Potentialsofoxymethylene-dimethyl-ether in diesel engine combustion

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Abstract

The increasing CO2 concentration in the atmosphere and the resulting climate change require an immediate and efficient reduction of anthropogenic carbon-dioxide emission. This target can be achieved by the usage of CO2-neutral fuels even with current technologies (Schemme et al. in Int J Hydrogen Energy 45:5395–5414, 2020). Diesel engines in particular are amongst the most efficient prime movers. Using oxymethylene-dimethyl-ether (OME) it is possible to solve the hitherto existing Soot-NOx-Trade-off. OME has bounded oxygen in the molecular chain. This reduces the formation of soot, but equally the calorific value. But in consideration of the physical and chemical properties of OME, it could be useful to optimize the standard diesel engine into an OME engine. As a result, single-cylinder tests were performed to obtain a detailed analysis of the differences between OME3-5 and commercially available DIN EN 590 Diesel. Based on the fact that OME has gravimetrically less than half the calorific value of diesel, twice the fuel mass must be injected for the same energy release in the combustion chamber. Therefore, at the beginning of the investigations, a variation of the injector flow rate was carried out by means of different nozzle hole diameters. The evaluation of the results included the fundamental differences in the combustion characteristics of both fuels and the determination of efficiency-increasing potentials in the conversion of OME3-5. Due to the lower ignition delay and the shorter combustion time of OME, potentials in the optimisation of the injection setting became apparent. Higher energy flows over the combustion chamber wall were noticeable in operation with OME. To get to the bottom of this, the single-cylinder investigations were supported by tests on the optically accessible high-pressure chamber and the single-cylinder transparent engine. The optical images showed a narrower cone angle and greater penetration depth of the OME injection jet compared to the diesel injection jet. This confirmed the results from the single-cylinder tests. This provides further potential in the design of the injector nozzle to compensate for these deficits. Overall, this work shows that operation with OME in a classic diesel engine is possible without any significant loss in efficiency and with little effort in the hardware. However, it is also possible to achieve more efficient use of the synthetic fuel with minor adjustments.

Keywords Oxymethylene-dimethyl-ether · Synthetic fuels · Diesel · Combustion · Optical analysis

1 Oxymethylene-dimethyl-ether

Oxymethylene-dimethyl-ether (OME) is a synthetic C1 oxygenate (no carbon–carbon bonds) which can be produced with methanol as an intermediate product from carbon dioxide and green hydrogen obtained from electrolysis. For a neutral CO2 balance, the production of OME takes place in a power-to-liquid process using renewable energies. In contrast to fossil Diesel fuel, the OME molecule chains have additional oxygen atoms between the carbon atoms, which inhibits the formation of acetylene (C2H2) as a soot precursor in the combustion process [1–6].

The chain length of the OME molecule [CH3O-(CH2O)n-CH3] determines the substance properties and the exact name (see Fig. 1). Depending on the atomic number of the oxymethylene group, these are mono-oxymethylene-dimethyl-ether (OME1) for n = 1, Di-OME for n = 2, Tri-OME for n = 3, up to the Hexa-OME for n = 6. [7]
The OME3-5 mixture used for the current investigation consisted of the following individual components: 47,1% OME3; 29,5% OME4; 16,7% OME5; 5,6% OME6.

The properties of the Diesel reference fuel and the OME3-5 fuel to be investigated are shown in (Table 1).

### 2 Basic investigations

Different publications give a look at the soot behaviour from OME in diesel engine. Härtl et al. [8] and Richter, Zellbeck [7] shown the significantly lower soot emissions in usage of OME in a diesel-combustion-engine. Jacob et al. [4] used a heavy duty single-cylinder engine. In a range from 0 to 25% EGR and a particle counter for particle size over 23 nm the particle number remained at a very low level. Beidl et al. [9] shows an increase of the particle number (< 23 nm) with OME and a EGR over 50% in a diesel combustion. Gelner et al. [10] used OME in a 6-cylinder heavy-duty-engine. With the synthetic fuel was a higher EGR possible and therefor in the emissions of NOx was reduced in the raw exhaust. In this context the after-treatment system could be optimized and regulated pollutant emissions could be further declined. This work shows the advantages of OME over diesel in a diesel engine. The following pages will show which adjustments can be made to the engine to increase the efficiency in OME operation without losing the advantages already determined.

