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Potential of using OMEx as substitute of diesel in the dual-fuel combustion mode to reduce the global CO_2 emissions

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ABSTRACT

To achieve the targets of extreme low emissions values for the transport sector, several technologies emerged in the last few years. In this sense, advanced combustion modes as the dual-fuel low temperature combustion showed great advantages in terms of NO_x and soot emissions reduction. At low and medium engine load, the operation is stable with virtually zero emissions. However, the exhaust gas recirculation rates at high load need to be increased to avoid excessive in-cylinder peaks, which leads to higher soot emissions. At these conditions, the use of non-sooting fuels as the oxymethylene dimethyl ethers (OMEx) allows avoiding the NO_x-soot trade-off. In addition, the e-fuel consideration of the OMEx makes it suitable to reduce the global GHG emissions. This paper assesses the potential of using OMEx as high reactivity fuel to reduce the CO_2 well-to-wheel emissions, and NO_x and soot tailpipe emissions, in a medium-duty truck operating under dual-fuel combustion in transient conditions. The cargo mass was varied between 0% and 100% (18 ton) in the World Harmonized Vehicle Cycle. The tank-to-wheel analysis shows slightly higher CO_2 production with OMEx-gasoline than with diesel-gasoline due to the ratio between the lower heating value and the carbon content. However, the well-to-wheel analysis shows the benefits of using OMEx to reduce the carbon dioxide footprint, which ranges from 13% (at full cargo mass) to 19% (at low cargo mass) compared to diesel-gasoline dual-fuel mode. This benefit is due to the large gains in terms of fuel production due to the carbon capture and the clean electric energy source necessary to produce the OMEx.

1. Introduction

The problem of air pollution in the cities around the world is aggravating along the years. Nowadays, a general trend towards to prohibit the old diesel vehicles entering into the cities to improve the air quality is being stablished. Diesel engines are accused to be major responsible for the high nitrogen oxides (NO_x) and particle matter (PM) levels in the ambient air of urban areas [1,2]. However, compression ignition (CI) engines offer better fuel economy, reliability, and less carbon monoxide (CO) and hydrocarbons (HC) emissions than the spark ignition (SI) engines [3]. In order to increase the acceptance of CI engines, a further reduction of their tailpipe emission is necessary.

To achieve this target, companies and researchers have developed several technologies to improve the combustion process: higher injection pressures, injector holes with lower diameter and optimized combustion chambers with sophisticated bowl geometries, among others. Also, to achieve the ultra-low emissions imposed by the regulations, more complex after-treatment systems (ATS) are needed to be installed in the vehicle to reduce the engine-out emissions: selective catalyst reduction (SCR) with urea dosing system, diesel particle filter (DPF) and diesel oxidation catalyst (DOC) [4]. In spite of this equipment is effective to achieve the current legislation targets, the cost is too high and the companies are looking for new technologies. In this line, advanced combustion modes as low temperature combustion (LTC) are receiving special attention due to the capabilities to reduce the engine-out emissions with high combustion efficiency [5,6]. It possible to achieve ultra-low NO_x and soot emissions thanks to using high amounts of exhaust gas recirculation rates (EGR) and a greater degree of premixed

Abbreviations: ATS, Aftertreatment systems; BSFC, Brake specific fuel consumption; CDC, Conventional diesel combustion; CI, Compression Ignition; CO, Carbon MoNO_xide; CO_2, Carbon Dioxide; DOC, Diesel Oxidation Catalysts; DPF, Diesel Particulate Filter; ECU, Engine control unit; EGR, Exhaust Gas Recirculation; EU, European Union; GHG, Greenhouse gas emissions; HCCI, Homogeneous Charge Compression Ignition; HRF, High Reactivity Fuel; ICE, Internal combustion engine; LHV, Lower Heating Value; LRF, Low Reactivity Fuel; LTC, Low Temperature Combustion; NO_x, Nitrogen Oxides; OEM, Original equipment manufacturer; OMEx, Oxymethylene dimethyl ether; PM, Particulate Matter; PER, Premixed Energy Ratio; PFI, Port fuel injection; TTW, tank-to-wheel; RCCI, Reactivity Controlled Compression Ignition; rpm, Revolution per minute; SCR, Selective Catalytic Reduction; SI, Spark Ignition; WHVC, Worldwide Harmonized Vehicle Test Cycle; WTT, Well to Tank; WTW, Well to wheel.

