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Additional Information

1 **Optimization of low carbon fuels operation on a CI engine under a simplified driving cycle for**
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16
17 **Abstract**

18 The study of internal combustion engines, and their associated energy conversion
19 processes, is currently focused on targeting the reduction of pollutant emissions while
20 maintaining or improving efficiency and fuel consumption. The research of alternative
21 fuels, in particular low carbon fuels (LCF), seems to be a promising strategy for solving
22 this problem. However, the characterization of a fuel with properties different than
23 those of diesel requires numerous tests and resources to prove the viability of the
24 substitution for another alternative. In Europe, for a vehicle to be homologated the
25 World harmonized Light vehicles Test Cycle (WLTC) must be complied with. This cycle

26 requires transient tests, that performed with a fuel for which an engine calibration is not
27 yet existent would be difficult and could hinder the evaluation of the potential of a given
28 fuel. This study proposes a cycle simplification methodology that seeks to reduce the
29 driving cycle to a discrete set of stationary conditions, for which each operational
30 calibration can be optimized. The optimization methodology is based on statistical
31 analysis and modelling, and is presented to select the most desirable operating
32 condition that can be reached using an LCF. For each testing point optimization NO_x,
33 soot, brake efficiency and fuel consumption are used as targets. Finally, the calibrated
34 operating conditions are applied within the simplified cycle to assess the homologation
35 potential of the studied fuel, as well as the equivalent CO₂ emissions under the criteria
36 of a well-to-wheel analysis (WTW).

37 **Keywords**

38 Low carbon fuel; engine optimization; WLTC; well-to-wheel; homologation; statistical
39 model

40

41 **1 Introduction**

42 Modern society is reliant on vehicles for the transportation of their individuals and their
43 goods. However, the road transport sector is one of the main sources of greenhouse gas
44 emissions [1]. Passenger vehicles in particular account for a significant percentage of
45 the total automotive fleet, and thus their polluting effect is aggravated by their quantity.
46 Recent years have shown the start of a transition towards the electrification of vehicles,
47 which is considered as a pathway for the de-fossilization of the whole sector, through
48 the use of electricity from low-carbon sources. The prospect is promising due to the
49 rapid growth of renewable energy capacity [2], the cost reduction of greener technology
50 against more contaminant energy production methods [3], and the general acceptance
51 of the consumer to the use of electricity sources like wind and solar [4]. Under this
52 panorama, and with policies supporting and accelerating the adoption of electric
53 vehicles (EV) [5], the intention is to phase-out internal combustion engines (ICE) in
54 vehicles by as early as 2030 [6]. Nonetheless, complete adoption of EVs will probably
55 take longer because complete vehicle fleet replacements are estimated to occur every
56 twenty years, and calculations indicate that even if half of new car sales were electric by
57 2035 only 30% of vehicles would be EVs [7]; some projections even indicate the
58 proportion of EVs in the road vehicle fleet will be much lower (7% by 2030 [5]). Knowing
59 that ICEs will still account for a significant percentage of all vehicles in the near-to-
60 medium term future, it is important to evaluate alternatives for road transport energy
61 carriers that can help reduce the pollution caused by combustion vehicles while they are
62 still in use. Of those alternatives, low-carbon fuels (LCF) represent an interesting option
63 because they provide the additional potential of being implemented under existent

64 commercially available powertrain systems, while at the same time reducing the carbon
65 dioxide lifecycle footprint of the fuel.

66 Alternative fuels for ICEs have been of interest for researchers since the first iterations
67 of the engine. In recent years the focus on fuels not coming from fossil sources has
68 increased due to the need of the sector to reduce CO₂ emissions and mitigate other
69 pollutant emissions -such as NO_x, CO, unburned hydrocarbons (HC) and particulate
70 matter (PM)- that can harm both the environment and human beings. Additionally,
71 these pollutants specifically regulated under norms such as Euro 6 [8]. LCF are a good
72 alternative because they can be synthesized from carbon, separated from captured
73 atmospheric CO₂ [9], and hydrogen from water electrolysis [10] (which can be obtained
74 from processes that use surplus electricity from renewable sources); or come from
75 biomass sources [11], as is the case for biofuels. For this study a
76 LCF blend with biofuel content, composed of hydrogenated vegetable oil (HVO) and
77 fatty acid methyl esters (FAME) is going to be used. The biofuel, in addition to the
78 contribution with the reduction of the equivalent CO₂ released can have properties that
79 aid in the reduction of NO_x, HC and CO emissions, such as a lack of sulfurs and aromatics
80 [12].

81 Different kinds of studies have been performed to evaluate ICEs. Some studies like the
82 one on [13] tested LCF blends with OMEx and HVO to characterize the combustion,
83 performance, and emissions by varying the composition of the blend at different speed
84 and loads. Other studies on biofuels and CI engines in general focus on the effect of the
85 variation of a single parameter on the combustion and emissions of the engine, like the
86 work of [14] [15] [16]. Due to the complexity of the combustion process, works where

87 several parameters are studied simultaneously require the approximation of models to
88 explain the effects of the variations observed. The models are empirical simplifications
89 of the phenomenon at hand and have already been proven effective in the study of
90 internal combustion vehicles. The work of [17], for example, studied the effect of a
91 gasoline-methanol mixture combined with metal nanoparticles by employing statistical
92 analysis to see the effect the throttle position, the engine speed and the presence of
93 nanoparticles had on the performance and emissions of spark-ignition (SI) engine.
94 Statistical models have also already been employed for Diesel engines calibration in the
95 work of [18] finding that this kind of models can accurately predict different responses
96 of the engine with generalizable results. The final kind of study to evaluate internal
97 combustion vehicles comprehends the adherence to regulations and the effect on
98 driving conditions. For these studies, tools like GT-Power have often been employed as
99 they can simulate driving conditions from stationary engine measurements as well as
100 test hybrid and fully electric powertrains to have a complete comparison [19]. Other
101 methodologies to assess probable driving scenarios can be seen in the form of the
102 discretization of a complete driving cycle into discrete operating conditions [20], as is
103 performed in this work.

104 After an overview of the current automotive scenarios where ICEs will continue to have
105 an important role, the potential of LCF to reduce both equivalent CO₂ emissions and
106 criteria pollutants, and the different studies methodologies capable of evaluating and
107 characterizing ICEs it is worth continuing the developing of works to further the
108 investigation on the improvement of ICEs. This work evaluates the use of an LCF with
109 moderate renewable content, inside a light-duty compression ignition (CI) engine and
110 proposes a simplified methodology for its assessment and operation calibration within

111 a statistical model framework that can be replicated for the study of other fuels with
 112 different renewable content proportions and intensive properties. The application of a
 113 simplified driving cycle assessment allows for the detailed study of the parameter
 114 modifications in ICEs because only a reduced set of experiments is needed to estimate
 115 the cycle results. Thus, for each of the operating conditions, complete optimization
 116 procedures based on statistical analysis can be done, obtaining relevant information on
 117 the combustion and operation parameters while allocating time and resources
 118 efficiently.