In a separate preliminary study, it was determined that OME can be used as a drop-in fuel in the current generations of diesel engines [11]. As an 7% OME/diesel-mixture without any changes or as 15% OME/diesel-mixture with a new injection setting is a reduction of CO2 and soot emissions in already driving cars possible. The soot emissions measured by means of EEPS spectrometers also showed that the addition of OME reduces the number of particles in all size classes (see Fig. 2) and that there is no shift in the particle size distribution to smaller size classes [11]. Because of this result, further recordings of the size distribution was not necessary and a CPC (Condensation Particle Counter) was used for particle counting in the following investigation.

The engine investigation of the oxymethylene-dimethyl-ether was carried out on a single-cylinder engine based on a 2.0 l series engine. The precise control of multiple parameters and the steady state operating point mapping allow for a detailed insight into the thermodynamics of combustion and pollutant formation.

An FTIR (Fourier-Transform-Infrared-Spectrometer) was also used to measure non-limited exhaust gas components. Particular mention should be made of CH4, which is a climate-relevant greenhouse gas and has been detected in various publications (e.g., [9, 4]) when 100% OME3-5 was
used. In addition, the FTIR was upgraded to detect OME1 in the exhaust gas. Table 2 shows the essential data of the single-cylinder engine.

The aim of the investigations was to find the fundamental differences in the conversion from Diesel fuel to oxymethylene-dimethyl-ether and to explore possible potentials to increase engine efficiency in OME operation.

To consider wide ranges of the engine map, the single-cylinder campaign was carried out at 6 characteristic operating points (see Fig. 3).

3 Discussion of the results of the nozzle design

The lower heating value of OME3-5 demands an increase in the flow rate of the nozzle to bring the same energy into the combustion chamber within the same time. However, there is only little risk of higher soot emission due to the larger nozzle holes and the resulting poorer jet decay compared to Diesel fuel, because nearly no soot is produced during the combustion of the synthetic fuel.

The flow rate of an injector nozzle is measured e.g., by the fuel flowing through the nozzle within 30 s at a differential pressure of 100 bar across the nozzle. This results in the following nozzle variations:

- HD325 (325 ml/30 s): this is the Diesel reference injector for this engine.
- HD650 (650 ml/30 s): double nozzle flow, compensating for half the lower heating value of OME3-5, compared to Diesel.
- HD590 (590 ml/30 s): smaller nozzle holes improve mixture formation.
- HD1000 (1000 ml/30 s): three times the nozzle flow of the reference injector, to investigate potential thermodynamic advantages of extremely short combustion durations.

For good comparability, the flow variation was run with the same engine boundary conditions and approximately the same injection settings. Although in operation with OME3-5, no post-injection would be necessary for the postoxidation of soot, this was nevertheless retained to enable a direct comparison with Diesel fuel. To obtain approximately the same heat release in the pre- and post-injection with the different OME injectors as in operation with Diesel and the HD325 nozzle, an adjustment of the energizing times was applied.

Due to the large number of results at different operating points, the following is limited to the medium part load, where the differences between OME and Diesel are most evident.

3.1 Medium part load

The medium part load represents the situation of a vehicle acceleration and is examined with an operating temperature of engine oil and coolant of 90 °C. The other boundary conditions are:

- Engine speed: 2280 min.⁻¹
- Ind. mean effective pressure: 14 bar
- Centre of combustion: 12°C a.TDC
- Boost pressure: 1950 mbar
- Injection pressure: 1600 bar

The variation of the EGR rate was from 0 to 20% for Diesel operation and from 0 to 25% for OME operation, each in 5% steps. For better comparability the results are shown over the NOX-emissions.

Despite increasing the injection mass of the synthetic fuel, the measured particulate mass (< 0.001 g/kWh) and number (< 70.000 #/cm³) were of a clearly lower level towards the diesel measurement results. This is shown in the overview in Fig. 4 for all three OME injectors, HD 590, 650 and 1000.

