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Additional Information

1 **Evaluating OME<sub>x</sub> combustion towards stoichiometric conditions in a compression**  
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12  
13 **Abstract**

14 Low energy density fuels combined with low temperature combustion modes have  
15 demonstrated a great contribution to engine-out NO<sub>x</sub> and soot reduction. Additionally,  
16 synthetic fuels have become an important way of reaching carbon neutral utilization of  
17 hydrocarbon-based fuels and internal combustion engines. Specifically, poly-  
18 oxymethylene dimethyl ethers (OME<sub>x</sub>) have demonstrated great advantages in  
19 combination with conventional fuels with higher energy content to compensate that  
20 aspect to reduce NO<sub>x</sub> emissions below the EU VI homologation normative while  
21 maintaining ultra-low soot emissions with a great benefit in CO<sub>2</sub> emissions in a well-to-  
22 wheel basis. Nonetheless, the properties of this fuel in single-fuel combustion strategies

23 are not thoroughly investigated in the literature. The objective of this work is to  
24 investigate the capabilities of OMEx fuel under conventional combustion modes  
25 compared to those of conventional diesel combustion. To do this, an experimental  
26 characterization under stoichiometric combustion has been carried out to evaluate the  
27 impact on engine hardware demand and total emissions. Additionally, a brief  
28 exploration under leaner conditions is performed. The results obtained from this work  
29 point out that, even under ultra-high EGR rates to reach high fuel-to-air ratios, OMEx  
30 fuel can emit ultra-low soot and NO<sub>x</sub> emissions with more than 90% reduction compared  
31 to diesel on engine out emissions. Under stoichiometric conditions, a significant increase  
32 appears on CO, UHC due to excessive usage of EGR and equivalent fuel consumption is  
33 penalized from 15% to 40% depending on the operating condition, but under slightly  
34 leaner conditions, a region where equivalent fuel consumption is improved with respect  
35 to CDC appears, and the four main pollutants investigated are almost EU VI compliant,  
36 exposing a very high potential for this fuel.

37

### 38 **Keywords**

39 OMEx; synthetic fuels; engine-out emissions; EURO VI;

40

41 **1. Introduction**

42 The current demanding regulations and the even more restrictive normative that will be  
43 imposed in the incoming years have put the internal combustion engines (ICE) in a  
44 critical situation [1]. For a vehicle using an ICE as its propulsive plant, they must ensure  
45 ultra-low emission levels of species that are harmful to the human health [2], like  
46 nitrogen oxides (NO<sub>x</sub>), carbon monoxide (CO), soot and unburned hydrocarbons (UHC),  
47 and additionally contribute to reducing the environmental impact by reducing their  
48 emissions of greenhouse effect gases [3], like the carbon dioxide (CO<sub>2</sub>) and water vapor  
49 (H<sub>2</sub>O).

50 The first type of pollutants is consequence of an incomplete combustion process of the  
51 fuel associated to imperfections during mixing and combustion process, which can be  
52 mitigated by improving the injection strategies and combustion modes, while the  
53 second group of emissions results from the complete oxidation process of the fuel and  
54 can only be lowered by reducing the total amount of fuel used if the same chemical  
55 composition is maintained [4]. As a result, the final objective is to produce an engine  
56 that can maintain very high combustion efficiency and thermal efficiency when  
57 obtaining energy from the burned fuel.

58 The current solution adopted by the manufacturers is to increase the thermal efficiency  
59 of the engine to reduce the fuel consumption while maintaining reasonable levels of  
60 emissions and then reduce the total emissions to values below the regulation limits by  
61 means of an aftertreatment system (ATS) [5]. The ATS has to be able to deal with  
62 different species, each one with different requirements for their reduction. Normally,  
63 an ATS for conventional diesel engines includes an oxidizer catalyst (DOC) for reducing

64 the CO and UHC emissions that originate from incomplete combustion reactions, a  
65 selective catalytic reducer (SCR) for reducing the NO<sub>x</sub> emissions, and a particulate filter  
66 (DPF) for treating the soot emissions [5]. As a result of this strategy based on ATS for  
67 emissions reduction, with more restrictive emission limits the ATS becomes more  
68 complex and expensive. For the current NO<sub>x</sub> emissions targets, some manufacturers  
69 have need to move to a dual-SCR strategy and even propose to move to a three-SCR  
70 architecture on the ATS [6-8]. This tendency only increases the manufacturing and  
71 operating costs of the ATS, especially with the SCR that consumes urea as a reactive  
72 agent for NO<sub>x</sub> reduction [9, 10].

73 The scientific community has put a great amount of effort in devising a way to reduce  
74 emissions from its source, the combustion process. For this purpose, several low  
75 temperature combustion (LTC) modes have been conceptualized and put into practice  
76 to evaluate their respective benefits and drawbacks compared to conventional diesel  
77 combustion (CDC) [11, 12]. In general, the LTC modes have brought great benefits in  
78 terms of reduced NO<sub>x</sub> emissions and improved thermal efficiency. Further development  
79 of the LTC strategies can allow to reach engine-out NO<sub>x</sub> emissions below the current  
80 normative levels and bring the possibility of removing the SCR from the ATS, reducing  
81 considerably the associated costs [10].

82 To reach such low levels of NO<sub>x</sub> emissions, the LTC strategies are combined with  
83 different strategies like ultra-high EGR (Exhaust Gas Recirculation) rates [13, 14] or  
84 alternative fuels [15, 16] with lower energy density to reduce the in-cylinder peak  
85 temperatures, one of the main drivers in the NO<sub>x</sub> production mechanism.  
86 Complementary to this, the use of alternative fuels with a very high oxygen content and

87 no carbon-carbon bonds provides the possibility of eradicating the soot emissions [17,  
88 18]. Specifically, the poly-oxymethylene dimethyl ether (OMEx) has demonstrated to  
89 provide zero-soot results when applied in dual-fuel systems with very high EGR rates  
90 and still be able to ensure a good combustion rate with its higher reactivity compared  
91 to diesel and reduced NO<sub>x</sub> emissions as a combined consequence of the high EGR rates  
92 and reduced lower heating values (LHV) [19, 20]. As a drawback, the use of such  
93 strategies produces a decrement on the reactivity of the fuel mixture and lower local  
94 temperatures that can end up in high CO and UHC emissions that do not have enough  
95 energy and time to complete their oxidation [21, 22]. Nonetheless, if the penalty in CO  
96 and UHC is not excessive, it can be manageable by means of alterations in the ATS [23].

97 As the literature shows, the use of oxygenated synthetic fuels like OMEx brings  
98 significant benefits for reducing the complexity and costs of the ATS as it allows to  
99 reduce the relevance of the SCR and the DPF or even remove them if the emissions are  
100 lower than the normative limits [19, 21]. On the other hand, the potential increase of  
101 CO and UHC could be managed by means of different strategies and devices depending  
102 on the exhaust gases composition. In this sense, two main streams are differentiated:  
103 stoichiometric combustion and diluted combustion. The first case is a solution normally  
104 used in spark ignition engines that work under stoichiometric conditions consuming  
105 most of the oxygen during the combustion process [24], which normally results in  
106 balanced emissions between NO<sub>x</sub>, CO and UHC. In this case, a three-way catalyst (TWC)  
107 is the preferred option to reduce the three contaminants simultaneously [25]. The  
108 second option is typical of diesel engines and it is used together with high air boosting  
109 conditions to improve the fuel consumption, but this can lead to very high emissions of  
110 NO<sub>x</sub> and unbalanced emissions of CO and UHC depending on the operating condition.

111 In this case, the NO<sub>x</sub> emissions are treated separately and CO and UHC are treated with  
112 a Diesel Oxidizer Catalyst (DOC) [26].