119 **2 Materials and methodology**

120 **2.1 Engine characteristics and test cell description**

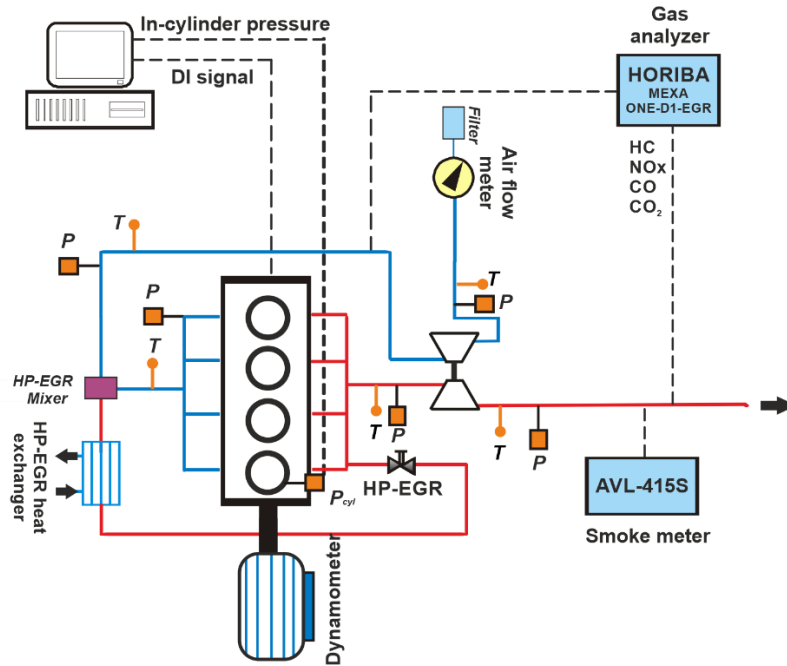
121 Table 1 Engine characteristics

General characteristics	
Number of cylinders [-]	4
Cylinder diameter [mm]	79.7
Stroke [mm]	80.1
Total displaced volume [cm ³]	1598
Connecting rod length [mm]	140
Compression ratio [-]	16.0
Rated power [kW]	100 @ 4000 rpm
Rated torque [Nm]	320 @ 2000 rpm

Injection system characteristics	
Type of injector	solenoid
Number of holes [-]	7
Hole diameter [μm]	141
Flow number [FN]	340
Maximum injection pressure [bar]	2000

122

123 A 4-cylinder commercially available 1.6 L CI engine provided with high-pressure EGR was
124 used to perform this investigation. More information on the engine can be found in
125 Table 1, including the type of injectors and compression ratio. The ECU was originally
126 provided with a baseline diesel B7 calibration, which through an INCA V5.2 virtual
127 environment (dedicated tool for ECU tests, diagnostics and calibration of electronically
128 controlled systems in the vehicle [21]) was modified in 8 main parameters to achieve
129 the desired calibration for the air management and injection systems. The parameters
130 to be controlled during tests were the fuel mass injected, the injection pressure, the
131 start of injection (SOI), the pilot injections fuel mass and dwell times, the in-cylinder
132 cycle air mass and boosting pressure.



133

134

Figure 1 Test cell scheme

135 The engine was installed in a completely instrumented test rig, provided with a Dynas₃
 136 LI dynamometer to measure the torque output, an Horiba MEXA 7100 to collect
 137 information on the main engine-out emissions of interest (NO_x, CO, HC, O₂ and CO₂), an
 138 AVL 415S smoke meter to measure soot in FSN number, and an air flow meter and a fuel
 139 balance to measure fuel mass flow. Additionally, pressure and temperature probes were
 140 present at the positions identified in Figure 1. The temperature and pressure values
 141 were recorded by an in-house LABVIEW controller, called CMT samaruc, which averaged
 142 the measurements. More information on the measuring equipment can be found in
 143 Table 2, including the accuracy each instrument has.

144

Table 2 Instrumentation accuracy

Variable measured	Device	Manufacturer/ model	Accuracy
-------------------	--------	---------------------	----------

In-cylinder pressure	Piezoelectric transducer	Kistler / 6125C	± 1.25 bar
Intake/Exhaust pressure	Piezoresistive transducers	Kistler / 4045A	± 25 mbar
Temperature	Thermocouple	TC direct / type K	± 2.5 °C
Crank angle, engine speed	Encoder	AVL / 364	± 0.02 CAD
NO _x , CO, HC, O ₂ and CO ₂	Gas analyzer	Horiba MEXA 7100	4%
FSN	Smoke meter	AVL 415S	±0.025 FSN
Fuel mass flow	Fuel balance	AVL 733S	±0.2%
Air mass flow	Air flow meter	AVL 422	±0.1%
Torque	Dynamometer	Dynas ₃ LI	

145

146 2.2 Fuel characteristics

147 This study is divided in two sections which will be performed with two fuels with
148 different proportions of EU fossil diesel and renewable content. The first fuel is EU fossil
149 diesel, while the second blend has 33% renewable content, with a composition of 7%
150 FAME and 26% HVO. Some important properties of the studied fuel blends are present
151 in Table 3. The fuel blends have different cetane index where the LCF blend has a higher
152 value which will reduce the combustion delay time. As can be seen, the fuels have a
153 similar energy density due to their similar carbon, oxygen and hydrogen content;
154 however, as they are not identical in terms of lower heating value (LHV), equation 1 is

155 used to obtain the equivalent fuel consumption excluding the effect of the lower heating
 156 value and using diesel as the reference and assessing the energy conversion each fuel
 157 blend can have; where \dot{m} is the mass flow rate of fuel, and P_{brake} is the brake power.

$$BSFC_{eq} \left[\frac{g}{kWh} \right] = \frac{\dot{m} \cdot \left(\frac{LHV_{fuel\ blend}}{LHV_{Diesel}} \right)}{P_{brake}} \quad (1)$$

158

159

Table 3 Fuel properties at standard conditions

	Diesel blend	LCF blend
EU fossil diesel composition [%v/v]	93	67
FAME [%v/v]	7	7
HVO [%v/v]	0	26
Cetane Index [-]	54.6	62.4
Density @ 15°C [g/ml]	0.834	0.821
KV @ 40°C [cSt]	2.86	2.90
Water content [ppm = 100 %m/m]	80.0	0.012
Lower Heating Value [MJ/kg]	42.81	43.04
Carbon [% m/m]	85.78	85.40
Hydrogen [% m/m]	13.45	13.84
Oxygen [% m/m]	0.77	0.76
Residue [%vol.]	1.30	1.4
K_{CO_2} [gCO ₂ /g _{fuel}]	3.22	3.13
TTW CI [gCO ₂ /MJ]	75.2	72.7

WTT CI [g _{CO2} /MJ]	15.8	-6.7
-------------------------------	------	------

160

161 The fuels' Well-to-Tank (WTT) carbon intensity was derived from the work performed in
162 [22], while the Tank-to-Wheel (TTW) CO₂ emissions come from equations 2 and 3, under
163 the premise of complete combustion. On equation 2, k_{CO_2} is the coefficient of
164 correlation of a unit of mass of fuel into a unit of mass of CO₂, $y_{C_{fuel\ blend}}$ is the carbon
165 proportion of the fuel in mass, while M_C and M_{O_2} are the molar masses of carbon and
166 oxygen respectively. Then, on equation 3, \dot{m}_{CO_2} represents the CO₂ mass flow rate.
167 These equations provide a relation between the available carbon content in the
168 composition of the fuel and the tailpipe CO₂. The hypothesis is supported, in part, by the
169 high efficiency (above 90% [23] [24]) that can be obtained in diesel oxidation catalysts
170 (DOC) which would make possible the complete oxidation of the fuel after the engine;
171 additionally, this consideration implies the worst case scenario for CO₂ emissions where
172 all the fuel used in the engine is exhausted from the vehicle as CO₂.

$$k_{CO_2} = y_{C_{fuel\ blend}} \cdot \left(\frac{M_C + M_{O_2}}{M_C} \right) \quad (2)$$

$$\dot{m}_{CO_2} = k_{CO_2} \cdot \dot{m}_{fuel\ blend} \quad (3)$$

173

174 **3 Driving cycle simplification methodology**

175 The Worldwide harmonized Light vehicles Test Procedure (WLTP) is the current
176 European standard to determine fuel consumption, and emissions of criteria pollutant
177 and CO₂ light duty vehicles have (both combustion, hybrids and electric) [25]. It consists
178 of chassis dynamometer tests cycles abbreviated as WLTC) that intend to reduce the

179 discrepancies between the results obtained in the laboratory and real driving conditions.
180 On this work, the Class 3 WLTC will be the focus as it is the cycle representative of light-
181 duty vehicles driven in Europe. In particular, the Class 3b cycle will be evaluated, which
182 has 4 phases, speeds above 120 km/h, a duration of 30 minutes and covers a distance
183 of 23.25 km.