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combustion than conventional diesel combustion (CDC) [7]. One of the potential LTC concepts is the reactivity controlled compression ignition (RCCI) [8], which uses two fuels to control the mixture reactivity [9]. This allows to operate at extreme low combustion temperatures with acceptable stability. Also, the ignition control is easier than in other advanced combustion modes as homogeneous charge compression ignition (HCCI) due to the possibility to change the proportion between the high reactivity fuel (HRF) and low reactivity fuel (LRF) [10].

In spite of the improvements of the dual-fuel concept in the brake thermal efficiency and tailpipe emissions, it is necessary to implement other strategies to drastically minimize the emissions of the greenhouse gasses (GHG) produced by the transport sector [11]. Advanced fuels extracted from renewable sources are one potential option to achieve the legislation targets [12]. The next generation of fuels must be scalable, extractable from renewable sources, and present good combustion properties. To be applied at large scales, the new fuels need to be easily adapted to the nowadays combustion devices to minimize the final emissions with a low cost of production and transportation. In spite of that the heavy-duty vehicles as trucks and buses represent a small part of the transport sector, it emits almost 50% of the CO_2 emissions [13]. Therefore, each effort to reduce the GHG emissions is well justified to achieve the desired emissions targets stablished by the governments [10]. The European community stablished reduction targets of 15% in 2025 and 30% in 2030 for heavy-duty vehicles together with achieving the Euro 6 levels for the rest of the emissions. This is a complex scenario for the internal combustion engines (ICEs) due to the necessity of direct reduction of fuel consumption and engine-out emissions at the same time. Synthetic fuels (e-fuel) have been proved to be an adequate solution both to reduce harmful emissions as well as the dependence on fossil fuels. In general, they are obtained by chemical processes from renewable electricity in a synthetic process that consumes carbon dioxide and water [10]. Therefore, it is considered a neutral or very low carbon fuel. Oxymethylene dimethyl ethers (OME*x*) are an electronic fuels, which are formed by a chemical structure CH_3–O–(CH_2–O) *x*-CH_3, being *x* in the range of 1–5 [13,14]. This fuel can be produced from methanol and formaldehyde [15]. Due to the large number of oxygen atoms and the absence of C–C bonds, the OME*x* combustion process has zero soot emissions [16]. In spite of that the average efficiency of the OME*x* production is comparable to the efficiencies obtained in the Fischer–Tropsch diesel, gasoline or methanol production, the demand for electrical energy is considerably lower for the OME*x* production [17].

This paper studies the combination of an e-fuel (OME*x*) together with a new combustion concept (RCCI) as a way to reach low CO_2, NO_x and soot emissions simultaneously. To do so, a numerical vehicle model is fed with experimental tests from a multi-cylinder heavy-duty engine to obtain the average fuel and CO_2 emissions in transient conditions. The results obtained with the OME*x*-gasoline calibration are compared to diesel-gasoline operation. Finally, a well to wheel (WTW) analysis is performed to have a global perspective of the benefits at the tailpipe as well as a global level.

2. Materials and methods

2.1. Engine and test cell

The experiments were performed in a multi-cylinder, 8 L, compression ignition engine, commercially available and designed to operate under conventional diesel combustion. Several modifications were performed to allow the engine to operate under dual-fuel combustion. In particular, an additional fuel line was installed to supply the LRF through the port fuel injector (PFI) in the intake port. The piston bowl was also optimized to improve the RCCI mode compared to the original design (used in the conventional diesel combustion mode). Moreover, the original compression ratio (CR) was reduced from 17.5:1 to 12.8:1 to allow the dual-fuel mode to operate at high loads due to the high peaks of in-cylinder pressure. The original engine design had only a high-pressure EGR line. To provide EGR with lower temperature and without reducing the mass flow in the turbine, a low-pressure EGR system was added. This solution provides higher flexibility on the turbine and the possibility to achieve high EGR rates. In addition, this system allows the possibility to control the EGR temperature with the mixture between high and low pressure EGR. Table 1 summarizes the main characteristics of the engine. More information could be found in previous publications [14].