113 In previous applications of OMEx in dual-fuel systems or in fuel blends, the fuel  
114 consumption was not highly penalized as there was a second fuel with higher energy  
115 density to compensate for the lower LHV of OMEx [20, 21]. However, when considering  
116 an application using OMEx as single fuel this cannot be solved and the total fuel  
117 consumption is significantly increased, meaning that the total CO<sub>2</sub> emissions are also  
118 proportionally increased. In a tank-to-wheel (TtW) analysis, there is no benefit in this  
119 application, and other alternatives like vehicle electrification [27-29] or fuel  
120 decarbonization [30] would be necessary. Nonetheless, if the OMEx production process  
121 is considered and the CO<sub>2</sub> emissions are analysed on a well-to-tank (WtT) basis, there is  
122 huge difference as OMEx is synthesized using CO<sub>2</sub> coming from the atmosphere with  
123 techniques like direct air capture (DAC) [31, 32]. If this factor is included, synthetic fuels  
124 formed through clean production paths can highly contribute to achieve the CO<sub>2</sub>  
125 reduction targets imposed for the next future. According to production data provided  
126 by the fuel supplier, the Well-to-Wheel (WtW) CO<sub>2</sub> emissions can be reduced between  
127 80% to 90% with respect to commercial diesel or gasoline depending on the energy pool  
128 and production path.

129 Considering all the benefits and drawbacks of using OMEx as single fuel in an ICE, this  
130 work aims to evaluate the potential of OMEx and its suitability with conventional ATS  
131 systems in terms of emissions. For that, pure OMEx combustion is evaluated in a single-  
132 cylinder compression ignition engine under stoichiometric conditions with the objective

133 of evaluating the suitability of using a cheap and easy-to-implement TWC as the sole ATS  
134 for an OMEx-fuelled ICE.

135

## 136 **2. Materials and Methodology**

### 137 **2.1. Engine characteristics**

138 The experimental evaluation has been carried out on a D5K engine from Volvo, a  
139 production four-cylinder engine dedicated to medium-duty transportation vehicles, and  
140 the main features of the stock engine can be found in Table 1. For this study, the stock  
141 engine has been modified into a single-cylinder engine by disabling three of the four  
142 cylinders and removing the turbocharging and injection system to be replaced by  
143 external devices that provide greater flexibility when defining the boundary conditions  
144 that are desired for the operating condition.

145

Table 1. Stock engine characteristics.

Characteristic	Value
Engine Type	4 stroke, Direct Injection diesel engine
Number of cylinders [-]	4 in-line
Number of valves [-]	4 per cylinder
Total displaced volume [cm <sup>3</sup> ]	5100
Stroke [mm]	135
Bore [mm]	110
Compression ratio [-]	17.5:1
Rated Power [kW]	177 kW @ 2200 rpm
Rated Torque [N·m]	900 N·m @ 1200-1600 rpm

146



## 147        **2.2. Test cell description**

148        The engine has been mounted on an AVL-APA 404 asynchronous dynamometer that  
149        governs the engine speed and is commanded from its own software platform AVL PUMA  
150        Open. As the stock air management system has been removed, the boosting is delivered  
151        by an externally driven screw compressor that can boost up to 3.7 bar. An air dryer is  
152        mounted after the compressor to remove the ambient humidity and a set heat  
153        exchanger and heating resistance are mounted in the circuit to control independently  
154        the intake temperature. To ensure the actual mass flow of fresh air, a volumetric air flow  
155        meter G-100 RVG from Elster is mounted in the intake circuit. Two settling chambers are  
156        used to remove undesired pressure waves coming from actuators and other devices  
157        mounted at the intake and outlet circuits. To control the back pressure at the exhaust  
158        manifold, an actuated valve is placed between the EGR circuit and the exhaust settling  
159        chamber. In the EGR circuit there is another set of heat exchanger plus flow heater  
160        mounted to control the EGR temperature and an EGR valve to better control the EGR  
161        flows and be able to emulate realistic operating conditions. External and independent  
162        coolant circuits were employed for the EGR and oil conditioning for greater operability  
163        of the test cell. Nonetheless, to avoid unrealistically cooling engine conditions, the oil  
164        and coolant temperature were maintained at temperature values representative of the  
165        stock engine. All these devices are controlled from the AVL PUMA platform, where  
166        different temperatures and pressures registered at relevant locations of the test cell are  
167        registered too and serve as inputs for the controllers of the auxiliary systems.

168        Regarding the injection system, a common rail injection system is used to deliver the  
169        desired injection pressure to the in-cylinder injector. The fuel pump used for this project

170 was an external Bosch CP3 fuel pump that allowed to reach rail pressures up to 2500  
171 bar. The fuel temperature was conditioned on a AVL 753C and the fuel mass flow was  
172 measured with a AVL 735S [33]. The injection settings like rail pressure, injection timing  
173 and energizing time were set using a driven engine controller to have full access to the  
174 injection parameters through the ECU (Engine Control Unit).

175 For the emissions characterization and EGR rate measurements, a five-gas analyser  
176 HORIBA MEXA-ONE-D1-EGR was used to account for the NO<sub>x</sub>, CO, UHC, CO<sub>2</sub> and O<sub>2</sub> [34].  
177 A heated line is included to avoid formation of condensates that can damage the  
178 equipment or affect the measurement accuracy. Additionally, an AVL 415S smoke meter  
179 was used to measure the smoke emissions and convert them into soot mass emissions  
180 in accordance to the methodology provided by the manufacturer [35].

181 Finally, the in-cylinder pressure was obtained by means of a piezoelectric transducer.  
182 This signal is processed online by INDICOM to provide with instantaneous reports of  
183 indicated magnitudes related to the energy liberation that takes place inside the  
184 combustion chamber, and this information is used for optimizing the injection settings  
185 and have a better control over the combustion process [36]. INDICOM provides this  
186 information with an increment of 0.2 CAD (crank angle degree) using as reference the  
187 crank position provided by the AVL 364 encoder.

188 The layout of the test cell with all the mentioned devices and relevant locations where  
189 the temperature and pressure are registered are shown in Figure 1, and a summary of  
190 the models and accuracy of the different measuring devices is included in Table 2.

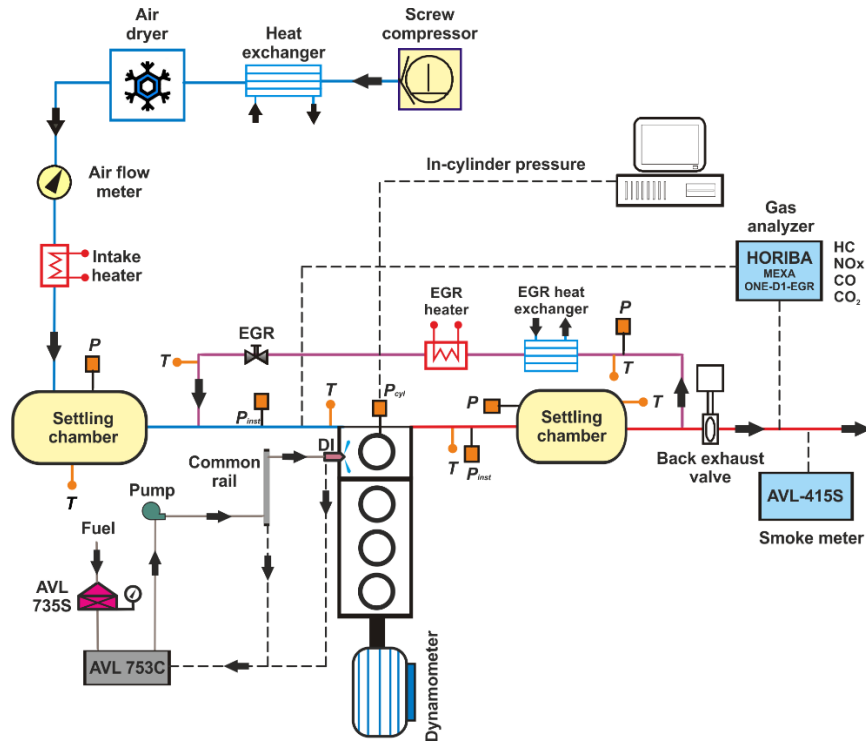


Figure 1. Test cell layout.

Table 2. Accuracy of the measuring devices used in the test cell.