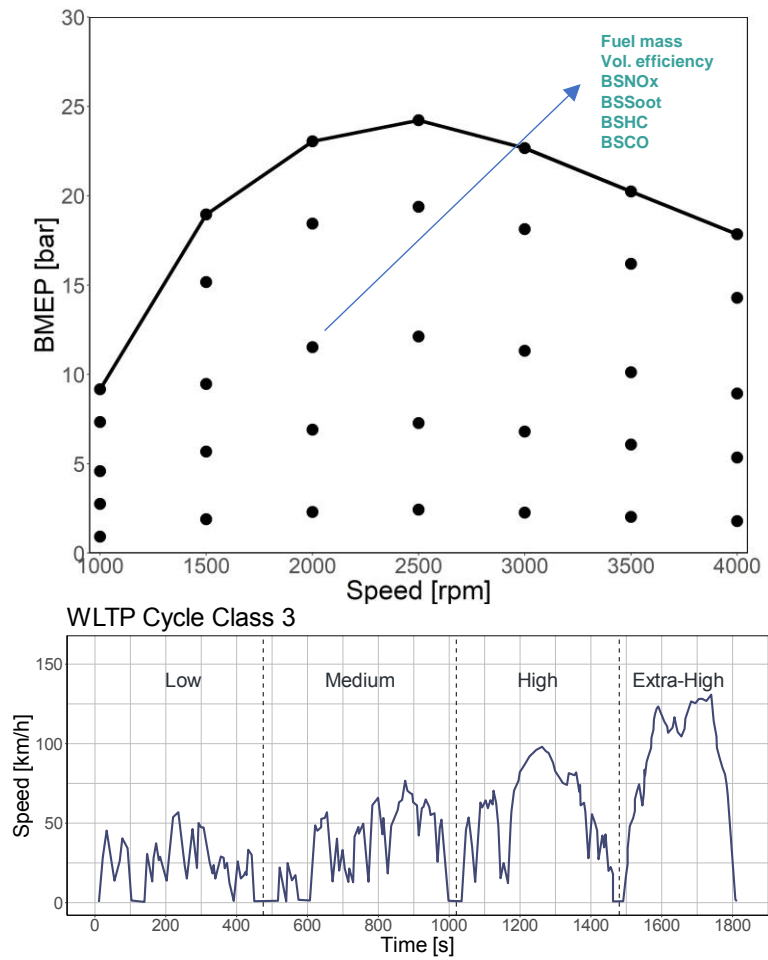
184 A methodology for the characterization of engine operation in the WLTC driving cycle is
185 proposed based on a simplified cycle which only requires a limited amount of
186 experimental data. In this approach the engine map is reduced to a few operating
187 conditions following a discretization methodology that seeks to reproduce the results of
188 the complete engine map with a limited and distributed dataset. The methodology
189 allows for the reduction of experimental measurements while still providing insightful
190 conclusions when correlated to a driving cycle, similarly to the work described in [20].
191 The interests in performing this kind of simplifications are the capability to work with
192 limited resources, for example reduced fuel quantities or testing time, that could
193 prevent the measurement of the complete engine map. For the case of this study the
194 simplification of the engine map model needs to be able to apply a dedicated calibration
195 strategy to each operating condition, which would be very cost and time intensive if the
196 complete engine map was given the same treatment.

197 The methodology to reduce a complete engine map to a limited set of points must
198 adhere to some considerations. Namely, the engine must already be characterized with
199 at least one fuel. Namely, complete engine maps should be available. For the Diesel
200 engine used in this study, because it is a commercial engine, information on the
201 performance and fuel consumption was accessible to compare with the measurements

202 and subsequently validate the proposed methodology. Additionally, measurements for
203 the complete engine map were performed with diesel to have information on both the
204 fuel consumption and main emissions that can later be compared with the results from
205 the simplified methodology that uses only a few selected operating conditions.

206 **3.1 Engine map characterization and GT-Power model**

207 The complete engine map was characterized by measuring 35 stationary operating
208 conditions distributed equally across the engine map with the diesel blend. The speed
209 allocation was made every 500 rpm, starting at 1000 rpm and ending at 4000 rpm, while
210 the load distribution was done every 10% of load at each speed. For each of these
211 operating conditions fuel consumption and emissions were measured, as well as the
212 instantaneous intake, exhaust and in-cylinder pressures and other boundary conditions.
213 The experimentally obtained values were then used to feed a GT-Power vehicle model
214 to calculate the WLTC (Figure 2).



215

216 Figure 2 Input information for the GT-Power model. [Top] Experimentally measured

217 engine map [Bottom] Speed profile for the Class 3b WLTC

218 For the GT-Power simulation, the vehicle modelled is an OPEL Astra J 1.6 CDT, which

219 equips the engine that was described in the previous section.

220

221 Table 4 shows the aerodynamic and mechanical characteristics of the original
222 equipment manufacturer (OEM) vehicle. Figure 3 illustrates the model and its sub-
223 assemblies to represent the different vehicle systems. Each timestep speed profile is
224 defined inside the object called "Driver", which consists of a PID controller which acts
225 on the accelerator position to provide the necessary power for the speed demand.
226 Additionally, the object called "Engine-1" has the information on the engine fuel
227 consumption and emissions that were experimentally measured, to be able to calculate
228 these results across the cycle. The "Vehicle" template has all the information necessary
229 to describe the operation, including the mass of both the vehicle and its cargo, the drag
230 coefficient, the tire information including rolling resistance and differential information,
231 as well as system strategies.

