 42.5        |
| Gaseous specific heat capacity | kj/kg K | 2.99 | 1.7           |
| Ignition limits              | vol% in air | 3.4/18.6 | 0.6/6.5 |
| Modulus of elasticity        | N/m²   | 6.37E+08| 14.86E+08 |
| Kinematic viscosity of liquid| cSt    | <1  | 3           |
| Surface tension (at 298 K)   | N/m    | 0.012 | 0.027     |
| Vapour pressure (at 298 K)   | kPa    | 530 | 10          |

2.2. Numerical Analysis Method

The software used for the simulations was AVL BOOST [44] version 2019.1, which provides a graphical user interface (GUI) with icons representing the components of the internal combustion engine (ICE). For the engine in Figure 1, a simulation model was constructed using the elements shown in Figure 2; the model was built in AVL BOOST [44] after all the necessary data had been collected. In the simulation model, initial and boundary conditions were established by modelling cylinders, turbochargers, valves or heat exchangers, and engine components. The modelled engine configuration considered the reference Cylinder 1 (C1), the main engine characteristics for the spatial distribution of the cylinders—namely, the explosion sequence C1-C2-C4-C6-C5-C3—and the firing angles of each cylinder. The model’s C1 was associated with Element 1 of Engine 1 (E1) and defined the engine type, operating speed, moment of inertia and brake average effective pressure (BMEP).
The combustion method adopted was an experimental mixed control combustion (MCC) model that predicted the amount of heat released (ROHR) and NOx emissions based on the amount of fuel in the cylinder and the turbulent kinetic energy from injection.

Figure 2. AVL BOOST model for a four-stroke marine diesel engine.

3. Results and Discussion

3.1. Characteristics of Combustion Pressure and Rate of Heat Release versus the Compression Ratio of the Turbocharger Nozzle Ring

Figure 3 shows the experimental results obtained using MDO and the simulation results using AVL BOOST; results showing the characteristics of the combustion and heat release rate according to the injection timing by using DME in the same marine engine are also presented. For DME, the experimental results and the numerical analysis results are, in general, in good agreement. Regarding the results of the combustion and heat release rate characteristics according to the injection timing, as the injection timing increased, the combustion start point occurred earlier and post-combustion was faster. In addition, as the injection time progressed, the combustion pressure increased. It is believed that this is the result of the complete combustion of the injected fuel owing to sufficient time for the fuel to combust. In the case of 100% load shown in Figure 3a, the characteristics of the heat release rate when MDO fuel and DME fuel are injected at the same time point show a tendency in which the heat release rate of DME increases more gradually than that of MDO. In the case of DME fuel, the diffusion combustion phase was more significant compared with that of MDO fuel. It seems that the higher cetane number and low autoignition temperature of DME fuel cause a fast start of combustion and promote a faster premixed combustion phase, and the flame created in premixed combustion and the excellent evaporation characteristics of DME fuel lead to diffusion combustion. Therefore, the diffusion flame presents a lower reactivity to the increment of accumulated heat release than that of MDO fuel.
3.2. Characteristics of Peak Combustion Pressure in Accordance with Injection Timing for MDO and DME Fuel

Figure 4 shows the results of peak pressure (PP) characteristics according to the injection timing of MDO and DME fuel according to BMEP. When using MDO and DME fuels, the combustion pressure tends to be similar under the same injection conditions. However, as the injection time advances, the combustion pressure increases. This is believed to be owing to the increased time to combust and the DME fuel characteristics.

Figure 5 shows the combustion characteristics according to the time when the highest pressure of MDO and DME fuel occurs. Through the experiment and numerical analysis results of MDO and DME fuel at the condition of BTDC 2.5CA injection timing, the position of the highest combustion pressure was detected and the highest combustion pressure was found to be greater for DME fuel than for MDO when the BMEP was below 12 bar; however, the position of the highest combustion pressure tended to advance when the combustion pressure was above 12 bar. This is thought to be because the diffusion flame of DME fuel is less responsive to the increase in accumulated heat release than that of MDO fuel, as described above. Moreover, as the injection time advanced, the position of the highest combustion pressure advanced.
Figure 4. Characteristics of the pressure peaks versus start of injection timing for marine diesel fuel and DME fuel.

Figure 5. Characteristics of the locations of the pressure peaks versus start of injection timing for marine diesel fuel and DME fuel.
3.3. Characteristics of NOx and PM in Accordance with Injection Timing and Nozzle Hole Diameter for MDO and DME Fuel

Figure 6 shows the combustion characteristics according to the injection timing of MDO and DME fuel for the case where the nozzle diameters are the same. Comparing the experimental and numerical analysis results of MDO and DME fuel at the same injection time, DME fuel promoted higher nitrogen oxide emissions than MDO when the BMEP was below 5 bar; however, the opposite was observed when the BMEP was above 5 bar. Nitrogen oxide emissions show a decreasing tendency for DME fuel. This is owing to the high cetane number and low autoignition temperature of oxygen-containing fuels such as DME, which also cause a rapid combustion start. Moreover, the premixed combustion time point progressed faster. This is because converted combustion caused by the excellent evaporation characteristics of DME fuel. In addition, from the characteristics of combustion and heat generation presented in Figure 3, it is believed that post combustion is reduced and nitrogen oxides are reduced owing to rapid combustion.