Fig. 3 Operating points

Table 2 data single-cylinder engine

| Type                  | Single-cylinder-engine                                      |
|-----------------------|------------------------------------------------------------|
| Injection system      | Continental Common-Rail; Servo-hydraulic piezo injector    |
| Displacement          | 500 cm³                                                    |
| Compression ratio     | 15.5                                                       |
| Stroke/Bore/Connection rod length | 88/85/145 mm                   |
| Charging system       | External; max. 6 bar abs                                   |
| Rated power           | 35 kW at 4000 min⁻¹                                        |
| Max speed             | 4000 min⁻¹                                                 |
| Max. cylinder pressure| 180 bar                                                    |
Due to the high exhaust gas temperatures, complete oxidation of methane residues occurs after combustion, both in Diesel and OME operation. The carbon monoxide and hydrocarbon emissions were lower in OME-mode, indicating a higher conversion of the synthetic fuel. But none of the OME injectors achieved an equal or better thermal efficiency than the HD325 with Diesel fuel.

An explanation of the lower efficiency in OME operation and further results of the medium part load point are considered below for closer examination at constant raw NOx emission of 1.5 g/kWh (area marked in pale yellow in Fig. 4).

As a result of the elevated load, unburnt hydrocarbons and carbon monoxide are low in the raw exhaust gas of both fuels, due to the general high combustion chamber and exhaust gas temperature in this load point. (see Fig. 5)
elevated temperatures in the combustion chamber reduce the ignition delay and the high exhaust gas temperatures promote the oxidation of combustion residues. With the use of oxymethylene-dimethyl-ether, the unburnt hydrocarbons and carbon monoxide are reduced further. The highest CO and HC output is reached with the HD1000 nozzle, but this still was only half the quantity compared to the HD325 with Diesel. In contrast, almost no formaldehyde (CH$_2$O) emissions are detected in Diesel operation. With OME, CH$_2$O remains in the exhaust gas due to the direct occurrence in the molecular structure of the fuel.

In contrast to the HD650 and HD590, the HD1000 produces the highest pollutant emissions due to the greatly enlarged nozzle holes and the consequently poorer mixture preparation. The HD650 and HD590 are on the same level due to only minimal difference in nozzle hole sizes. The lower exhaust gas temperatures of the HD590, HD650 and HD1000 compared to the HD325 are due to the fast conversion rate and therefore the almost non-existent burnout phase of the OME. This needs to be taken into account when designing the exhaust after-treatment system of a vehicle powered for pure OME.

The HD650 achieves the highest thermal efficiency among the OME injectors, but doesn’t reach that of the HD325 with Diesel fuel. This is also evident in the CO$_2$ emissions. With its lower flow rate, the HD590 has a disadvantage in the higher-load range, as the injection time is longer compared to the HD650 and HD1000. With elongated injection duration the heat release is shifted to the thermodynamically less favourable range after TDC. As a result, the HD590 performs worse in efficiency and CO$_2$ emissions than the HD1000, which bears the disadvantages in mixture formation.

With the increase in injection pressure with higher load and with increasing nozzle hole diameter, the expected increase in noise emissions is observed. This is due to the increase in fuel flow with the increasing nozzle hole diameter and the resulting high conversion rate. Also, mixture preparation and penetration change with nozzle hole diameter, which may increase the ignition delay and, hence, the premixed fraction of fuel before ignition. In the cases shown in Fig. 6 the instantaneous heat release increases with increasing nozzle hole diameter, which results in a steeper pressure gradient and thus a higher combustion noise.

The heat release and pressure curves of the OME injectors show higher maxima and shorter burn durations with increasing flow rate. This results in steeper pressure and heat release gradients as well as in higher gas temperature peaks.

Due to the very short burnout phase in OME combustion, the start of injection of the HD590, HD650 and HD1000 is only 5°CA later than for the HD325 with Diesel, for a constant centre of combustion of 12°CA after top dead centre for all nozzles. Due to this late combustion of the synthetic fuel, the maximum cylinder pressure of the OME injectors is below that of the HD325 with Diesel fuel. This offers potential for thermodynamic optimisation by advancing the centre of combustion. This would also reduce exhaust gas losses.