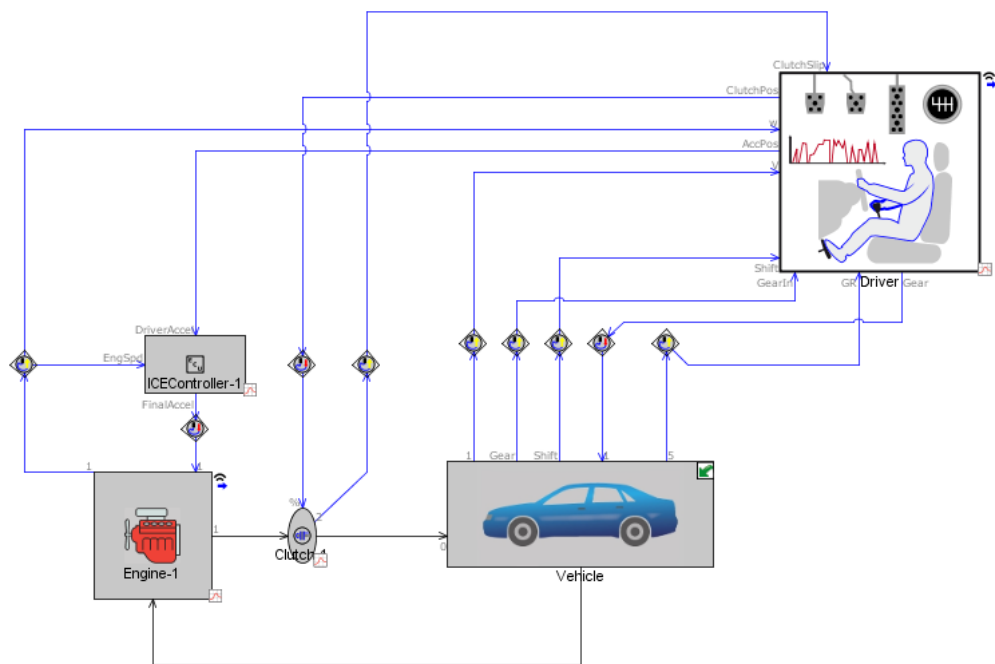
232

233 Table 4 Vehicle characteristics and driving strategy characteristics for the GT-Power

234 modelling

Vehicle characteristics	
Base vehicle mass [kg]	1364
Passenger and cargo mass [kg]	145
Vehicle drag coefficient [-]	0.28
Frontal area [m ²]	2.8
Tires size [mm/%/inch]	225/50/R17
Differential ratio [-]	3.2
Wheelbase [cm]	268.5
Driving strategy	
Driver mode	Speed targeting
Transmission type	Manual
Gear shift-up [rpm]	2500
Gear shift-down [rpm]	1200

235

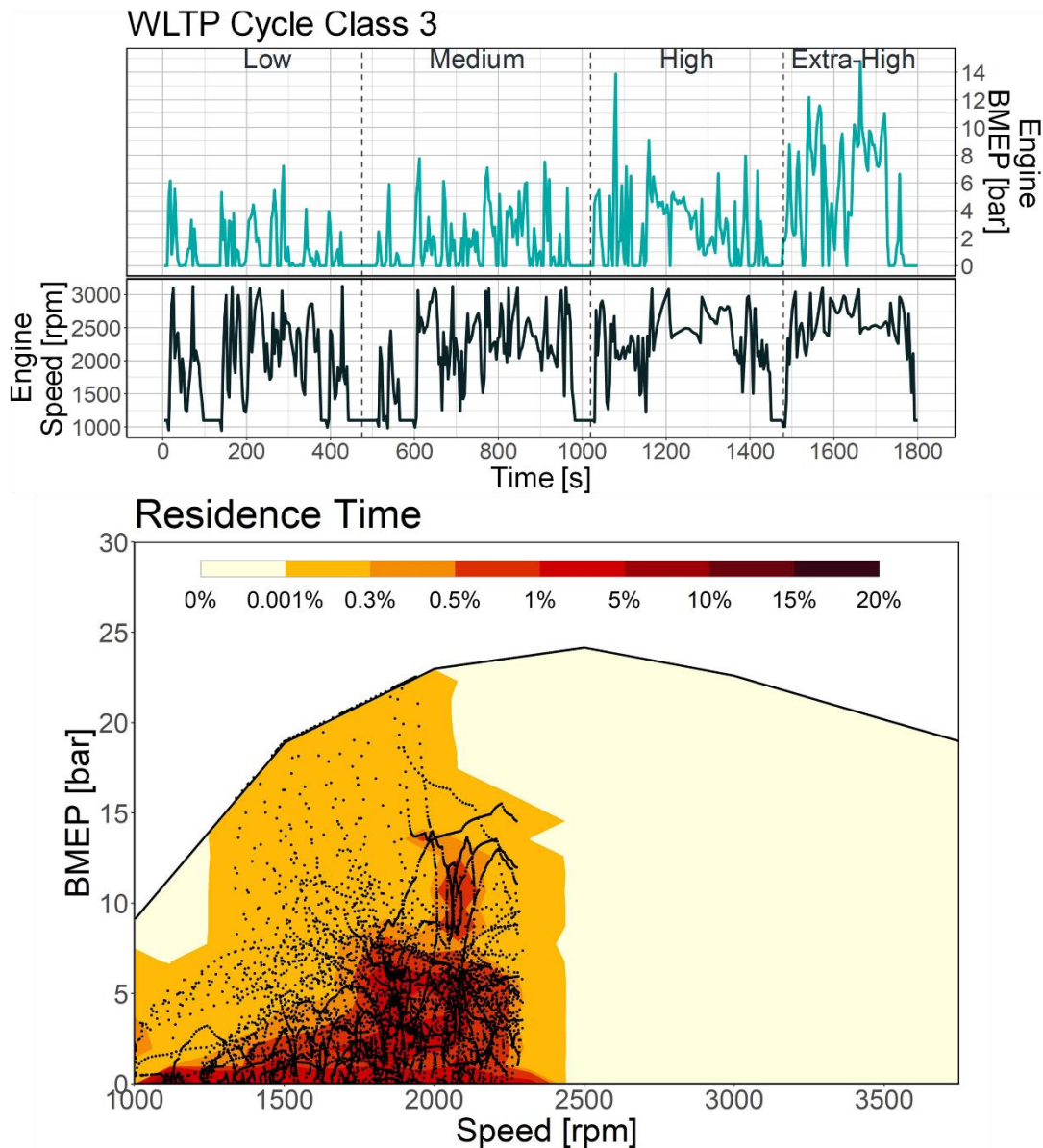


236

237

Figure 3 GT-Power vehicle model

238 For this study, the driver mode was set to speed targeting in order to be able to follow
 239 the speed profile of the WLTP cycle. With the model, the brake mean effective pressure
 240 (BMEP) and engine speed are determined for each instant, providing the information
 241 necessary to calculate the residence time for each engine operating condition (defined
 242 as the time the engine remains on a given speed and load). This output is represented
 243 in Figure 4, where it can be seen that most of the engine operation is concentrated at
 244 low loads and speeds, not exceeding 2500 rpm. It is important to highlight that the
 245 residence time results are dependent on the gear up shift strategy used, and the results
 246 may vary depending on whether a longer or shorter one is used.



247

248 Figure 4 GT-Power model output [Top] Engine speed and load profiles [Bottom]

249 Residence time map showing the distribution of operating conditions

250 3.2 Characterization of the engine map with limited operating conditions

251 Once the engine cycle operating conditions are characterized, it is desired to simplify

252 the operation of the engine to a reduced quantity of operating points where each can

253 be optimized individually, but a global overview of the driving conditions can still be

254 obtained. The selected operating conditions for this study are based on the work of [26],

255 and provide a low-speed low-load point, two mid-load points, and two high-load points.
256 These operating conditions are distributed across the engine map in such a way that
257 they can be representative of the engine operation. Table 5 describes the speed and
258 BMEP for each one of the testing points.