Table 1
Main ICE characteristics.

Parameter	Value
Engine type	4 Stroke, 4 valves, direct injection
Number of cylinders	6
Displacement volume	7.78 L
Stroke	135 mm
Bore	110 mm
Piston bowl geometry	Bathtub
Compression ratio	12.75:1
Rated power	235 kW @ 2100 rpm

Table 2
Main fuel properties.

Property	Diesel	OME*x*	Gasoline
Fuel use	HRF	HRF	LRF
Density [kg/m^3]	838	1067	720
Viscosity [mm^2/s]	2.67	1.18	0.55
Cetane Number [dimensionless]	54.0	72.9	–
RON [dimensionless]	–	–	95.6
MON [dimensionless]	–	–	85.7
LHV [MJ/kg]	42.61	19.04	42.40
Carbon content [$\%_{mass}$]	85.9	43.6	84.2
Hydrogen content [$\%_{mass}$]	13.3	8.8	15.8
Oxygen content [$\%_{mass}$]	0.8	47.1	0
Nitrogen content [$\%_{mass}$]	0	0.5	0
CO_2 formation [g_{CO2}/g_{Fuel}]	3.17	1.60	3.09

2.2. Fuels

Three diferent fuels were used to perform the CO_2 analysis shown in this work. Diesel and OME*x* are propesed as HRF and gasoline as LRF. The calibration of the whole engine map was performed with diesel-gasoline, and a tentative scenario is proposed with OME*x*-gasoline. Table 2 shows the main properties of the fuels used. It is worth to note the large difference in lower heating value (LHV) between diesel and OME*x*. This will increase the fuel injected for the OME*x* case. However, the carbon content for OME*x* is strongly lower. Therefore, for the tailpipe or tank-to-wheel analysis, this factors will push for oppossite sides.

To understand which parameter is more important, the CO_2 formation ($CO_{2formation}$) is calculated as the mass production of CO_2 (m_{CO_2}) in a complete combustion process per mass of fuel (m_{fuel}):

$$CO_{2\,\mathrm{formation}} = \frac{m_{CO_2}}{m_{\mathrm{fuel}}} = \frac{n_{CO_2} * MW_{CO_2}}{m_{\mathrm{fuel}}} = \frac{n_c * MW_{CO_2}}{m_{\mathrm{fuel}}} \tag{1}$$

with n_{CO_2} the number of moles of CO_2 and MW_{CO_2} the molecular weight of CO_2. An interesting parameter, when the substitution of a fuel is proposed, is the ratio between the CO_2 mass production. Eq. (2) shows the ratio between the HRF substitution, OME*x*/Diesel:

$$\frac{m_{CO_{2_{\mathrm{Omex}}}}}{m_{CO_{2_{\mathrm{Diesel}}}}} = \frac{m_{\mathrm{OMEx}} * CO_{2\,\mathrm{formation,OMEx}}}{m_{\mathrm{diesel}} * CO_{2\,\mathrm{formation,diesel}}} \tag{2}$$

In this work, it was assumed that the substitution of diesel as HRF by OME*x* is made by the same premix energy ratio (PER). The PER is calculated as follows:

$$PER = \frac{m_{\mathrm{LRF}} * LHV_{\mathrm{LRF}}}{m_{\mathrm{LRF}} * LHV_{\mathrm{LRF}} + m_{\mathrm{HRF}} * LHV_{\mathrm{HRF}}} \tag{3}$$