Variable Measured	Device	Manufacturer / Model	Accuracy
In-cylinder pressure	Piezoelectric transducer	Kistler / 6125C	$\pm 1.25$ bar
Pressure	Piezoresistive transducer	Kistler / 4045A10	$\pm 25$ mbar
Temperature	Thermocouple	TC direct / K type	$\pm 2.5$ °C
Crank angle, engine speed	Encoder	AVL / 364	$\pm 0.02$ CAD
NO <sub>x</sub> , CO, UHC, O <sub>2</sub> , CO <sub>2</sub> , EGR	Gas Analyzer	HORIBA/MEXA-ONE-D1-EGR	$\pm 4\%$
Smoke	Smoke meter	AVL / 415S	$\pm 0.025$ FSN
Fuel mass flow	Fuel flow meter	AVL / 735S	$\pm 0.12\%$
Air mass flow	Air flow meter	Elster / RVG G100	$\pm 0.1\%$

### 2.3. Injector and fuel properties

Low energy density fuels suffer from increased fuel mass consumption as it requires

higher mass to have the same energy input. This also means that the injection durations

198 must be significantly increased compared to conventional fuels when using the same  
 199 injector. Anticipating this effect when using OMEx, it was decided to use an injector with  
 200 higher flow rate capacity to not reach excessively long injection durations that cannot  
 201 be managed by the ECU limitations, the properties of which can be found in Table 3. This  
 202 injector was used during all the experimental evaluation, including the reference  
 203 performance with diesel and the calibration using OMEx. For a reference on the  
 204 differences between both fuels in terms of relevant physical properties and combustion  
 205 properties, Table 4 includes a summary of the most relevant properties. Note that the  
 206 OMEx used in this study is a mixture of different poly-oxymethylene dimethyl ethers  
 207 mainly ranging between OME<sub>3</sub> and OME<sub>5</sub> (OME mix 3-5).

208

Table 3. Injector properties.

Injector property	Value
Actuation Type [-]	Solenoid
Steady flow rate @ 100 bar [cm <sup>3</sup> /min]	2200
Included spray angle [°]	140
Number of holes [-]	6
Hole diameter [μm]	244
Maximum injection pressure [bar]	2500

209

Table 4. Summary of fuel characteristics.

	EN 590 diesel	OMEx
Lower heating value [MJ/kg]	42.44	19.21
Density [kg/m <sup>3</sup> ] (15 °C)	842	1067
Viscosity [mm <sup>2</sup> /s] (40 °C)	2.93	1.18

Cetane number [-]	55.7	72.9
Carbon content [% m/m]	86.2	43.6
Hydrogen content [% m/m]	13.8	8.82
Oxygen content [% m/m]	0	47.1
Vapor pressure [hPa] (T=40 °C)	1-10	32
Stoichiometric Air-to-Fuel ratio [-]	14.5:1	5.85:1

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210

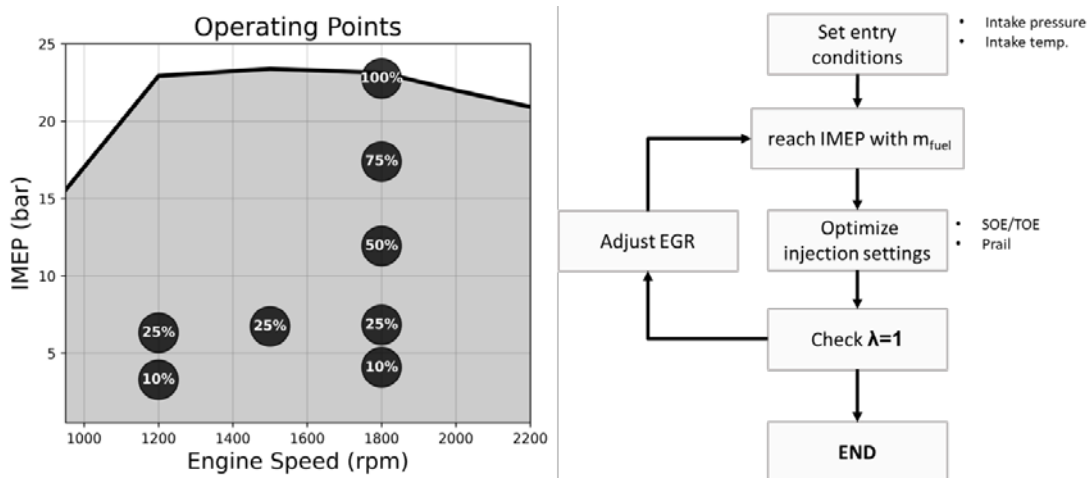
#### 211 **2.4. Testing methodology**

212 Eight operating points from the engine map have been chosen as representative of the  
213 complete engine operation based on previous vehicle simulations under different  
214 driving scenarios [21]: 10% and 25% engine load at 1200 rpm, 20% load at 1500 rpm and  
215 10%, 25%, 50%, 75% and 100% engine load at 1800 rpm. These eight operating points,  
216 represented in Figure 2, have been evaluated first with diesel using the injection settings  
217 from the original engine calibration. These points serve as a reference of the real  
218 performance of the engine even if the injector has been replaced by one with higher  
219 flow rate capacity than the stock one. For the OMEx combustion optimization under  
220 stoichiometric conditions, it was decided to use a simple injection strategy with a single  
221 injection as this allows to have a first insight on the performance of the concept with a  
222 good trade-off between testing time and results.

223 For the definition of the cylinder boundary conditions, some hypotheses were applied  
224 based on relevant literature. First is that the low  $AF_{st}$  (stoichiometric air-to-fuel ratio) of  
225 OMEx makes necessary to significantly reduce the amount of fresh air as stoichiometric  
226 conditions would be reached [37, 38]. For this reason, the fresh air density was

227 decreased using the intake flow heater to reach a consistent intake temperature of 80  
 228 °C in all the engine map [39]. The air mass flow reduction will also diminish the power  
 229 output, so it was decided to reach a compromise and loose some benefit from heating  
 230 the intake by boosting the engine. To have consistent and realistic boundary conditions,  
 231 the same boosting map used for the results with diesel was used as it is representative  
 232 of the real conditions of the stock engine turbocharger. Also, as the OME<sub>x</sub> energy  
 233 density is lower than that of diesel, the injection pressures were consistently higher  
 234 than for diesel to reduce the injection durations, maintaining the coherence of the  
 235 original map with an increasing injection pressure with the engine load [40, 41]. Finally,  
 236 stoichiometric conditions were achieved by increasing the EGR fraction to further  
 237 displace the fresh air. The injection duration and timing were optimized looking for the  
 238 minimum specific fuel consumption to then evaluate the impact on the engine-out  
 239 emissions. In any case, the mechanical limitations of the engine were respected and the  
 240 limitations of 190 bar of maximum in-cylinder pressure and 15 bar/CAD of maximum in-  
 241 cylinder pressure gradient were imposed as limitations of the calibration strategy.

242



243

244

Figure 2. Summary of the testing methodology.

245 For a reliable data acquisition strategy, emission measurements from the five-gas  
246 analyser were averaged during a period of 40 seconds after a stationary operating  
247 condition was achieved to remove the possible noise and scattering on the output. The  
248 variable sampling smoke meter was set to perform three consecutive measurements  
249 that were averaged afterwards. For the in-cylinder measurements, INDICOM was set to  
250 record 100 cycles that were then averaged to minimize the effect of the possible cycle-  
251 to-cycle variation and the coefficient of variation of the IMEP provided by INDICOM  
252 during the test has to be lower than 3% to consider the operating condition as stable.  
253 Together with this measurement, INDICOM also provided with combustion parameters  
254 on an indicated analysis. For a more detailed thermodynamic analysis of the results,  
255 these results were post-processed using the in-house code CALMEC [42]. This software  
256 uses 0D models to include thermodynamic phenomena like heat transfer and obtain  
257 effective burning rates and a more detailed analysis of the combustion process.