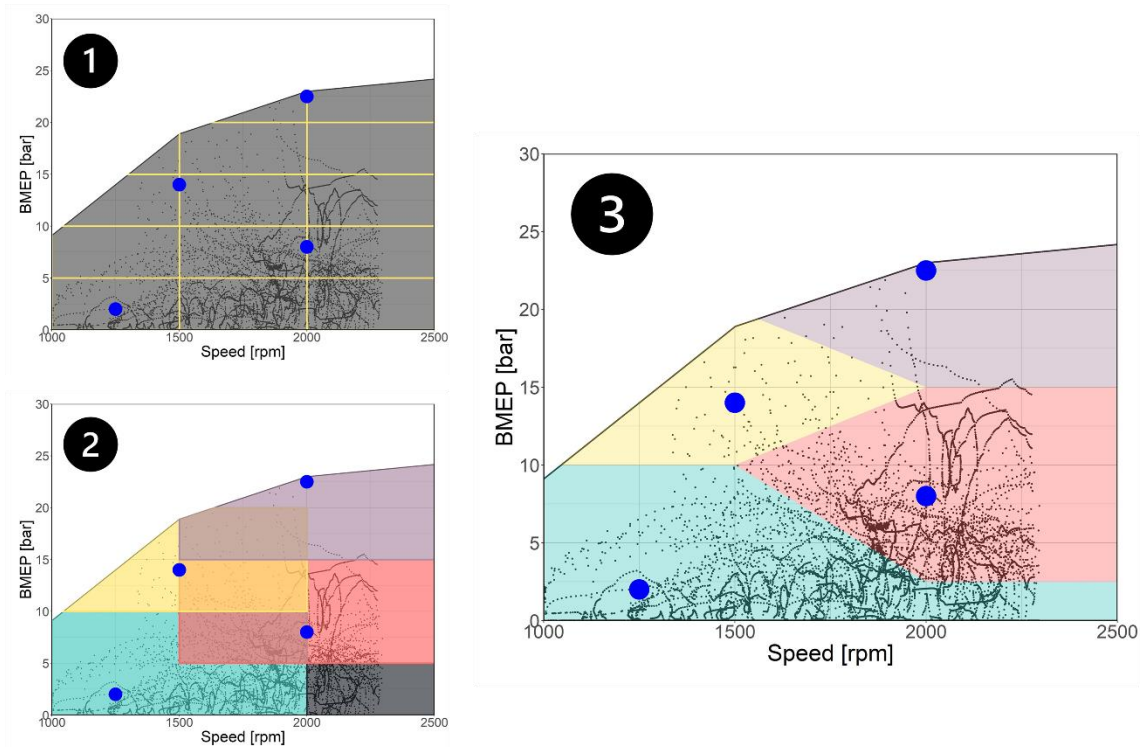
259 Table 5 Engine operating conditions

Test Label	Speed [rpm]	BMEP [bar]	Cycle weight [%]
1250 rpm @ 2 bar	1250	2	52.00
1500 rpm @ 14 bar	1500	14	1.65
2000 rpm @ 8 bar	2000	8	44.42
2000 rpm @ 22 bar	2000	22	1.43

260

261 The simplification methodology for the WLTC cycle, is based on the discretization of the
262 engine map into equal bin sizes with dimensions speed \times load. The speed ranges cover
263 a span of 500 rpm while the load is divided every 5 bar of BMEP (which is the maximum
264 sized area that allows equally sized bins in the engine map), as can be seen in the first
265 step in Figure 5. The second step of the process consists of using the operating
266 conditions of interest as centroids, where multiple bins from the first step are grouped
267 to form bigger bins that contain all the operating conditions of the cycle with their
268 respective centroids. The bins in this step have a range of 1000 rpm and 10 bar of BMEP,
269 and there can be overlap between them. To resolve the overlapping of bins and assign
270 each of the centroids a unique area, the regions that overlap are divided in half, thus

271 delimiting 4 singular regions within the engine map (as can be seen in the third step
272 shown in Figure 5.

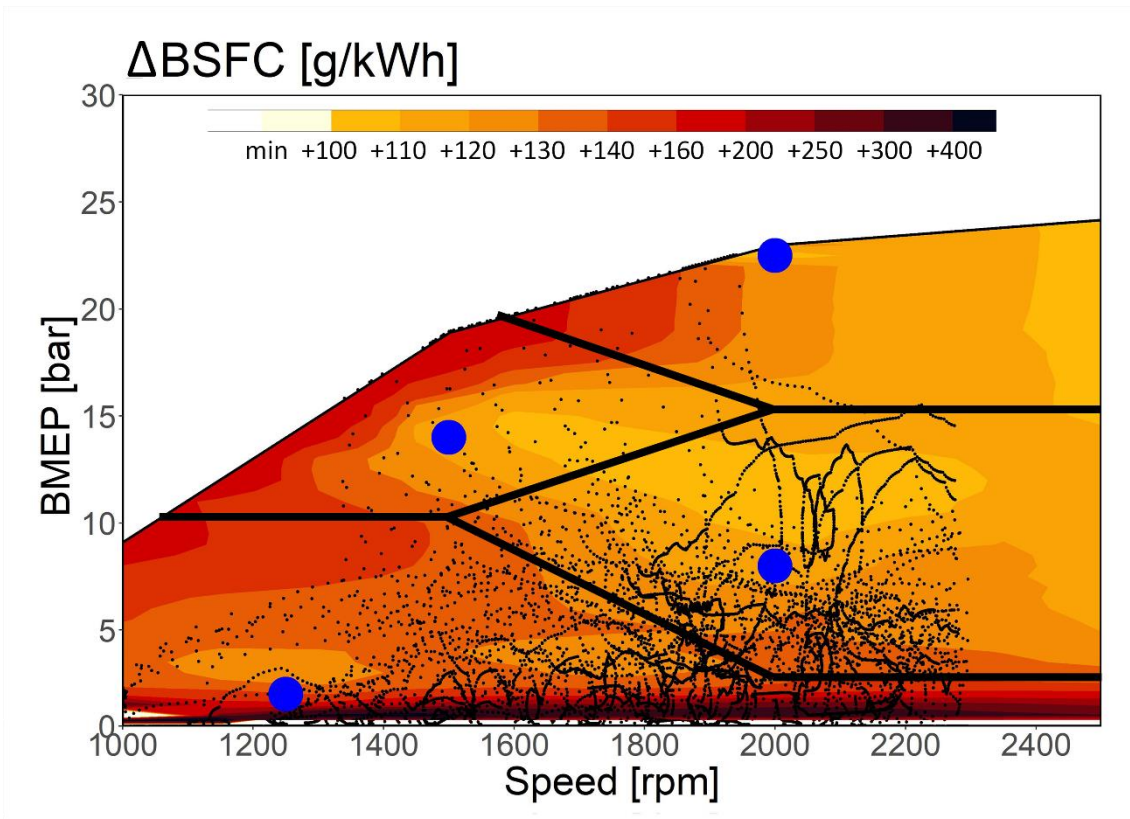


273

274 Figure 5 Engine map discretization procedure schematic

275 After the discretization in regions, the percentage of time within each region is
276 calculated by counting the number of operating conditions that fall inside each area,
277 where each point represents an equal amount of time in the respective condition. The
278 proportion value is then assigned as the weight to be used in the simplified driving cycle
279 that can be seen in Table 5. From both Table 5 and Figure 5, it should be noted how most
280 of the weight of the cycle falls in the zones that correspond to the lower load operating
281 conditions (1250 rpm @ 2 bar and 2000 rpm @ 8 bar).