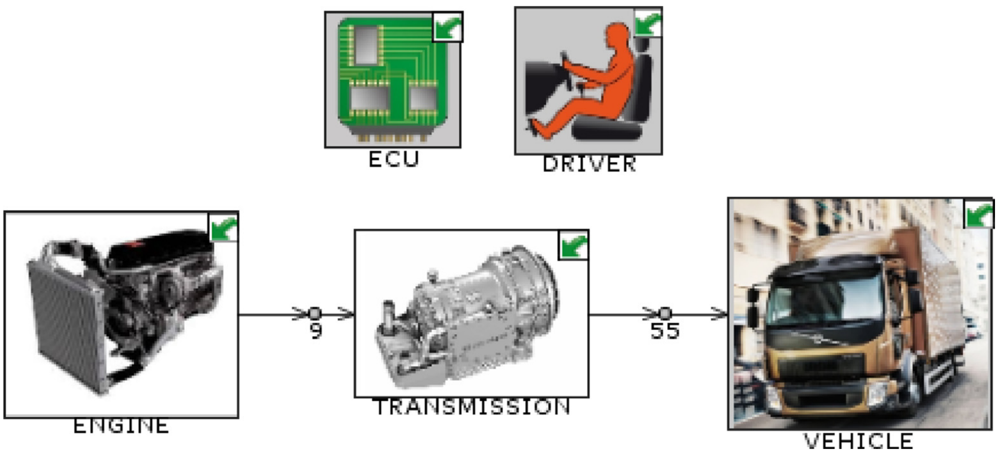

Fig. 1. Powertrain numerical model.

Therefore, the mass of OME*x* used in each condition can be obtained from the diesel-gasoline dual-fuel calibration as follow:

$$m_{\mathrm{diesel\_tot}} * LHV_{\mathrm{diesel}} = m_{\mathrm{OMEx}} * LHV_{\mathrm{OMex}} \tag{4a}$$

$$m_{\mathrm{OMEx}} = m_{\mathrm{diesel\_tot}} * \frac{LHV_{\mathrm{diesel}}}{LHV_{\mathrm{OMex}}} \tag{4b}$$

Using Eqs. (4b) and (2) it is possible to obtain the CO_2 mass production ratio between the two HRF:

$$\frac{m_{CO_{2_{\mathrm{Omex}}}}}{m_{CO_{2_{\mathrm{Diesel}}}}} = \frac{42.5}{19.04} * \frac{1.6}{3.17} = 1.125 \tag{5}$$

This means that the OME*x* will increase the tank to wheel (TTW) CO_2 emissions, if the premix energy ratio is maintained. Therefore, with this preliminary analysis, it is possible to affirm that the final benefits will be due to the well to tank (WTT) CO_2 reduction and not due to differences in the combustion process. For this reason, a WTT section was added to obtain a global perspective on the real potential to reduce the GHG emissions.

2.3. Truck numerical model

The experimental engine test in stationary conditions were used to feed a 0D vehicle numerical model to simulate the truck operation in transient conditions (driving cycles). The GT-Suite interface (v2019, Gamma Technologies, LLC., Westmont, IL, USA) was used with a calibrated medium-duty truck platform that originally equips the 8 L multi-cylinder engine. The software includes several modules to model the vehicle traction forces, transmission and control units (electronic control unit (ECU), brakes control, etc.). The speed-time profile of the driving cycle to be studied is inserted in the driver module, which determines the pedal accelerator, brake and clutch positions as a real driver. The driver aggressiveness was use as default, typically used for a moderate driving condition.

As mentioned, the vehicle selected for the study is a medium-duty truck capable to transport up to 12 tons of cargo mass. This means that the total truck mass is around 20 tons at maximum load. The truck has the powertrain layout showed in Fig. 1 with the engine coupled to a 6-gear manual transmission and finally coupled by a conventional differential with the rear wheels. This original equipment manufacturer (OEM) powertrain layout was used to compare both HRF fuels (OME*x* and Diesel) with gasoline as LRF. The main truck parameters are described in Table 3.

In the ICE model, the brake specific fuel consumption map (BSFC) in total mass (HRF+LRF) per kWh was inserted as well as the PER map. Therefore, it is possible to determine the fuel consumption of each fuel with the following equation:

Table 3
Main vehicle characteristics.

Parameter	Value
Truck mass	8000 kg
Max cargo mass	12,000 kg
Frontal area	5.24 m^2
Cd	0.65
Differential ratio	5.29
Transmission ratios	3.36/1.91/1.42/1.00/0.72/0.62

$$\dot{m}_{\mathrm{LRF}} = \frac{\dot{m}_{tot} * PER * LHV_{\mathrm{HRF}}}{LHV_{\mathrm{LRF}} - PER * LHV_{\mathrm{LRF}} + PER * LHV_{\mathrm{HRF}}} \tag{6a}$$