As for the efficiency (Fig. 5), the difference in fuel energy supplied into the combustion chamber is minimal between the HD325 with Diesel and the HD650 with OME. (see Fig. 7) Due to the shorter heat release, the losses via the exhaust gas heat flow are lower in OME operation. The wall heat losses, on the other hand, are significantly higher with OME than in the reference with diesel. The heat release is higher with OME and this leads to higher gas temperatures (see Fig. 6). Consequently the wall heat flow is greater. But that combustion is taking place closer to the combustion chamber wall could be possible too.

3.2 Conclusion nozzle design

To achieve future emission targets, oxymethylene-dimethyl-ether shows great potential to replace conventional Diesel fuel. Even with high inert gas contents in the combustion chamber, the influence on the conversion of OME remains low. The molecular structure of OME drastically reduces the formation of soot as well as the emission of carbon monoxide and hydrocarbons. The higher fraction of formaldehyde and unburnt OME1 is due to the molecular structure of the fuel, but the concentration is low enough and can be minimised with simple catalytic exhaust gas after treatment.

4 Extended consideration of the OME combustion process

Optical measurement methods were used to analyse the mixture formation more precisely. The LVAS has an optically accessible high-pressure chamber as well as a “transparent” single-cylinder research engine. The single-cylinder engine is located in an air-conditioned chamber which allows for cold start studies down to $-25$ °C. The analysis of the injection is carried by means of four different methods, which are explained in the following.

4.1 Optical measuring methods

The optical measurement methods are categorised into self-emitting methods (solid-state-radiation and chemiluminescence) and externally excited methods (MIE scattered light and shadow/ Schlieren-measurement-techniques).

MIE scattering and shadowgraph techniques are often used in combination (see Fig. 8 bottom right) to examine lateral and longitudinal spray penetration. Data on the cone angle, penetration depth and penetration velocity of the liquid and vapour phases of the fuel jet are recorded, to
conclude on mixing with the cylinder charge and possible emission formation.

During the chemical reaction of hydrocarbons, OH radicals are formed, which emit light with a wavelength in the ultraviolet range. By means of filters, the UV radiation is recorded in the combustion images and the OH concentration can be deduced from the radiation intensity. A high OH concentration indicates a high fuel conversion. UV images only allow for a relative evaluation between different measurements.

The combustion of Diesel fuel on a injected jet shows clearly visible soot radiation. Similar to the glow of the OH radicals, the intensity of the yellow soot radiation is directly related to the conversion rate. A brighter, more yellowish light intensity indicates more soot burnt.

Since the combustion of OME is nearly soot-free, only the inherent OH luminescence can be used for solid-state radiation.

4.2 Optical investigation in the high-pressure chamber

For a more detailed analysis of the mixture formation of oxymethylene-dimethyl-ether injected into the combustion...
chamber, the temperature and pressure conditions prevailing in the single-cylinder engine at the time of injection were simulated in a high-pressure chamber located at the LVAS. These investigations serve for the direct comparison of the injection behaviour between the conventional Diesel fuel with HD325 nozzle and OME with the optimum HD650 nozzle, found in the single-cylinder investigations.

Boundary conditions:

- Injection pressure: 2000 bar
- Gas temperature: 1010 K
- Chamber pressure: 72 bar
- Gas density: 2282 kg/m$^3$
- Injection duration: 1.2 ms

Figure 9 compares the HD325 with Diesel and the HD650 with OME. The image shows the spray pattern after half of the injection time, when the jets of both injectors are fully developed. The blue lines near the nozzle indicate the penetration length of the so-called liquid fuel. The inner and outer yellow rings indicate the bowl edge and the cylinder wall, respectively. The red lines are the penetration length of the fuel vapour, which has already penetrated to the edge of the image due to the absence of a piston bowl in the high-pressure chamber.

The difference in penetration length of the two fuels is too small for the conclusion a significant influence on combustion. However, more decisive are the cone angles of the liquid and vapour fuel phases. These are much narrower in the case of the OME spray, which causes a higher fuel concentration at the position of the combustion bowl. This is also indicated by the shadow of the OME vapour phase, which is clearly darker than that of the Diesel spray at the inner yellow ring. Due to the higher fuel concentration, the combustion and thus the heat input into the bowl and rim is also more concentrated. This behaviour is also reflected in the combustion images in Fig. 10. To make the different OH concentrations more visible, both images were converted into false colour images using a fixed colour scale, where blue indicates low OH concentration, red high OH concentration.