### 258 **3. Results and discussion**

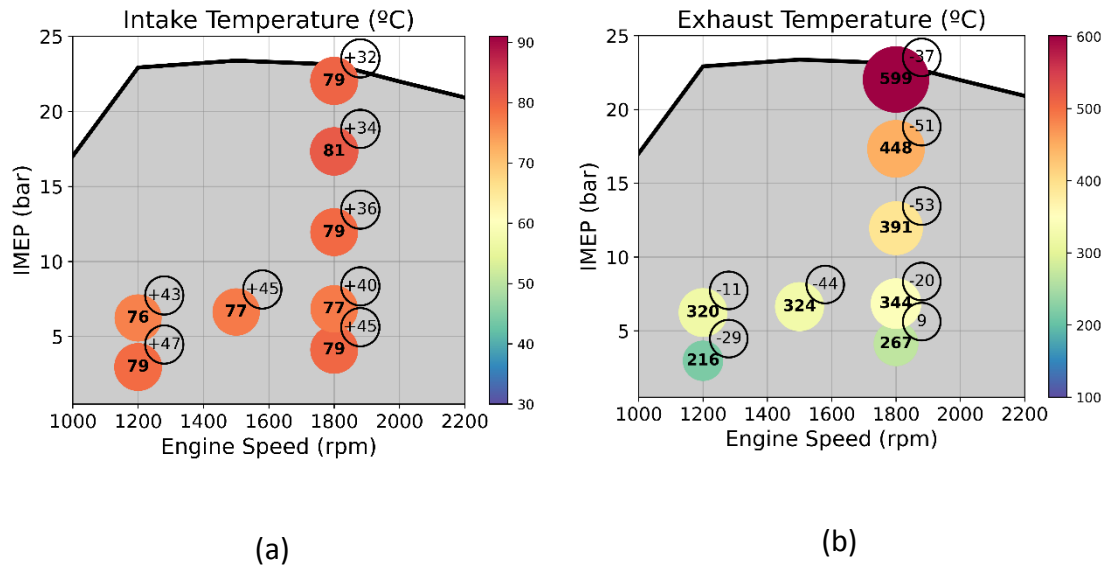
#### 259 **3.1. Boundary conditions**

260 Promoting a stoichiometric combustion of a fuel with low  $AF_{st}$  and low energy density  
261 has certain implications that must be discussed. The first difference that can be noticed  
262 is the increased intake temperature that has been almost doubled in all the engine map,  
263 as shown in Figure 3a. Depending on the application, having such an increase in the  
264 intake temperature may seem to be unrealistic for the requirements of the flow heater,  
265 but it has to be noticed that the boundary conditions for diesel results belong to a  
266 turbocharged and intercooled engine. The hotter intake requirements for the OME<sub>x</sub>  
267 points could be easily achieved by implementing a less demanding thermal management

268 strategy for the intercooler and the EGR circuit. Additionally, the increased EGR rates  
269 will also contribute to increase the intake temperature as there will be a higher mass  
270 fraction of hot gases in the intake mixture.

271 Contrary to what could be expected, the exhaust temperature, included in Figure 3b, is  
272 not increased with respect to the reference, but it is reduced up to 53 °C depending on  
273 the operating condition. This is a consequence of several factors like having a more  
274 advanced combustion phasing, higher EGR rates that acts as a heat sink during all the  
275 combustion process due to its higher specific heat and its non-reactivity that acts as a  
276 quenching factor, and finally, the reduced energy density of OMEx plays a great role in  
277 produced lower peak and local temperatures within the combustion chamber. Even if  
278 this trait of oxygenated fuels will be beneficial for NO<sub>x</sub> reduction, the fact that for this  
279 combustion strategy the EGR has been increased and the in-cylinder temperatures have  
280 been reduced will reduce the reactivity of the mixture and the CO and UHC emissions  
281 will be increased. Considering that the DOC will play a more important role on the ATS,  
282 the operational requirement of having temperatures above 200°C - 230°C at the inlet of  
283 the DOC for a reasonable conversion efficiency [26], reducing the exhaust temperature  
284 is going in the opposite direction, especially considering that the expansion at the  
285 turbine (as it is not mounted in the test facility) is not being considered.





286 Figure 3. Intake (a) and exhaust (b) temperatures for OME<sub>x</sub> results (colored balls) and their difference with CDC  
 287 reference (black bordered balls).

288 The other important change on the cylinder boundary conditions is the EGR fraction  
 289 needed to reach stoichiometry on a turbocharged diesel engine. As can be seen in Figure  
 290 4, the EGR rates have been increased from 40% to 50% depending on the operating  
 291 point. From the feasibility point of view of this requirement for the engine, these EGR  
 292 rates are excessively high, but considering that fresh air density has been reduced  
 293 significantly, it can be displaced easier and such an increase in EGR could be doable with  
 294 proper turbo-matching. Nonetheless, from the applicability point of view, having such  
 295 high EGR rates with high intake temperature will drastically reduce the volumetric  
 296 efficiency of the engine and penalize the power output or fuel consumption in addition  
 297 to the reduced reactivity and lower outlet temperature for the DOC and the possibility  
 298 of having unbalance emissions. These implications will be analysed in more detail in the  
 299 following sections.

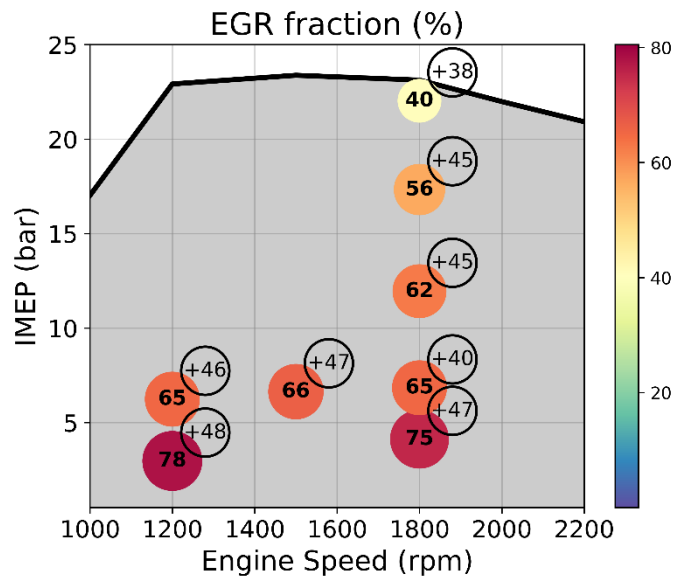


Figure 4. EGR rate for OMEx results and its difference with CDC reference.

300

301

302

303 Regarding the intake and exhaust pressures to control EGR and boosting, the intake

304 pressure followed the turbocharger conditions from the reference in all the cases except

305 for the full load condition. To achieve stoichiometric conditions by means of EGR, the

306 exhaust pressure was tuned by commanding the exhaust back pressure and leaving fully

307 open the EGR valve. It is important to remark that the changes in the exhaust back

308 pressure were not greater than 0.1 bar, and this could be interpreted as an indicator of

309 the feasibility to obtain a turbocharger design that could reach such high EGR rates.

310 Finally, regarding the injection pressure, it was observed that increasing the injection

311 pressure with optimum combustion phasing resulted in greater pressure gradients, so

312 the same injection pressure was used for both fuels except for the full load condition.

313 A comment on the limitations found to reach the full load condition should be made. As

314 it was observed that maximum power output could not be achieved using the

315 designated strategy, the injection pressure was increased to the maximum capacity of

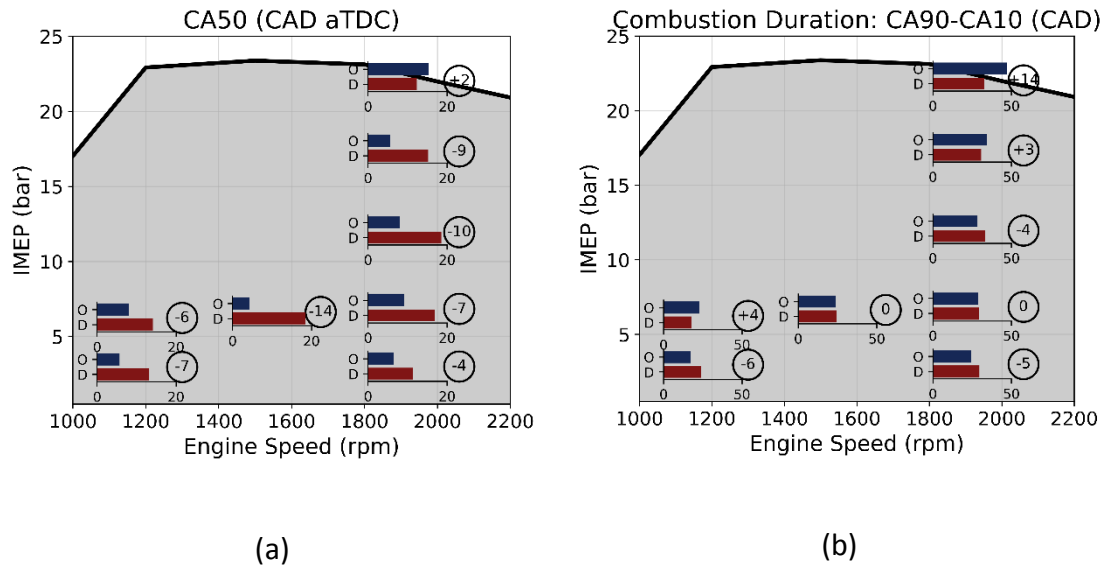
316 the system, 2500 bar, to increase the amount of fuel injected. Then, the injection  
317 duration was increased to 4 ms, the maximum injection duration allowed by the ECU  
318 per injection. Finally, a pilot injection was included, and its duration was increased  
319 together with the boost pressure, that was increased by 0.15 bar with respect to the  
320 reference value for that operating point. As it can be seen, to reach such condition, the  
321 injection system capacity and boosting capacity are pushed to the limit to achieve the  
322 desired power output, but the final setting may result in an unrealistic application. This  
323 clearly states the main limitation of the concept to reach high power rates.