$$\dot{m}_{\mathrm{HRF}} = \dot{m}_{tot} - \dot{m}_{\mathrm{LRF}} \tag{6b}$$

with $\dot{m}_{tot}$ the total mass fuel rate at each instant along the driving cycle. The total mass of each fuel is calculated with:

$$m_{\mathrm{HRF}} = \int_{t=0}^{t=cycle\ end} \dot{m}_{\mathrm{HRF}} * dt \tag{7a}$$

$$m_{\mathrm{LRF}} = \int_{t=0}^{t=cycle\ end} \dot{m}_{\mathrm{LRF}} * dt \tag{7b}$$

and can be calculated in energy basis as follows:

$$HRF_{\mathrm{energy}} = m_{\mathrm{HRF}} * LHV_{\mathrm{HRF}} \tag{8a}$$

$$LRF\_\mathrm{energy} = m_{\mathrm{LRF}} * LHV_{\mathrm{LRF}} \tag{8b}$$

Therefore, it is possible to estimate the fuel consumption of the dual fuel CI ICE along transient conditions.

For this work, the World Harmonized Vehicle Cycle (WHVC) was used [18]. The main reason is due to the extend range for homologation test in Europe for the heavy-duty transport sector. The EU VI limits applied for this type of vehicles are referenced to the WHVC when the vehicle is tested in transient conditions. The normative uses a range between 50% of cargo mass of the truck to do this test. In this work, 0%, 50% and 100% cargo mass conditions were analyzed. As shown in Fig. 2, the duration of the WHVC is 30 min (1800 s). The test includes segments as urban, rural and highway areas.

2.4. Well to Wheel analysis

The WTW analysis is a method that allows to quantify the GHG emitted for a selected energy source. Specifically, two fuels were compared in this work (Diesel and OME*x*), operating as HRF in a dual-fuel combustion mode with gasoline as LRF. To better detect the source of CO_2

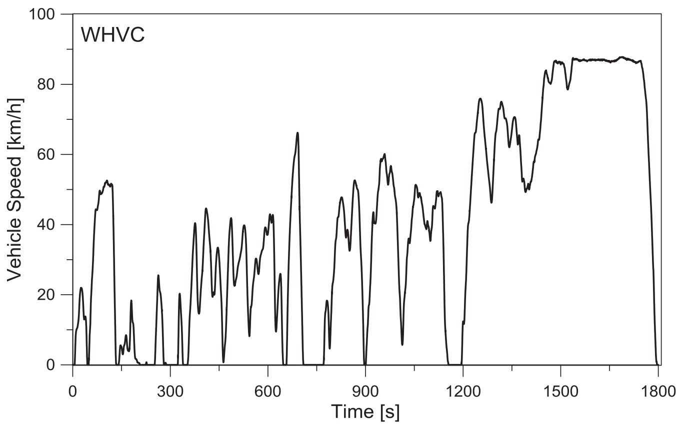

Fig. 2. WHVC homologation driving cycle for heavy duty transportation.

Table 4
Well-to-tank CO_2 production by fuel.

Fuel	WTT CO_2 [g_{CO2}/MJ_{fuel}]
Diesel	18.6
OME*x*	−16.8
Gasoline	17.2

production in each phase, the analysis was divided into two different types: WTT and TTW, which sum becomes the WTW.

The WTT analysis comprehends the estimation of the GHG emissions during the production and distribution of a determined fuel. In the case of the OME*x*, as is a synthetic fuel, the emissions generated by the construction, use and end-of-life of the fuel production infrastructure was included. The calculation was performed using the software application GaBi®, licensed by thinkstep®. Table 4 lists the final values of each fuel used in the experimental tests. CO_2 production was expressed in mass of CO_2 by the energy content of each fuel [gCO_2/MJ_{fuel}]. It is possible to see that OME*x* provides large advantage in terms of CO_2 saving. The carbon capture in the process of fabrication together with a clean energy mix allows negative values in terms of WTT. In this case, the necessary energy to produce the OME*x* was supposed to be taken entirely from wind sources. This means an extra low carbon source. More information about the possible energy sources to produce OME*x* can be found in a previous article of the authors [14]. Lastly, the difference between Diesel and Gasoline are minimum, as expressed in previous works [14].