As in the spray image, the HD650 injector with OME has a much narrower flame cone in contrast to the HD325 injector with Diesel. The areas with the highest OH concentration are also located much further inwards in the images with Diesel. Due to the higher density of the OME, the fuel spray has a higher swarm inertia, i.e., droplets travel in the wake
of other droplets. In addition, the lower viscosity/surface tension reduces the internal friction in the liquid fuel. As a result, OME droplets are also broken up less intensively and thus penetrate further into the combustion chamber than Diesel droplets. This is obviously a trade of between break up mechanism and evaporation rate. These properties also produce a lower cone angle of the OME spray lobe.

The consequence of this largely different OME fuel jet is a strong shift in heat release towards the outer regions of the combustion bowl. On the one hand, this leads to greater wall heat losses compared to Diesel operation, and on the other hand, if the injection period is long enough, the constantly high and concentrated temperature load on the piston surface is likely to cause damage.

The engine effects of these properties of the OME fuel jet will be examined in more detail in the next Section, on the basis of the results from the transparent engine.

### 4.3 Investigation of the temperature behaviour of OME on the optically accessible transparent motor

#### 4.3.1 Test engine

OME has a lower viscosity and higher density than conventional Diesel. Due to this, the single-cylinder tests showed larger wall heat transfer with OME, which suggested a higher penetration length. This was confirmed in the previous chapter in measurements in the high-pressure chamber.

To understand the processes in the combustion chamber and also to investigate the cold start behaviour as well as the combustion at low operating temperatures, the transparent engine located at the LVAS (see Fig. 11) was employed. This is based on the same base engine as the metal single-cylinder research engine used for the OME tests.

The design for optical access required a reduction of the compression ratio. To recreate the combustion chamber pressures and temperatures at the time of injection with the reduced compression ratio on the metal single-cylinder research engine, the boost pressure was adjusted. This adaptation was carried out in a preliminary investigation on the transparent engine by initially operating it with a metal replacement instead of the glass window. This reproduces the referenced pressure and heating curves from the full-metal single-cylinder tests.

To realise the operating temperatures of $T_{\text{coolant}} = 90$ °C, 25 °C and −7 °C, the transparent motor was located in a climatic chamber. This chamber allows for the control of pressures and temperatures of the ambient air as well as oil, cooling water and charge air to the desired temperature.

#### 4.3.2 Result in medium part load

The investigated part load point has one pilot injection, a postinjection and was run at the following boundary conditions:

- Engine speed: 2280 min.$^{-1}$
Ind. mean effective pressure: 8 bar
Centre of combustion: 12°CA a.TDC
Boost pressure: 2050 mbar
Injection pressure: 1600 bar

Over the entire combustion process and at all operating temperatures, no soot radiation was recorded with OME. In the case of Diesel fuel yellow-orange soot radiation appeared at an operating temperature of 90 °C from -3°CA before TDC (top dead centre), became more intense in the further course of combustion and spread further into the combustion chamber (see Fig. 12). As the coolant temperature decreased the soot radiation became weaker due to the increase in pre-mixed combustion and lower diffusive combustion.

The single-cylinder tests already showed higher energy inputs into the engine media in OME compared to Diesel combustion, which suggests greater wall heat losses. The previously presented results from the high-pressure chamber tests supported this assumption, which was confirmed in the UV images of the transparent engine. It is clearly shown that the OME fuel jet penetrates further into the bowl and forms a more intensive ring of fire along the combustion bowl rim (see Fig. 12). As described previously, this behaviour is caused by the high density and low viscosity/surface tension of the OME compared to Diesel.