### 324 **3.2. Combustion analysis**

325 The changes in the calibration strategy combined to the modifications of the boundary  
326 conditions have a direct impact on the burning rate and other combustion properties.  
327 The first indicator of a change in the combustion control is the CA50 (crank angle for  
328 which 50% of the energy has been released, represented in Figure 5a). In the case of  
329 OMEx, the injection timing is optimized to reach the best specific fuel consumption and  
330 not from an emissions control strategy standpoint, as in the case of the diesel reference.  
331 For this reason, the injection timings are advanced, and the combustion takes place near  
332 the TDC. This can be observed in the CA50, that takes values around 4 to 8 CAD aTDC.  
333 For the results with diesel, the CA50 takes place around 15 to 20 CAD aTDC as the  
334 purpose of the calibration is to reduce the peak temperatures and have a certain control  
335 over the NO<sub>x</sub> emissions to have acceptable levels that can be treated on the ATS that  
336 would be equipped with an SCR. Despite the change in the objectives of both  
337 calibrations, a similar trend can be observed in the distribution of the combustion  
338 phasing along the engine map with a certain offset. Considering the fact that the diesel

339 reference is an already optimized calibration, it is valid to assume that the single-  
340 injection strategy with OMEx is enough to have a consistent engine calibration with  
341 acceptable results and is valid for further comparisons. Nonetheless, an exception to  
342 this trend of having more advanced combustion with OMEx appears at full load  
343 conditions. This change in the trend appears as a consequence of the limitations of the  
344 concept and the hardware, as the injection system is pushed to the limit in terms of  
345 injection duration and rail pressure to achieve the targeted power output regardless of  
346 the combustion or emissions performance.

347 Differences can be also found in the burning rate, evaluated through the CA10 to CA90  
348 difference to avoid distorted trends as a consequence of the signal noise and that can  
349 be consulted in Figure 5b. In general, OMEx results in a very similar or even shorter  
350 combustion duration than diesel. Considering the significantly increased EGR rate, the  
351 higher reactivity of OMEx combined to the higher intake temperature is enough to  
352 compensate for the almost doubled total mass of fuel that must be burned due to its  
353 LHV, which is less than half of that of Diesel. In this sense, it is possible to obtain a faster  
354 combustion despite the increase in the fuel flow. Again, the outlier at full load condition  
355 is not considered when analysing these trends as it is the result of a hardware limitation.

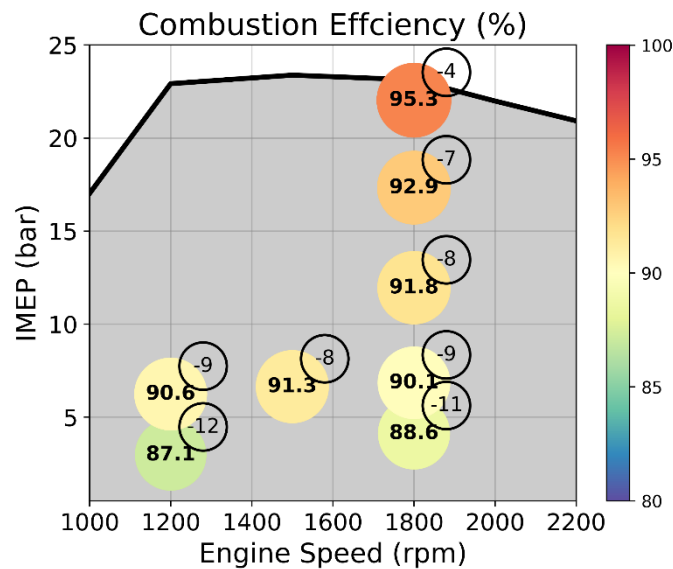


356 Figure 5. Comparison of combustion phasing (a) and combustion duration (b) for OMEx results and the Diesel  
 357 reference.

358 Initially, by considering that the combustion phasing is advanced, and the combustion  
 359 duration has been kept to similar values, the direct consequence of having the end of  
 360 combustion displaced towards the TDC may lead to think that less combustion  
 361 inhomogeneities may appear and the soot emissions and the penalty in UHC and CO  
 362 associated to combustion at cooler stages of the expansion stroke may be reduced.

363 Contrary to this, the increased EGR has the opposite effect, leading to less oxygenated  
 364 regions that are easily saturated with the long fuel injections, rapidly consuming the  
 365 oxygen available and leading to an increase of combustion imperfections. To evaluate  
 366 the compromise between these two effects, the combustion efficiency obtained from  
 367 the post-processing based on exhaust composition is analysed in Figure 6. It is observed  
 368 in Figure 6 that combustion efficiency, which usually has values greater than 99% for  
 369 conventional fuels, in the case of OMEx has suffered an important penalty, going down  
 370 to 87% in the worst case [43]. This means that the remaining fraction is the fraction of  
 371 fuel that has not been fully oxidized, therefore, a significant penalty in fuel consumption

372 is expected as not the energy available in the fuel is being profited during the work  
 373 extraction. From this, it can be concluded that the excessive EGR rates lead to an  
 374 unacceptable combustion performance that is not suitable for a real application and  
 375 needs significant improvements.



376

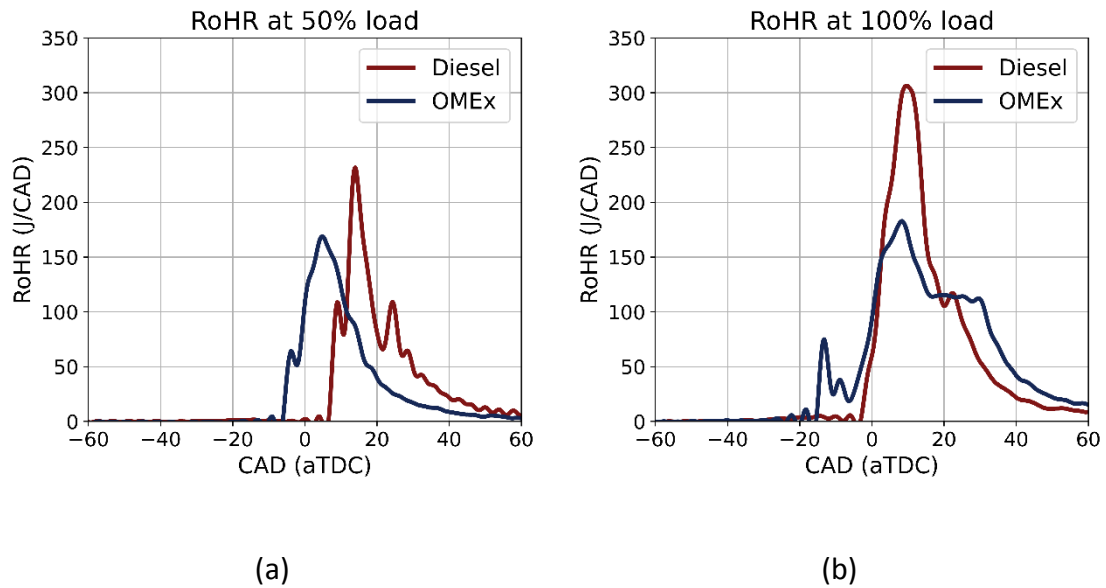
377

Figure 6. Combustion efficiency for OME<sub>x</sub> results and its difference with CDC reference.