282



283

284 Figure 6 BSFC engine map and region delimitation after the discretization procedure.

285 The blue dots represent the selected operating conditions for the discretized regions

286 Figure 6 shows the BSFC engine map which illustrates the different fuel consumption

287 zones can be appreciated for the WLTC operating conditions. In the figure, it can be

288 observed how the lower load conditions present the highest BSFC gradients and how,

289 when the speed and load are increased, the variation in BSFC is less variable with lower

290 values. This information is presented in Table 6, where the minimum, maximum and

291 mean values of each region are given. It is also shown, how in terms of BSFC the selected

292 operating conditions have values that are similar to the mean inside the corresponding

293 region. To accept the proposed discretized regions, it was verified that the BSFC

294 difference between extreme values and the selected operating point did not exceed 30%

295 to ensure a good representation in terms of fuel consumption. In the same table, values

296 for the main criteria pollutants can also be appreciated, highlighting that although the
 297 mean value for the region and the selected operating condition show relatively good
 298 agreement, emission values are harder to be represented with only a few stationary
 299 conditions. The results in Table 6 are presented as differences according to Equation 4
 300 to preserve the intellectual property of the OEM.

$$\Delta X_{value} = X_{value} - X_{global\ min} \quad (4)$$

301 Table 6 Discretized engine map BSFC and emissions values represented as difference
 302 with respect to the global minimum value

		Δ BSFC [g/kWh]	Δ BSNOx [g/kWh]	Δ BSSoot [g/kWh]	Δ BSHC [g/kWh]	Δ BSCO [g/kWh]
Area 1 1250 rpm @ 2 bar	min	21.0	0.00	0.030	0.12	0.35
	max	502.9	3.02	4.886	6.01	13.22
	mean	80.8	1.55	0.455	0.82	4.21
	1250 rpm @ 2 bar	106.7	0.46	0.111	1.03	5.07
Area 2 1500 rpm @ 14 bar	min	2.2	0.19	0.051	0.02	0.97
	max	98.5	2.68	5.946	0.22	12.32
	mean	38.7	1.68	1.826	0.09	5.18
	1500 rpm @ 14 bar	36.1	1.43	0.066	0.07	3.83

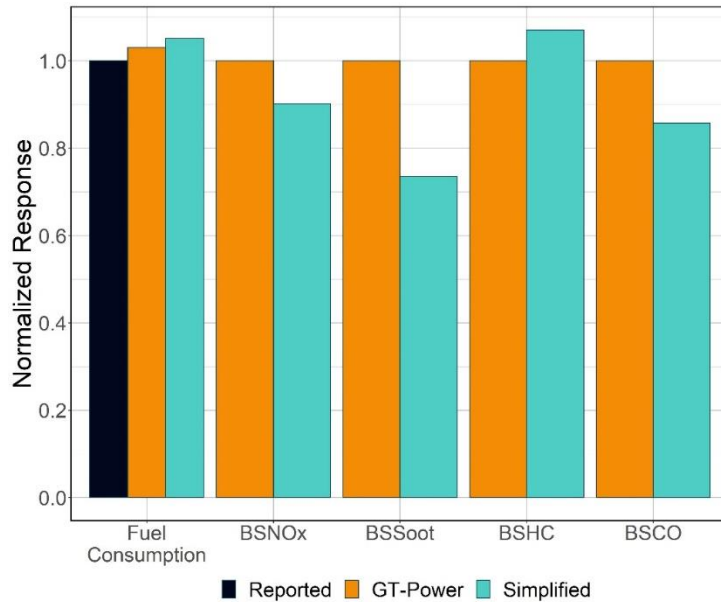
Area 3 2000 rpm @ 8 bar	min	0.0	1.01	0.005	0.05	0.07
	max	34.5	4.63	0.104	0.66	4.40
	mean	17.0	2.16	0.053	0.16	0.91
	2000 rpm @ 8 bar	23.5	1.30	0.077	0.13	0.80
Area 4 2000 rpm @ 22 bar	min	5.8	0.19	0.000	0.00	0.00
	max	89.1	5.89	5.866	0.15	11.02
	mean	24.4	3.13	0.846	0.04	4.12
	2000 rpm @ 22 bar	26.8	2.71	0.348	0.02	10.07

303

304 **3.3 Simplified engine map characterization validation results**

305 With the selected operating conditions assigned their relative weight in the WLTC, the
306 cycle calculation was performed and compared with the results yielded from the GT-
307 Power model presented in previous sections. It has been shown in previous studies [27]
308 that GT-Power models closely approximate experimentally measured driving cycle
309 results for fuel consumption, but however struggle to accurately predict emissions due
310 to the high effect transient operation has on pollutants, although relatively good
311 approximation can be achieved for NO_x emissions (difference below 4%) [28]. The
312 results of the simplified cycle proposed in this study will be compared with the GT-Power
313 results to serve as baseline of how well the methodology can provide information on a

314 given driving cycle, with a small set of operating points. As an additional reference, the
315 OEM-reported fuel consumption is also compared to have a fuller assessment of the
316 results.



317

318 Figure 7 Simplified WLTP cycle results compared to the results obtained with the
319 complete engine map GT-Power model and OEM reported fuel consumption values.

320 Figure 7 shows the simplified cycle results compared with the GT-Power model results
321 and the OEM reported fuel consumption. In terms of fuel consumption, it can be noticed
322 that the simplified methodology is around 5% higher than the reported values and 2%
323 higher than the GT-Power results, which under real driving conditions is a feasible
324 variation. Regarding the pollutant emissions it should be noted that the simplified cycle
325 methodology shows lower values than GT-Power (except for HC), which under a real
326 driving scenario are expected to be higher than GT-Power's results. Even though
327 emissions might not be as well captured with this methodology as they would be with
328 experimentally measured transient results, the simplified methodology provides a first
329 insight into the emissions homologation potential of different fuels with a small

330 operating point sample. The approach allows the characterization of the engine
 331 operation and the calculation of the CO₂ emissions of the engine in a given cycle,
 332 allowing the assessment of the carbon footprint of the engine. More importantly, having
 333 few operating conditions allows the calibration of each operating condition in a
 334 dedicated manner, as will be described in the following section.

335 **4 Statistical model and optimization for a light-duty compression ignition engine**

336 The current section will explain the engine optimization methodology. The methodology
 337 seeks to achieve a balance within the NO_x-soot tradeoff prevalent in CI engines, while
 338 maintaining the highest possible efficiency and lowest fuel consumption using a low
 339 carbon fuel blend. The engine calibration process consists of defining various control
 340 parameters to obtain the desired responses from the engine in terms of emissions and
 341 performance. In this study the LCF blend, described in Table 3, will be evaluated and
 342 calibrated at the operation conditions corresponding to the simplified engine map areas
 343 (1250 rpm @ 2 bar, 1500 rpm @ 14 bar, 2000 rpm @ 8 bar and 2000 rpm @ 22 bar),
 344 without exceeding the constraints specified in Table 7 to guarantee a safe operation of
 345 the engine and, in the case of the emissions, to serve as targets for the optimization.

