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Potential of oxymethylenether-diesel blends for ultra-low emission engines



Ahmad Omari*, Benedikt Heuser, Stefan Pischinger

Institute for Combustion Engines, RWTH Aachen University, Germany

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ABSTRACT

In the race to counteract global warming, fossil fuel dependency and urban air pollution, it is clear that vehicle emissions have to be reduced considerably. A pathway out of today's limitations in engine technology is synthetic fuel. In particular, oxymethylenether (OME) is an attractive candidate due to its soot free combustion. In this work, OME₁ – diesel blends are considered aiming to outline their potential as a near future alternative fuel. Various blends ranging from 0% to 80% vol OME₁ in diesel fuel were investigated in a single cylinder research engine. Results show that tradeoffs of NO_x-soot and NO_x-HC/CO are in general retarded with increasing OME₁ content in the fuel. With 50% (vol) OME₁ in diesel, the NO_x-soot tradeoff is completely eliminated up to the higher end of moderate loads ~10 bar. Furthermore, with increasing content of OME₁ in the blend, exhaust gas temperatures reduce down to –7% (°K) and indicated thermodynamic efficiency increases up to +2% with respect to pure diesel. Due to the lower cetane number (CN) of blends containing OME₁, the combustion noise level increase at lower loads compared to diesel combustion. At higher loads, the lower heating value of the OME₁-containing blends results in a reduction of combustion noise. To identify an optimal blending range for OME₁ in diesel, the soot reduction potential is systematically analyzed by a Gaussian process regression analysis at the higher load points. From the analysis an optimal blend ratio of 35% OME₁ in diesel is suggested, being the best compromise between soot reduction (~90%) and the deterioration of fuel properties like heating value (–15%) and cetane number. With a CN of 51, the 35% OME₁-diesel blend still complies with the CN lower limit in the current EN590 Norm. Finally, we conclude that from the combustion and emission point of view, OME₁ is a superior diesel fuel substitutive, in particular when higher blending ratios (20–40%) are considered.

1. Introduction

Aiming to reduce greenhouse gas emission, fossil fuel dependency and mitigation of urban air pollution, upper limits for vehicle emissions are continuously reduced by the legislation authorities [1]. Upcoming Real Driving Emission (RDE) legislations are expected to confront engine developers with new challenges mostly leading to complex and costly exhaust aftertreatment systems [2,3]. Consequently, alternative fuels tend to become a vital pathway for the future. For diesel engines, such fuels must not only reduce the carbon footprint, e.g. biofuels, but also have the potential for drastic soot reduction. Thereby, new flexibilities are created to comply with strict limits for Nitrogen oxide (NO_x) emissions. In this regard, oxygenated fuels are considered very promising [4–8]. In particular, the synthetic fuel oxymethylenether (OME₁), which was already recognized within the last two decades [9,10], has recently drawn new attention [4,11–19]. Pure OME₁ combustion shows no soot formation at all [20], not only because of the high amount of oxygen bounded in the molecule (42%), but also due to the lack of C-C bonds (CH₃-O-CH₂-O-CH₃) [16]. In addition, a high

volatility and a low reactivity contribute to soot suppression as well. In a recent work of Härtl et al. [4] OME₁ was identified to have the highest soot reduction potential among a broad range of oxygenated fuels. From the availability point of view, OME₁ can be easily synthesized from methanol [14,21] thus having the potential for near future implementation as a pollution mitigating blending component in diesel fuel. In a long term view, OME₁ might be produced via direct synthesis routes with recaptured carbon dioxide (CO₂) and renewable hydrogen [22,23], making it a sustainable alternative fuel candidate for the future. In a recent work of Schmitz et al. [14] the production costs of OME₁ out of methanol were predicted for a large scale production scenario. A conservative synthesis route was chosen with methanol and water as feedstock and formaldehyde as an intermediate step towards OME₁. With this route, 1.33 kg of methanol is needed to synthesize 1 kg of OME₁. The OME₁ cost was varied over a wide range of methanol cost leading to the finding that the feedstock price is the major factor dominating the OME₁ price. In an exemplary case it is shown that a methanol cost of 300US\$/t leads to an OME₁ price of 559US\$/t, corresponding to an increase of 86% [14]. However, when accounting for

* Corresponding author.

E-mail address: Omari@vka.rwth-aachen.de (A. Omari).

the lower heating value of methanol compared to OME₁, the cost of 1 MJ OME₁ exceeds the cost of 1 MJ methanol by 60%. Considering an exemplary diesel fuel price of 0.5US\$/liter at the refinery in comparison with the above mentioned OME₁ price, the OME₁ cost exceeds diesel by 70% per energy unit. The latter cost penalty can be further reduced when synthesis routes are optimized for OME₁ production. Deutz et al. [24] have compared the environmental impact and the exergy balance of two OME₁ synthesis routes (formaldehyde route vs. novel direct route according to [22]) and found that the exergy efficiency from H₂ to OME₁ could be improved from 74% to 86%.

An additional concerning aspect of OME₁ is the high vapor pressure. Vertin et al. [9] reported a Reid vapor pressure of ~1 bar (at 37.8 °C) for pure OME₁ in a closed tank. At 71 °C, ~2.75 bar was measured. The consequence would be high fugitive emissions when opening the tank in addition to a flammability hazard. Hence, a sealed fuel tank to contain the fuel vapors and a quick-disconnect dispensing nozzle was proposed in their work. To evaluate the flammability hazard of the trapped fuel vapors in the tank, Vertin et al. [9] measured the upper and lower temperatures at which a self-propagating flame could be maintained in the tank. For blending ratios in the range of 20% to 50% OME₁ in diesel, the flammability region was found to be within –30 °C to +6 °C. Above 6 °C, the vapor-air mixture was too rich for flame propagation.