378 All these effects are clearly observed when analysing the rate of heat release (RoHR) at  
 379 different operating points. Comparing the RoHR at 50% load and 1800 rpm for both fuels  
 380 (Figure 7a), several observations can be extracted. The main difference is obviously the  
 381 advance in the injection strategy for the case with OME<sub>x</sub>, but despite this, both heat  
 382 release curves follow a very similar shape with an initial portion of fuel that is premixed  
 383 and burns rapidly (the first peak) that is then followed by a diffusive combustion. In  
 384 general, the capacity of OME<sub>x</sub> to produce high peaks is limited compared to that of  
 385 diesel and this can be observed in the local peaks that are always lower even if the total  
 386 mass injected is significantly higher. This results in a lower efficiency when extracting  
 387 energy from the combustion to convert it into effective work [44]. Also, the combustion  
 388 duration for OME<sub>x</sub> is slightly shorter given its enhanced reactivity. It can be said that for

389 this operating condition, OMEx is able to operate on a very similar manner compared to  
390 diesel and the calibration strategies may not be very different apart from the total mass  
391 flows required.

392 For full load condition (Figure 7b), OMEx does not operate in a normal way and several  
393 conclusions can be obtained from it. First thing to observe is that the peak values of  
394 RoHR do not differ much between 50% load and full load. This is the first limitation  
395 imposed by the reduced LHV of OMEx. Independently on the fuel mass injected, the EGR  
396 rates used or the combustion phasing, there is a very restrictive limit on the energy that  
397 can be transferred effectively to the crankshaft. Even if a pilot injection is added, as in  
398 this case, the fuel burns rapidly and does not contribute to the premixed phase of the  
399 spray combustion, resulting in split combustion stages that do not produce a smooth  
400 burning rate as in the first case. Then there is the impact of total injection duration. Even  
401 with a greater injection pressure (2500 bar for OMEx and 1900 bar for diesel), it is  
402 observed how a constant burning rate appears after the most energetic combustion  
403 stage. This is caused by a constant inflow and fuel burning that are stabilized. It is  
404 observed that the fuel is being injected during more than 30 CAD and, as more advanced  
405 is the expansion stroke, the lower power is obtained from the fuel injected at that late  
406 stage. As it can be expected, this prolonged fuel injection results in very long  
407 combustion duration that makes very difficult to properly match the combustion  
408 phasing, which reduces the fuel economy significantly. In addition to this, the exhaust  
409 temperatures are increased up to 600°C, which is near the usual safety limit of a  
410 conventional turbine.



411 Figure 7. Comparison of rates of heat release for OMEEx and diesel at 50% load (a) and full load (b) operating points  
 412 at 1800 rpm.

413 From this analysis, it is possible to conclude that there is a power limit up to which a  
 414 high-reactivity fuel with low LHV like OMEEx can operate in a similar way to a  
 415 conventional diesel, independently of other restrictions imposed by EGR strategies or  
 416 hardware limitations. In case that a conventional engine architecture is used with a low  
 417 LHV fuel, a certain de-rating of its maximum power output is expected to maintain  
 418 smooth operation and coherent strategies with assumable engine performance in terms  
 419 of fuel consumption.

### 420 3.3. Fuel consumption and engine-out emissions

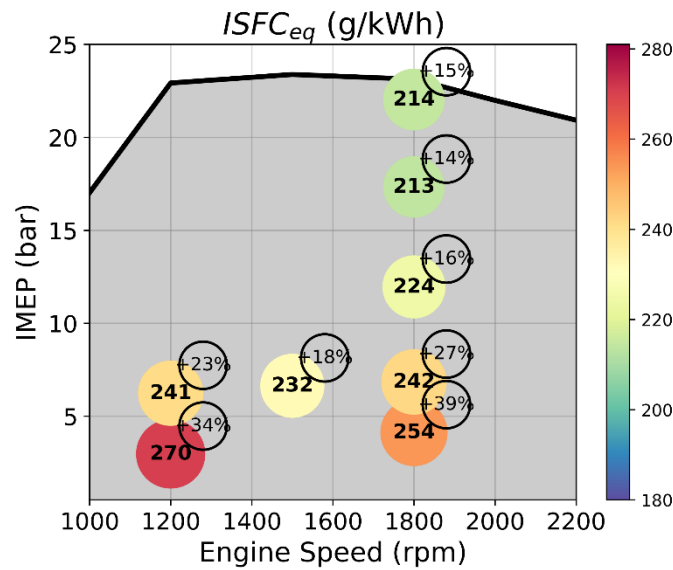
421 Previous sections showed that the boundary conditions and combustion strategy  
 422 modifications followed in order to reach stoichiometric operation utilizing OMEEx have a  
 423 detrimental effect in terms of fuel consumption. In this section, the indicated specific  
 424 fuel consumption (ISFC) of OMEEx under  $\lambda=1$  is represented in equivalent terms and it is  
 425 represented in Figure 8. This equivalent ISFC accounts for the total ISFC scaled by the



426 energy density ratio of OMEx and diesel as expressed in Eq. 1 to have a more  
427 representative comparison in terms of energy utilization efficiency and equivalent diesel  
428 fuel consumption.

$$ISFC_{eq} = ISFC \cdot \frac{LHV_{OMEx}}{LHV_{Diesel}} \left[ \frac{g}{kWh} \right] \quad \text{Eq. 1}$$

429 The added effect of combustion worsening coming from the high EGR rates and reduced  
430 in-cylinder trapped mass leads to a total penalty on engine performance in terms of  
431  $ISFC_{eq}$  that varies from 15% at high load to almost 40% at lower loads. It can be observed  
432 that the trends in this penalty are very similar to that of the increment in the EGR rates,  
433 so it reasonable to assume that this parameter is the one with the highest relevance of  
434 fuel economy as it may be the main cause for increasing the combustion imperfections  
435 and limited RoHR peaks. From these results, the final fuel consumption on a real  
436 application would be much higher than that of conventional diesel engines, with a  
437 significant increase in re-fuelling costs and an unavoidable reduction of the vehicle  
438 autonomy, therefore the application of this concept may not be interesting for road  
439 vehicles. Nonetheless, it may still hold certain attractive for off-road applications.



440

441

Figure 8. Equivalent BSFC for OME<sub>x</sub> results and its difference with CDC reference.

442 To finish with the evaluation of this combustion concept, the engine-out emissions of  
 443 most relevant controlled species: NO<sub>x</sub>, soot, UHC and CO are shown in Figure 9. In the  
 444 figure, the red circles denote the operating condition that fulfils the EU VI limit for the  
 445 corresponding specie. In general trends, the concept performs exceptionally well for  
 446 NO<sub>x</sub> and soot emissions, while greatly penalizes the UHC and CO emissions.

447 The NO<sub>x</sub> emissions are practically removed up to 50% load, for 75% load there is a small  
 448 increase, but still insignificant, and then at full load there are greater NO<sub>x</sub> emissions that  
 449 go beyond the EU VI limit, but still, it greatly reduces NO<sub>x</sub> emissions compared to diesel.  
 450 To explain this, it is necessary to consider that the two main factors affecting NO<sub>x</sub>  
 451 production in this case are local hot spots with high temperature and the residence time  
 452 at that high temperature. As can be deduced from the analysis of the combustion  
 453 process, the RoHR peak limit also limits the maximum temperatures contributing to the  
 454 NO<sub>x</sub> reduction. This, combined with the enormous amounts of EGR that act as a heat  
 455 sink and slows down the reactivity of the mixture, can reach virtually-zero NO<sub>x</sub>  
 456 emissions. For 75% and 100% load, the phenomenon of constant heat release due to a

457 long diffusive flame creates a hot region that is maintained during a significant amount  
458 of time, allowing for the progressive formation of NO<sub>x</sub> emissions. Given this scenario, it  
459 can be concluded that the SCR of the ATS could be removed as almost no NO<sub>x</sub> is being  
460 produced, and the only point that emits above the regulation limit is a point that is  
461 scarcely used during normal driving conditions and it would be possible to easily fulfil  
462 during a homologation cycle.