346 Table 7 Experimental constraints for the optimization of the testing operating
 347 conditions

Test Label	BSNO _x [g/kWh]	Soot [FSN]	Pmax [bar]	PRR [bar/CAD]
1250 rpm @ 2 bar	0.2 — 1	< 2	<180	<8

1500 rpm @ 14 bar	<3	< 3	<180	<8
2000 rpm @ 8 bar	0.7 – 2	< 3	<180	<8
2000 rpm @ 22 bar	< 4.5	< 3	<180	<8

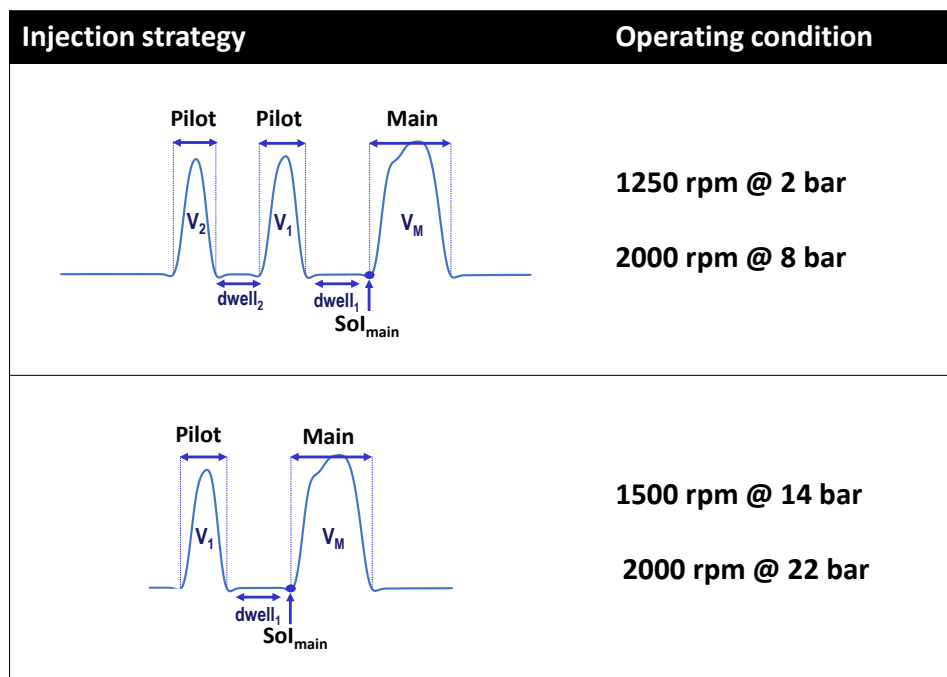
348

349 The study of each operating condition will be performed by a design of experiments
350 (DoE) considering different variables corresponding to the fuel injection pressure, SOI of
351 the main injection, the volume of the pilot injections, the dwell time between injections,
352 as well as the air mass quantity and the boosting pressure. The design of experiments is
353 done in two levels, a minimum and a maximum. The test matrix design depends on the
354 operational condition; low and medium load conditions are explored with a 6-factor 2-
355 k factorial design [29] with a central point, while the higher load points are studied with
356 a modified Plackett-Burman design [30] with central points and also 6 factors. Both types
357 of DoE allow to assess the interaction between factors. The use of two Plackett-
358 Burmann design at higher loads follows the need for a shorter test run under these
359 conditions. The shorter DOE promotes less permanence on straining engine conditions
360 where in-cylinder and exhaust temperatures can be extremely high, or pressure rise rate
361 (PRR) can surpass safety levels, and thus guarantees a safer engine operation, although
362 the reduced amounts of test can slightly increase the error in the modeling. To overcome
363 this issue, the modification on the Plackett-Burmann design is done by adding more
364 experimental data points after the creation of a first model, where parameters
365 necessary for the minimum achievable NO_x, soot and BSFC operating conditions are
366 found, as well as maximum efficiency and an efficiency-emissions-fuel consumption
367 balanced operating point are found. The prediction accuracy is later checked in the
368 engine. If after the initial screening, the operating conditions responses have an

369 accuracy of less than 90%, this process is repeated, adding the new experimental results
 370 into the data set and finding new parameters until the error is below 10%.

371 As can be seen in Figure 8, the different operating conditions use different injection
 372 strategies which can include one or two pilot injections. The cases with two pilot
 373 injections, which are the lower load points, have 8 possible variable parameters,
 374 however for the study only 6 were modified during the optimization and the other 2
 375 remained fixed. Additionally, it was important to know beforehand the minimum and
 376 maximum levels achievable with each parameter. For those reasons, preliminary tests
 377 were performed with two defined objectives: individually test each factor to see the
 378 limit at which the previously mentioned constraints are exceeded (which
 379 consequentially allows to ensure a monotonous behavior); and provide a factor removal
 380 criterion, based on the standardized response of each parameter, for the operating
 381 conditions that have two pilot injections.

382



383

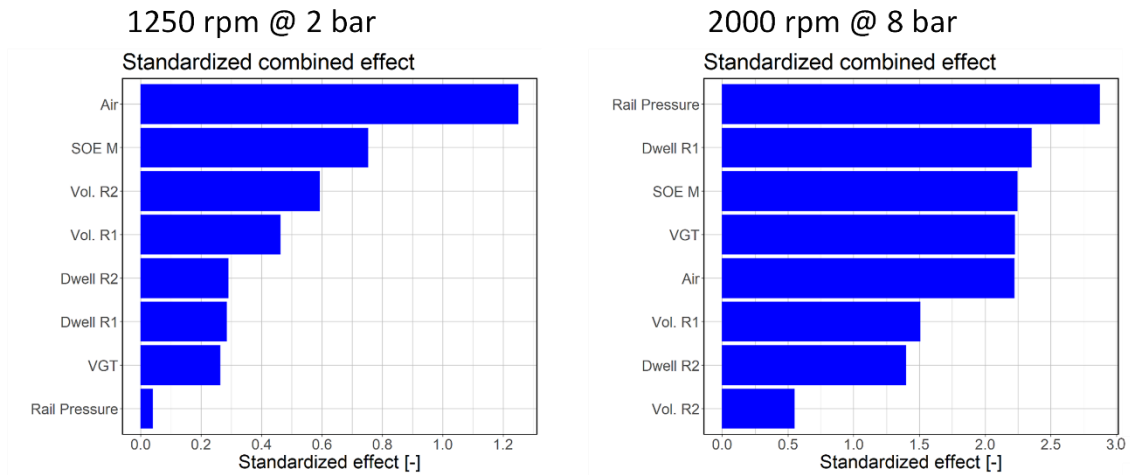
384 Figure 8 Injection strategy for the different tested operating conditions

385 The factor removal criteria involve the evaluation of the standardized effect [31] of the
386 variables on the responses of BSNO_x, gross brake efficiency (GBE), BSFC and soot (in FSN
387 number). To select which variables to remove the responses are normalized and
388 combined according to equation 5. On the equation, SR_x is the standardized effect of a
389 parameter x on a given response [32] [33]; which is normalized to equally weight the
390 effects of interest, and CR the combined sized effect for each of the parameters studied.

$$CR = \sum_{y=responses} \frac{|SR_x|}{\max(|SR_x|)_{response}} \quad (5)$$

391

392 The combined sized effect results for both low load points can be seen in Figure 9, where
393 for the single parameter tests on the operating condition 1250 rpm @ 2 bar the boosting
394 pressure (represented as VGT) and the rail pressure have the least significant effect and
395 will thus be kept fixed. While, for the operating point 2000 rpm @ 8 bar it is observed
396 how the variation of the characteristics of the second pilot injection have the least
397 important effect.



398

399 Figure 9 Standardized responses for the operating conditions with two pilot injections

400 to define which 6 factors are studied during the calibration procedure with an LCF

401 blend

402 After selecting the variables to test for each of the operating conditions, the variables

403 and their testing levels can be seen in Table 6. And, in accordance with the types of DoE

404 selected, different combinations of the factor levels are observed to better understand

405 the parameter effects.