The second step on the GHG quantification is the TTW. This means to determine the average emission of CO_2 due to the use of the fuel in the vehicle. The WHVC was used to represents the average driving pattern. The tailpipe CO_2 emissions was used instead the measurements at engine-out due to the legislation requirements. Therefore, Eqs. (1) and (7) was used to obtain the CO_2 produced with the fuel consumption measurements. The $CO_{2formation}$ allows to performs this calculus with good accuracy by the hypothesis of complete combustion. As nowadays the normative is strict in terms of HC and CO emissions at tailpipe, this assumption is widely used in the bibliography.

3. Results and discussion

3.1. Tank-to-Wheel analysis

The three different cargo mass (0–50–100%) were simulated in the WHVC. The fuel mass consumption and emissions were computed instantaneously as well as an average value of the cycle. Fig. 3 shows the premix energy ratio at each step time for zero and full load of cargo mass. The peak values achieve the 80% of LHV energy in the total energy. The zero phases are due to idle conditions were the engine works with pure HRF fuel (diesel or OME*x*). In general, at higher loads, the PER increases due to better mixture and easy engine control. The average PER value of the cycle is shown in Fig. 4, being 32% at low cargo mass and 53% at the highest load.

With the PER and the total mass values at each time step, it is possible to determine the amount of HRF and LRF fuels with Eq. (6). Table 5 shows the fuel and energy mass for diesel and gasoline dual-fuel mode along the WHVC. The CO_2 at tailpipe was estimated with the $CO_{2formation}$ parameter. In spite that the emission increases strongly with the cargo mass, when the values are normalized by the total truck mass (vehicle + cargo), a decrease in the TTW CO_2 emissions it is seen (last colum of Table 5, CO_2 tailpipe mass [g] per cargo mass [t] and distance [km]. Also, it is seen a more balanced contribution between the CO_2 production due to diesel and gasoline. Mainly, by the increase near to 50% of the PER.

As mentioned in the methodology, the OME*x*-gasoline case was supposed to maintain the PER ratio as well as the brake thermal efficiency of the diesel-gasoline case. This means that the fuel energy used to perform

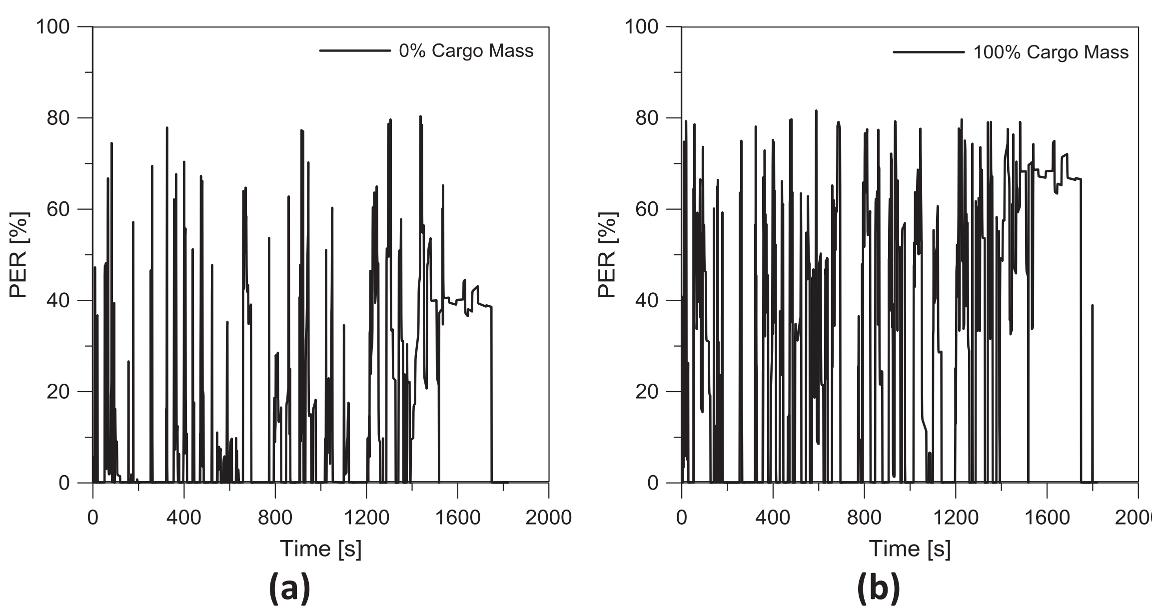

Fig. 3. Instantaneous premix energy ratio (PER) for the WHVC at 0% cargo mass (a) and 100% cargo mass (b).