463 In the case of soot emissions, OMEx is able to maintain ultra-low emissions in every  
464 operating condition, reaching less than a tenth of the limit. The molecular structure of  
465 OMEx with no carbon-to-carbon bonds allows to avoid the creation of soot precursors  
466 like polycyclic aromatics and produce a significant improvement in this aspect. In other  
467 applications like dual-fuel combustion, OMEx has produced virtually zero soot  
468 emissions, and the small presence of soot measurements in this case may be the result  
469 of having a slightly rich mixture due to uncertainties in the definition of stoichiometric  
470 conditions. Nonetheless, it is important to remark that the measuring device employed  
471 for this study may have a certain under reporting when working with oxygenated fuels  
472 [45, 46].

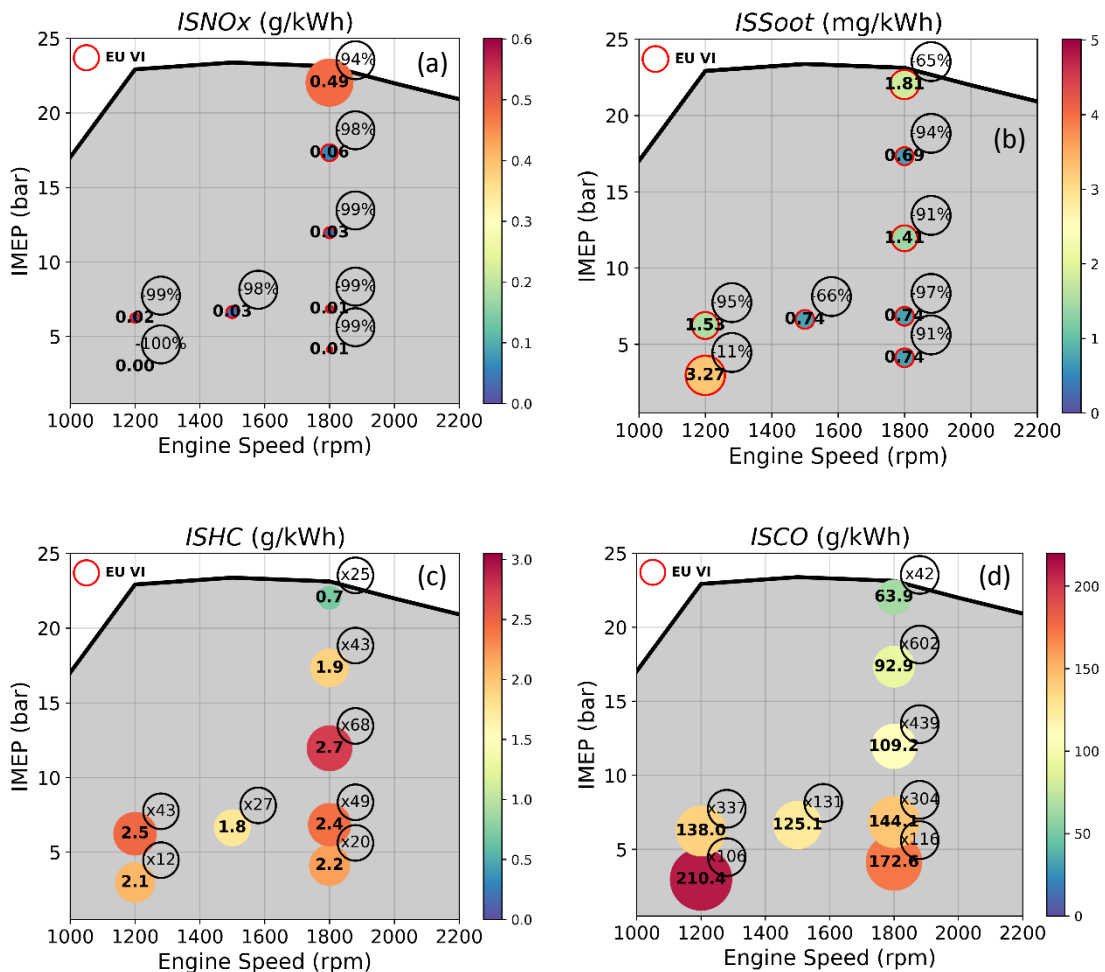
473 Regarding UHC and CO emissions, the effect of the recirculated gas is the main cause.  
474 The great amount of EGR rates imply that pockets with almost no oxygen presence may  
475 appear in the cylinder, inhibiting the hydrocarbons oxidation. Additionally, the low in-  
476 cylinder temperatures also reduce the reactivity of said oxidation reactions and  
477 contribute to increase the amount of fuel that is not fully utilized. As can be seen in  
478 Figure 9c, the amount of UHC is increased between 10 and 70 times compared to  
479 conventional diesel operation, but it is necessary to remark that CDC usually produces

480 very low levels of these emissions. Of course, such great amounts of UHC do not fulfil  
481 EU VI regulations and would require the utilization of an ATS system capable of  
482 completing the oxidation reactions. It is interesting to note that the UHC emissions levels  
483 are relatively similar to those of other LTC concepts, and it has been previously  
484 demonstrated that conventional DOCs are able to deal with such high emissions [21,  
485 23]. Nonetheless, it is important to mention that unburned hydrocarbons produced by  
486 oxygenated fuels can contain aldehydes, ketones and other species that cannot be  
487 reduced by conventional DOC [47] and dedicated evaluations would be necessary to  
488 select or design an appropriate aftertreatment device considering the specific speciation  
489 of UHC coming from OMEx.

490 To explain the CO emissions increase, the effect of high EGR rates is combined with the  
491 excessively long injection times, producing large regions with very rich concentrations  
492 that rapidly consume all the oxygen available. The reduction of CO to CO<sub>2</sub> has one of the  
493 longer characteristic times, therefore, by the time this reaction would take place, there  
494 is no oxygen available for it within the spray structure, specially at late stages if the  
495 injection process. This leads to an unacceptable level of CO emissions that are increased  
496 up to 600 times.

497 Considering the final balance of emissions with almost no NO<sub>x</sub> and soot, high UHC and  
498 unacceptable CO emissions, the impact on a conventional ATS system is significant. The  
499 SCR for NO<sub>x</sub> reduction and the particulate filter can be removed as the engine-out  
500 emissions do fulfil the EU VI regulation. In the case of UHC, a conventional DOC could do  
501 the work with adequate resizing and catalyst material composition. Nonetheless, when  
502 considering CO, there is no possibility to use any conventional system to reduce it to

503 acceptable levels. A TWC could not be used as there is no adequate balance between  
 504 NO<sub>x</sub>, UHC and CO, and a DOC cannot be considered as there is not sufficient oxygen at  
 505 the exhaust given the combustion strategy utilized. The only conclusion on this side is  
 506 that there is no conventional ATS capable of dealing with such high emissions of CO and  
 507 HC simultaneously without a significant stage of development. Added to this, the 30%  
 508 of penalty in the equivalent fuel consumption makes this concept not viable for its  
 509 implementation in a real application.  
 510



511 Figure 9. Emissions of NO<sub>x</sub> (a), soot (b), unburned hydrocarbons (c) and CO (d) from OMe<sub>x</sub> results and their  
 512 difference with diesel reference.

513 **4. Global lambda sweep study**

514 At this stage, it is clear that the concept of reaching stoichiometric combustion with an  
515 oxygenated fuel with low LHV is not a viable option for commercial applications. It was  
516 thought that even with such high EGR rates, the maximum power output would not be  
517 that difficult to reach and that NO<sub>x</sub> emissions would not decrease so much.