In the Diesel case there are correspondingly more areas with a strong OH concentration closer to the centre. In the OME case no such maxima occur, but there is a uniformly distributed OH concentration at the bowl rim. The strongest OH concentration in the Diesel case exists at the glow plug. This is due to the fact that one of the fuel jet plumes passes the glow plug very closely. This leads to a high fuel concentration around and possibly on the glow plug, probably due to a slowed down charge motion and/or slight glow plug wetting. This is reflected in the strong OH and soot radiation. Due to the narrower cone angles in OME operation, this phenomenon does not occur. The generally weaker concentration of OH radicals during OME combustion originates from the molecular structure and the greater penetration length as described above. The OH concentrations for OME and

![Fig. 11 Transparent motor](image-url)
Diesel fuel indicate much more inhomogeneous combustion process for Diesel compared to OME. This can probably be attributed to the very wide variation of molecule chain length in Diesel, while OME is restricted to short chains of formaldehyde groups. This is confirmed by the good ignitability of OME, which also becomes evident, when operating temperatures are low.

The reduction of the operating temperature has a greater influence on the ignition delay for Diesel fuel than for OME. In addition to the heat release curves (see Fig. 13), the increased ignition delay is also evident in the photographs in Fig. 12. At 25 °C, the pilot injection of the Diesel no longer ignites, but premixes and burns together with the premixed phase of the main injection/combustion. In contrast, with OME the pilot still ignites and ensures a uniform increase in the heat release of the main injection. There is only little difference in the heat release and pressure curves at 90 and 25 °C operating temperature (see Fig. 13, pilot heat release, bottom right and top left diagrams, dark and middle blue).

If the temperature is reduced further to −7 °C, the main injection is hardly ignited during Diesel operation. From 3°CA onwards, individual injection jets close to the glow plug begin to burn, but the top injection jets remain unburnt. Figure 13 shows a very late combustion with low pressure rise (light green trace), indicating incomplete combustion. Only with the postinjection at −9°CA the Diesel fuel ignites. The steep rise in heat release after 12°CA aTDC indicates the combustion of the premixed fuel of the pilot and parts of the main injection.

OME combustion at −7 °C still shows a relatively homogeneous combustion of all jets, if at a lower OH intensity. This is also shown in Fig. 13, light blue trace, which similar to the light green Diesel curve, displays later combustion. However, with OME there is still a faint rest of a pilot combustion present. In the OH images the ignition of the postinjection can be detected at 18°CaTDC. Although OME also shows an increased ignition delay with lower temperature, the ignition readiness still ensures a faster and more homogeneous combustion event.
5 Summary and outlook

The current investigations show that OME3-5 has the potential to be used as an alternative Diesel fuel in future diesel engines. One big advantage of OME is the lack of soot emission. This means the soot-NO\textsubscript{x} trade-off is omitted and much higher EGR rates are possible. This allows for a further reduction of nitrogen oxide emissions, especially also at cold start, where SCR catalysts do not work yet.

The reason for this are the oxygen atoms in OME, which prevents the formation of soot precursors. The reason for the drastic reduction of particle emission is that OME is made up from –CH\textsubscript{2}–O– repeating units. As a result OME lacks the C–C bonds, which are the molecular prerequisite for soot precursors. In addition, this special molecular structure ensures that other pollutant emissions such as carbon monoxide and hydrocarbons are much lower than with Diesel fuel. The disadvantage, however, is that the presence of oxygen in the molecule reduces the gravimetric energy content by half compared to Diesel. As a result, fuel consumption with OME doubles for the same engine output. Therefor the destination of this research was to find the optimal nozzle from three different nozzle hole diameters.

The results from the single-cylinder engine research shows only a small deficit in efficiency of all three OME nozzles against the diesel nozzle. The carbon monoxide and hydrocarbon emissions and the exhaust gas losses are lower with OME. In addition to the emission benefits, the single-cylinder tests and the optical recordings demonstrated the need for a further development of the injection system. The increased wall heat loss in the single-cylinder tests already indicated greater penetration length of the OME fuel jet. This assumption was confirmed with the optical recordings in the high-pressure chamber and the transparent engine. The higher density and the lower viscosity of OME yield a narrower OME spray, penetrating further towards into the combustion bowl. To compensate for this an altered nozzle hole design would be necessary. This also means that there is still some potential for increasing efficiency by means of an optimised injection system for OME.

Finally, in an investigation of the cold-running behaviour, OME finally showed a lower ignition delay and better conversion in the combustion chamber compared to diesel due to the high cetane number.

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