Table 5
TTW WHVC Diesel–Gasoline result by cargo mass.

Cargo mass [%]	Fuel	Fuel mass [g/km]	Fuel energy [MJ/km]	CO_2 tailpipe [g/km]	CO_2 tailpipe [g/tkm]
0	Diesel	116	5.0	369	46.2
	Gasoline	54	2.3	168	21.0
	Total	171	7.3	537	67.2
50	Diesel	128	5.4	404	28.9
	Gasoline	111	4.7	343	24.5
	Total	239	10.1	748	53.4
100	Diesel	143	6.1	453	22.6
	Gasoline	164	7.0	507	25.3
	Total	307	13.0	960	48.0

Table 6
TTW WHVC OMEx-Gasoline result by cargo mass.

Cargo mass [%]	Fuel	Fuel mass [g/km]	Fuel energy [MJ/km]	CO_2 tailpipe [g/km]	CO_2 tailpipe [g/tkm]
0	OME*x*	260	5.0	416	52.0
	Gasoline	54	2.3	168	21.0
	Total	314	7.3	584	73.0
50	OME*x*	285	5.4	455	32.5
	Gasoline	111	4.7	343	24.5
	Total	396	10.1	799	57.1
100	OME*x*	319	6.1	510	25.3
	Gasoline	164	7.0	507	25.5
	Total	483	13.0	1017	50.9

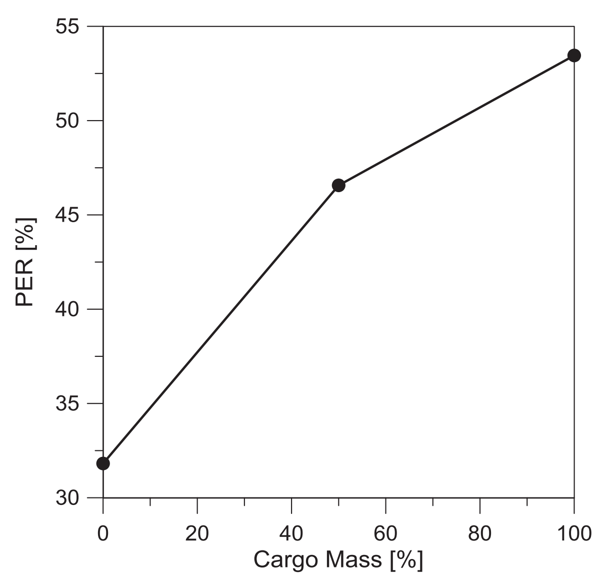

Fig. 4. Average WHVC premix energy ratio (PER) against the cargo mass.

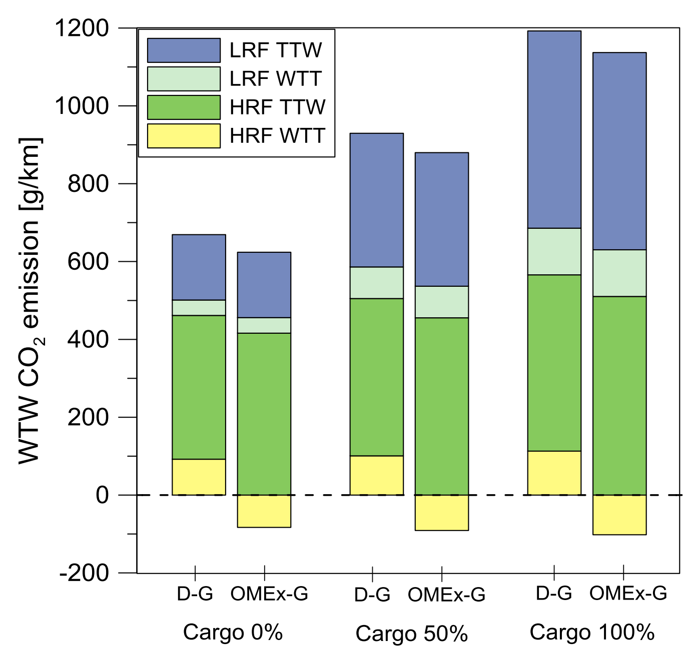

Fig. 5. Well-to-Wheel CO_2 emissions divided by dual fuel mix at different cargo mass.