Nevertheless, OME₁ properties are not optimal to be used as a pure fuel, not only due to its low boiling point which imposes handling and storage issues similar to those of gaseous fuels. The low reactivity and lubricity are further shortcomings although they might be overcome with proper additives [4]. Finally, the low heating value (20.1 MJ/l) may put dedicated OME₁ vehicles in an unattractive perspective compared to electric vehicles. Considering the above, the vision followed in this work is the partial substitution of OME₁ in diesel fuel. Such an approach provides several benefits over the use of pure OME₁ as a fuel. For example, small amounts (~5%) of OME₁ could be considered already nowadays thereby enhancing it's the large-scale production and market introduction. In a future scenario, where the production capacities of OME₁ by re-captured CO₂ and renewable hydrogen have increased, higher blend ratios shall be considered. In such a scenario, OME₁ availability is still limited, and the question arises whether it would be preferable to use the given amount of OME₁ as a pure fuel or as a blend with diesel. It is anticipated by the authors that by utilizing the OME₁ as a blend, a higher pollutant emission reduction can be achieved. In other words, running one vehicle on pure OME₁ and one on diesel is anticipated to give less pollutant reduction potential than running two vehicles with a 50:50 OME₁-diesel blend. Considering the latter, the fundamental question arises: What blend ratio would be the optimal one? This question is investigated in this work. In addition, a combustion and emission characterization was performed for several OME₁-diesel blends on a single cylinder engine.

2. Methodology

Four OME₁-diesel blends in addition to EN590 diesel (B7) as a reference were investigated on a single cylinder engine. Furthermore, the cetane number (CN) was measured for various blend ratios with the advanced fuel ignition delay analyzer AFIDA 2805. The properties of the considered fuels are given in Table 1. Except for CN, blend properties are calculated according to the mass fractions of OME₁ and diesel in the blend. Being a solvent, no miscibility issues of OME₁ in diesel were observed in the complete blending range. Due to the low boiling temperature of OME₁, a pressurized fuel tank was used to avoid possible cavitation in the supply fuel pump. Also, the fuel tank was hermetically sealed to prevent fumigation of OME₁ out of the blend.

Specifications of the single cylinder engine and emission measurement system are given in Table 2 and Table 3 respectively. In order to measure the fuel consumption a Coriolis flow meter is used. For the intake air flow an ultrasonic gas meter is used. The exhaust gas

Table 1
Fuel properties.

Property	unit	diesel (B7)	OME ₁ -diesel blends				OME ₁
OME ₁ content	vol%	0	20	35	50	80	100
Oxygen content	w.%	0.8	9.3	15.6	21.8	34.1	42.1
Hydrogen content	w.%	13.5	12.9	12.4	12.0	11.1	10.5
Carbon content	w.%	85.8	77.9	72.0	66.2	54.8	47.4
Density	kg/L	0.835	0.836	0.840	0.845	0.853	0.859
Lower heating value	MJ/kg	42.8	38.8	35.9	33	27.2	23.4**
Cetane number	–	55	53	51	48	37	24
Lubricity (HFRR)	µm	< 460	–	–	–	–	759 [4]
Kinematic viscosity	mm ² /s	2–4	–	–	–	–	0.36 [11]
Flashpoint	°C	> 55	–	–25*	–	–	–32 [25]

*DIN EN ISO 3679, **DIN 51900–2 mod.

Table 2
Specification of single cylinder engine.

Feature	Value
Bore/Stroke	75 mm/88.3 mm
Displacement	0.39liter
Number of valves	4
Compression ratio	15
Maximum boost press.	4 bar (abs)
Peak firing pressure	220 bar
Piston bowl geometry	ω-shaped reentrant

Table 3
Emission measurement devices.

Emission	Device	Accuracy
Soot	AVL 415s (Filter paper method)	2%
NOx	Chemiluminescence detector*	1%
HC, as C ₃ H ₈ equiv.	Flame ionization detector**	1%
CO, CO ₂	Non dispersive infrared**	1%
O ₂	Paramagnetic detector**	1%

*EcoPhysics CLD 700 EL **Rosemount – NGA 2000 Series.

recirculation (EGR) rate is determined by the CO₂ concentration in the intake plenum. The in-cylinder pressure is measured by a water cooled piezo electric pressure transducer (Kistler 6041A) and logged at a 0.1° crank angle resolution. Subsequently, cylinder pressure traces were processed with FEV's "Combustion Analysis System". Combustion and emission characteristics of the OME₁-diesel blends were obtained at predefined screening load points (LP) given in Table 4. The boundary conditions were determined based on data from the equivalent four cylinder engine. The center of combustion was set constant for a given load point. Thus, changes in combustion and emission characteristics could be related to the fuel only. Finally, the screening data were evaluated by a Gaussian process regression analysis method. Here the

Table 4
Engine load points and boundary conditions.

Name	IMEP [bar]	Speed [min ⁻¹]	MFB50° [°C AaTDC]	Boost [bar]	Rail press. [bar]
LP1	4.3	1500	6.6	1.07	720
LP2	6.8	1500	5.8	1.5	900
LP3	9.4	2280	9.2	2.29	1400
LP4	14.8	2400	10.8	2.6	1800

*MFB50: degree crank angle where 50% of the fuel mass has burned.

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