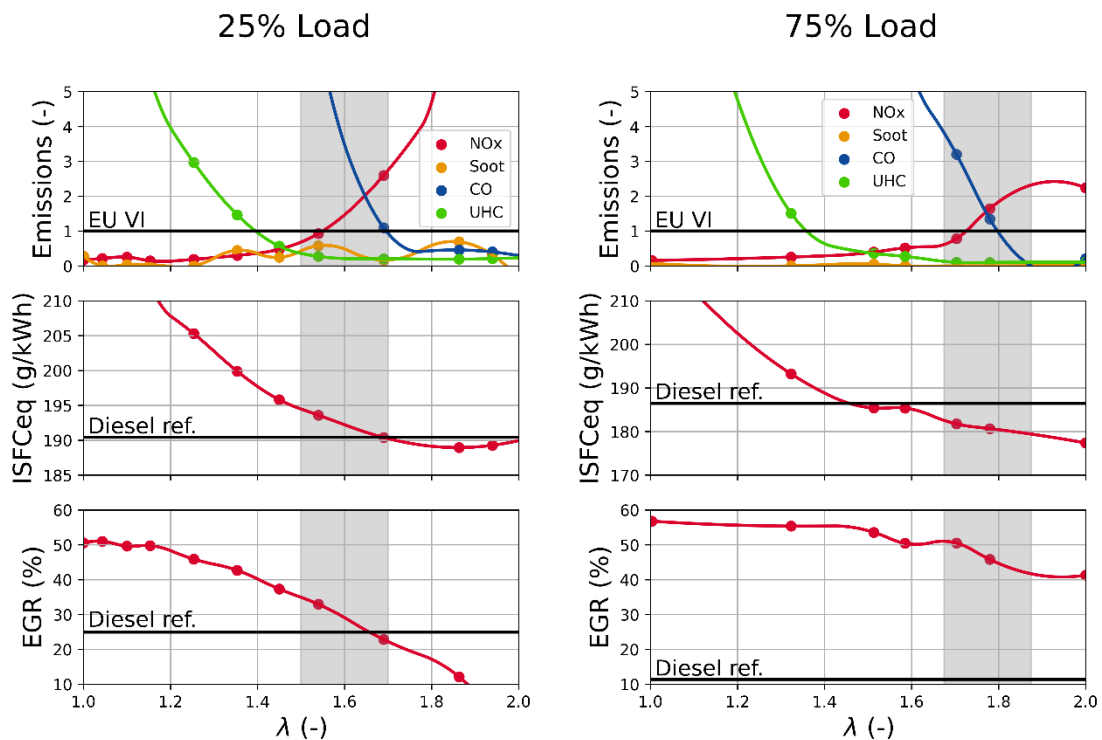
518 Considering the current scenario, with an excessive amount of EGR, OMEx is still able to  
519 have almost zero NO<sub>x</sub> and soot emissions and there seems to have room for lowering  
520 the EGR rates towards mixture conditions of  $\lambda > 1$  and have a more diesel-like operation  
521 while maintaining certain benefits. The authors decided to perform a preliminary re-  
522 evaluation of how OMEx performs under other conditions of dilution to decide if there  
523 is any interesting direction for the application of OMEx as a single-fuel in an ICE.

524 This study consisted of a lambda sweep at two operating conditions: 1800 rpm at 25%  
525 and 75% engine load. The results shown in Figure 10 depict the evolution of regulated  
526 emissions normalized with the EU VI limits (when lower than 1, it fulfils EU VI),  
527 equivalent fuel consumption and EGR requirements when moving towards leaner  
528 conditions.

529 It is observed how the reduction of EGR utilization produces a rapid decrease in UHC as  
530 temperatures and oxygen availability are slightly increased. As the combustion goes  
531 leaner, CO emissions are also reduced below accepted limits while NO<sub>x</sub> start to go over  
532 the regulation limit. At the same time, engine performance is improved, and energy  
533 utilization efficiency can even surpass that of conventional diesel operation having lower  
534 equivalent fuel consumption. At every condition, soot remains virtually null. These  
535 trends are maintained for both engine loads, and the most interesting finding is that in  
536 both cases there is a region in a narrow gap of  $\lambda$  for which all emissions are very near to

537 be EU VI compliant and engine efficiency is slightly better than that of diesel. In this  
 538 region, the EGR levels are still high compared to conventional strategies, but they remain  
 539 below 50%, which is a more reasonable demand for the air management system.

540 The authors think that a detailed calibration around this region with more complex  
 541 multi-injection strategies has a great potential to reach results that can fulfil the EU VI  
 542 regulation in engine-out basis, not requiring any ATS while increasing engine thermal  
 543 efficiency at the same time. As a next step, the authors consider carrying out this  
 544 detailed calibration and report the viability of extending these trends to all the engine  
 545 operating map.



546 Figure 10. Effect of global lambda on OMEx combustion.

## 547 5. Conclusions

548 This work explores the concept of utilizing an oxygenated fuel with low LHV like OMEx  
 549 in a turbocharged compression ignition engine under stoichiometric conditions as a low-

550 emission architecture to evaluate the impact of the fuel properties on the engine  
551 performance. For this, a preliminary calibration for best fuel consumption is obtained  
552 with OMEx and compared against a conventional diesel calibration. From this study it  
553 was possible to obtain the following conclusions:

- 554 • Excessively high EGR rates of almost 80% are required to maintain stoichiometric  
555 conditions, and this has a huge impact on combustion efficiency and engine  
556 performance in terms of equivalent specific fuel consumption reaching a penalty  
557 of 34% compared to that of diesel.
- 558 • Peak heat release is limited by the LHV of the fuel and allows to maintain low in-  
559 cylinder temperatures that contribute to significantly reduce NO<sub>x</sub> emissions. This  
560 property combined with the high EGR rates permits to almost erase NO<sub>x</sub>  
561 emissions in most of the engine map ranging from 95% to 100% reduction.
- 562 • The limitation imposed by the reduced LHV of the fuel cannot be easily overcome  
563 by increasing injection pressure to reduce injection times, establishing a power  
564 limit up to which normal combustion strategies can be maintained.
- 565 • Oxygenated fuels with no carbon-to-carbon bonds in their molecular structure  
566 like OMEx are able to maintain almost-zero soot operation in all the engine  
567 operational range.
- 568 • Due to the low temperatures and high EGR fraction, UHC and CO emissions are  
569 greatly increased. For UHC, the values are typical of other LTC, but for CO, the  
570 increase of up to 600 times is too high and associated to extended local regions  
571 with very rich fuel concentrations.



572 • No suitable ATS based on conventional components can be established as a  
573 preferred option to deal with these emissions levels, which together with the  
574 significant penalty in fuel consumption make this concept not attractive for real  
575 applications.

576 Based on these conclusions, the authors performed a brief exploration of other  
577 combustion strategies under leaner stoichiometric ratios and found out that there is a  
578 region of lambda at which OMEx combustion can fulfil almost all controlled species on  
579 engine-out measurements with a more efficient usage of the energy content in the fuel  
580 compared to conventional diesel engines. Due to the interesting properties found, the  
581 authors have proposed as next steps of this OMEx combustion evaluation to perform a  
582 detailed calibration to evaluate the complete potential of this combustion strategy.

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755

## 756 **Abbreviations**

757 AFst: Stoichiometric Air-to-fuel ratio

758 ATS: Aftertreatment System

759 CA50: Crank Angle at which 50% of fuel mass has been burned



- 760 CDC: Conventional Diesel Combustion
- 761 CO: Carbon Monoxide
- 762 CO<sub>2</sub>: Carbon Dioxide
- 763 DAC: Direct Air Capture
- 764 DOC: Diesel Oxidation Catalyst
- 765 DPF: Diesel Particulate Filter
- 766 ECU: Engine Control Unit
- 767 EGR: Exhaust Gas Recirculation
- 768 EU VI: EURO VI regulation for engine homologation
- 769 H<sub>2</sub>O: water vapor
- 770 ICE: Internal Combustion Engine
- 771 ISCO: Indicated Specific CO emissions
- 772 ISFC: Indicated Specific Fuel Consumption
- 773 ISFCeq: Equivalent Indicated Specific Fuel Consumption
- 774 ISHC: Indicated Specific UHC emissions
- 775 ISNOx: Indicated Specific NOx emissions
- 776 ISSoot: Indicated Specific Soot emissions
- 777 LTC: Low Temperature Combustion
- 778 NOx: Nitrogen Oxides
- 779 OME: Poly-oxymethylene Dimethyl Ether

780 OME<sub>x</sub>: Poly-oxymethylene Dimethyl Ether mixture

781 RoHR: Rate of Heat release

782 SCR: Selective Catalytic Reducer

783 TtW: Tank-to-Wheel

784 TWC: Three-Way Catalyst

785 UHC: Unburned Hydrocarbons

786 WtT: Well-to-Tank

787 WtW: Well-to-Wheel

788