the driving cycle is the same in both cases (Diesel-Gasoline and Diesel-OME*x*) as shown Tables 5 and 6. With the LHV of each fuel was determined the OME*x* fuel mass consumption. In spite of this strong hypothesis, it is a conservative analysis due to the good properties of the OME*x* to reduce the WTT emissions as well the zero soot emissions that allows other strategies to achieve better energy consumption. Table 6 shows the results for the OME*x*-gasoline case. The CO_2 tailpipe was calculated with the CO_2 formation for each fuel from the results of fuel mass. Comparing the two HRF fuels, the tailpipe CO_2 increase between 8.7% and 6.0% at zero and full load, respectively. Therefore, from a TTW perspective the OME*x* presents a worse behavior. This was expected from the consideration of the ratios between CO_2 production and LHV values (Eq. (5)).

3.2. Well-to-Wheel analysis

After the study of the TTW emissions, it is time to analyze the impact of the fuel production and the results in terms of global values (WTW).

Fig. 5 shows the results for each cargo mass with the two dual-fuel cases (diesel or OME*x*). The HRF WTT is negative for the OME*x* according to the previous study shown in Table 4. This compensates the higher TTW emissions seen in the previous section and the final result is the cumulative bar graph. For all cargo masses, the results were better for OME*x* than diesel.

Fig. 6 shows the cumulative results, which show an improvement in the total CO_2 emissions of 19% for zero load and 13% for full load. The main reason of the lower benefit with the increase of the load are the PER values used. As was seen in Fig. 4, the PER increases with the cargo mass. This means that higher amount of gasoline is used, instead of HRF. For the OME*x* dual-fuel case, this is the worst scenario due to the high benefits in the fuel production (e-fuel condition).

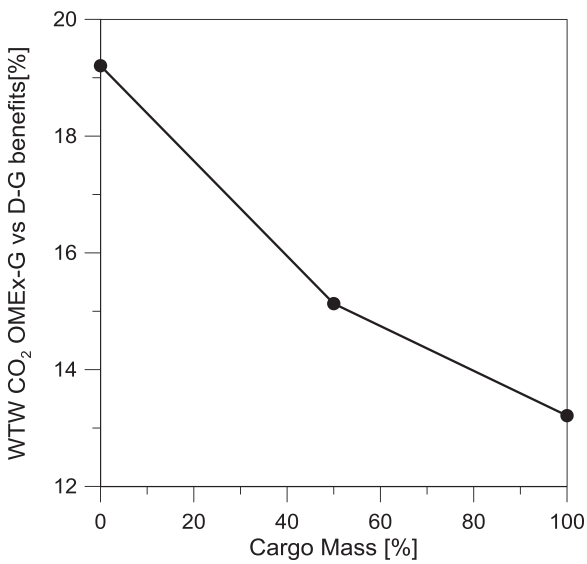

Fig. 6. Well-to-Wheel CO_2 emissions benefits between OME*x*-Gasoline against Diesel–Gasoline depends on the cargo mass.

4. Conclusions

This study shows the benefits of using OME*x* as replacement of diesel in a dual-fuel LTC mode with gasoline as LRF. A complete diesel-gasoline calibration was performed, achieving ultra-low NO*x* and soot emissions levels. After that, a theoretical analysis is proposed to study the potential of use OME*x* instead of diesel as direct-injected fuel. The main assumption is to maintain the premix energy ratio and brake thermal efficiency between fuels.

The fuel preliminary study shows a disadvantage of using OME*x* due to the higher CO_2 formation when is evaluated together with the lower heating value (1.125 times the Diesel tailpipe CO_2 production). These results were confirmed in the driving cycle analysis with an increase of 9% at low loads and 6% at high cargo mass. The change is due to the increase of the premix fuel ratio. However, the trend was reverted for the WTW analysis in which the OME*x* shows CO_2 emissions reduction between 19% and 13% for low and high cargo mass, respectively.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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