Figure 7 shows the nitrogen oxide emission results according to the diameter and injection timing of the nozzle using MDO and DME fuel. From these results, when the diameter of the nozzle hole is large and the injection timing is decelerated, nitrogen oxide emissions are reduced. For this reason, it can be seen that the size of the nozzle hole must be increased in order to inject the same amount of fuel because the density of DME fuel is lower than that of MDO. Therefore, it is believed that it is necessary to optimise the pore hole of the nozzle considering the fuel density when using MDO or DME.

Figure 6. Characteristics of NOx emission versus start of injection timing for marine diesel fuel and DME fuel.
Figure 7. Characteristics of NOx emission versus start of injection timing and nozzle hole diameter for marine diesel fuel and DME fuel.

Figure 8 shows the combustion characteristics according to the injection timing of MDO and DME fuel for the case where the nozzle diameters are the same. From the results of Yang [39], the emission of smoke or PM was not emitted at the region of all loads. Comparing the experimental and numerical analysis results of MDO and DME fuel at the same injection time, the overall PM emissions of DME fuel were significantly lower than those of MDO. These results were very similar to those obtained through experiments presented by Yang [39]. This is because DME is an oxygen-containing fuel and therefore causes a rapid combustion start owing to its high cetane number and low autoignition temperature. Moreover, converted combustion is caused by the excellent evaporation characteristics of DME fuel. However, as a result of the characteristics of nitrogen oxide and PM emissions when using MDO and DME fuels, the two emissions are considered to present a trade-off relationship: PM emissions decreased when nitrogen oxide emissions increased, and PM emissions increased when nitrogen oxide emissions decreased. However, owing to the fuel characteristics of DME, PM emission is very low overall, indicating that it is not necessary to consider the PM emission characteristics owing to the effect of nitrogen oxides.

Figure 9 shows the smoke (PM) emission results according to the diameter and injection timing of the nozzle using MDO and DME fuels. These results show that the PM characteristics present a dominant effect according to the change in the diameter of the nozzle hole compared with the injection timing. It is considered that the case where the nozzle’s pore hole is small is a factor affecting PM reduction. This is because DME fuel requires a smaller nozzle pore hole size to reduce PM in order to inject the same amount of fuel owing to its lower density than MDO. However, considering the characteristics of the PM emitted as a whole, it was found that the effect of the hole of the nozzle was greater than the effect of the injection timing. Finally, when considering the emission characteristics of nitrogen oxide and PM, it is believed that it is necessary to design the combustion chamber considering nitrogen oxide characteristics rather than the effect of PM.

Figure 10 shows the results of nitrogen oxide and PM measurement for MDO fuel and the nitrogen oxide and the PM reduction rates according to the injection timing and the change in the hole diameter of the nozzle for DME fuel. As the BMEP increased, the results of this study showed
that nitrogen oxide emissions decreased. When the BMEP was 23.5 bar, the nitrogen oxide and PM reduction rates were 40% and 98%, respectively, compared with MDO fuel.

Figure 8. Characteristics of black carbon emission versus start of injection timing for marine diesel fuel and DME fuel.

Figure 9. Characteristics of smoke emission versus start of injection timing and nozzle hole diameter for marine diesel fuel and DME fuel.
4. Conclusions

Herein, the characteristics of nitrogen oxide and black carbon emission reduction in accordance with injection timing and the hole diameter of the fuel nozzle using MDO and DME fuel were studied by using a numerical method on experimental data. The results are as follows:

1. As a result of the combustion and heat release rate characteristics of MDO and DME fuels according to the injection timing, as the injection timing advanced, the combustion start point occurred earlier and post-combustion was faster.

2. When MDO and DME fuels were injected at the same time point, the heat release rate of DME increased more gradually than that of MDO. The diffusion combustion phase of DME fuel was more significant than that of MDO fuel. It seems that the higher cetane number and low autoignition temperature of DME fuel cause a faster start of combustion and promote a faster premixed combustion phase, and the flame created in premixed combustion and excellent evaporation characteristics of DME fuel lead to diffusion combustion.

3. Comparing the experimental and numerical analysis results of MDO and DME fuels at the same injection time, the nitrogen oxide emissions for DME fuel were higher than those of MDO when the BMEP was below 5 bar and the opposite was observed when the BMEP was above 5 bar. This is owing to the high cetane number and low autoignition temperature of oxygen-containing fuels such as DME, which cause a rapid combustion start. Moreover, it is believed that the premixed combustion time point progressed faster.

4. The results of nitrogen oxide and PM emission measurement for MDO fuel and nitrogen oxide and PM reduction rate assessment according to the injection timing and the change in the hole diameter of the nozzle with increasing BMEP for DME fuel indicated that, when the BMEP was 23.5 bar, the nitrogen oxide and PM reduction rates for DME fuel were 40% and 98%, respectively, compared with MDO fuel.
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