406 Table 8 Experiment design matrix with variables and levels

Variable	1250 rpm @ 2 bar	1500 rpm @ 14 bar	2000 rpm @ 8 bar	2000 rpm @ 22 bar
Sol [deg bTDC]	[-4; 5.5; 7]	[-4; 0; 4]	[2; 5; 8]	[5; 8; 11]
Rail Pressure [bar]	[240; 275; 310]	[800; 875; 950]	[780; 860; 940]	[1050; 1150; 1250]

Vol. pilot 1 [mm ³]	[0.9; 1.4; 1.9]	[1.0; 2.0; 3.0]	[0.9; 1.6; 2.3]	[1.2; 1.8; 2.4]
Dwell pilot 1 [ms]	[0.680; 0.723; 0.765]	[0.500; 0.75; 1.000]	[0.590; 0.700; 0.810]	[1.000; 1.250; 1.500]
Vol. pilot 2 [mm ³]	[0.9; 2.0; 3.0]	[-]	[0.9; 1.7; 2.4]	[-]
Dwell pilot 2 [ms]	[0.630; 0.710; 0.790]	[-]	[0.500; 0.600; 0.700]	[-]
Air [mg]	[180; 196; 212]	[610; 625; 640]	[412; 424; 435]	[610; 625; 640]
Boost pressure [kPa]	[102; 103.5; 105]	[162; 171; 180]	[140; 150; 160]	[162; 171; 180]
Type of DOE	2-k factorial with center	Modified Plackett- Burman	2-k factorial with center	Modified Plackett- Burman

407

408 **4.1 Statistical analysis and model development**

409 The design of experiments allows to obtain polynomial regression equations that follow
410 the form shown in Equation 6. The regressions represent the responses obtained by the
411 variation of the different factors. The b_0 coefficient is the mean of the analyzed
412 responses, while coefficients b_i and b_{ij} represent the effect of the variables X_i and the
413 interaction between X_iX_j , respectively. Interaction between factors was limited to only
414 first order interactions (b_{ij}), or coefficient of effectiveness of second grade, due to this

415 being able to represent the main effects without providing excessive degrees of freedom
 416 to the model.

$$Y = b_0 + \sum_i^k b_i X_i + \sum_i^k \sum_{j \neq i}^k b_{ij} X_i X_j \quad (6)$$

417 The best polynomial model was selected for each of the responses of interest and each
 418 operating condition, including the mechanical constraint responses. The final
 419 polynomial equation for each case was then used to obtain the curve predicted by the
 420 model. The polynomial models obtained contain only significant terms (following the
 421 convention of $p < 0.05$), r-square above 80% and an F-statistic that allows the rejection
 422 of the null hypothesis.

423 **4.1.1 Model evaluation**

424 One of the main interests in generating model is to be able to characterize the engine
 425 behavior with the modification of the different parameters and to be able to predict the
 426 conditions necessary to obtain a combustion that fulfills the constraints criteria, while
 427 also maintaining good performance and efficiency values. That objective demands that
 428 the models can closely reflect experimental values. Table 9 shows the r-square values
 429 for the main responses indicating there is good agreement between both experimental
 430 and modelled values. It is important to highlight that the accuracy of the models can
 431 only be ensured within the ranges studied.

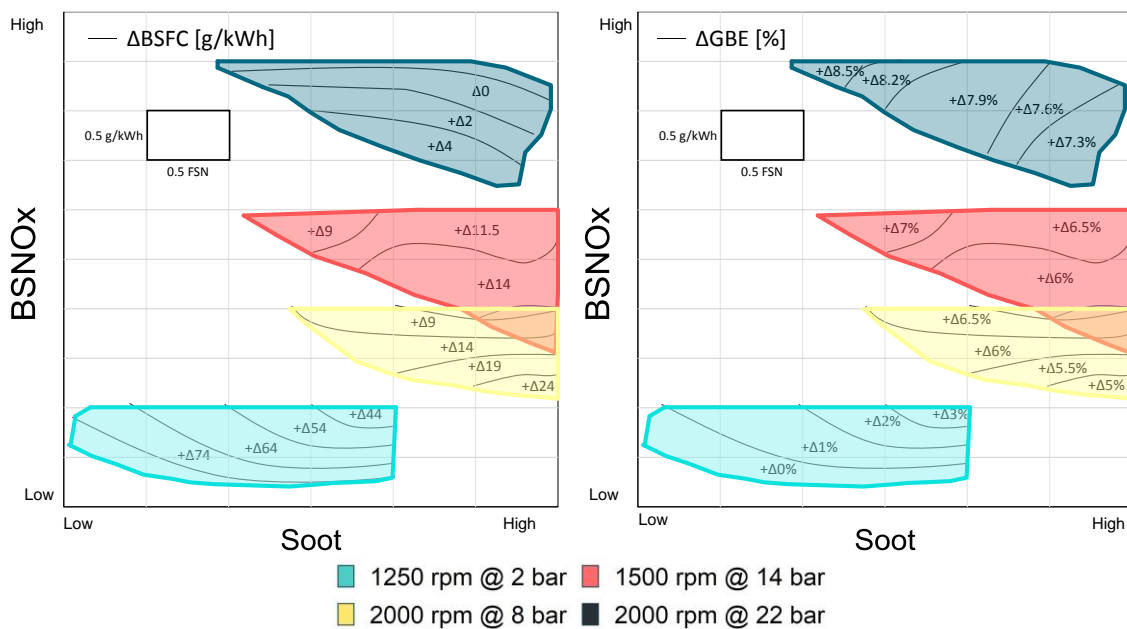
432 Table 9 R-square values for the main studied responses across all operating conditions

	BSNOx	Soot	BSFC	GBE
1250 rpm @ 2 bar	93.8	84.1	82.2	83.9

1500 rpm @ 14 bar	95.6	85.9	89.4	91.2
2000 rpm @ 8 bar	99.4	93.0	91.2	96.8
2000 rpm @ 22 bar	95.1	92.1	90.4	83.3

433

434 **4.2 Operating condition optimization based on modelling results**



435

436 Figure 10 BSNO_x-FSN tradeoff [Left] Including BSFC maps; [Right] Including GBE maps.

437 Values are expressed as absolute differences following the convention specified in

438 equation 4.

439 The developed models for the different responses allow the augmentation of the data

440 to test not experimentally measured operating conditions. Figure 10 shows the relation

441 between the modelled NO_x and soot emissions for the operating conditions that comply

442 with the previously defined constraints. In terms of emissions, it can be seen how the

443 NOx emissions increase when the load is increased. The 1250 rpm @ 2 bar condition has
444 both the lowest NOx and soot emissions . The relation between BSFC and the emissions'
445 tradeoff is also reflected in the figure. It can be observed that within each operating
446 condition the increased in NOx is inversed to the fuel consumption increase; when the
447 BSFC is reduced, the BSNOx are increased and vice versa. The correlation with soot,
448 however, is not as strong. Similar inferences can be extracted from the GBE maps; the
449 difference being that for the operating condition 2000 rpm @ 22 bar a well-defined
450 correlation is found between GBE and soot, where a reduction of 1 FSN can see an
451 increase of 0.6% of efficiency.

452 This work also intends to propose an optimized operating condition that has both low
453 NOx and soot emissions. As these two emissions present a strong tradeoff between
454 them, the implementation of optimization criteria is necessary to select the best
455 operating condition. Additionally, it is of interest to be able to have the highest possible
456 GBE and the lowest BSFC. The operating condition is selected by applying the
457 optimization functions described on equations 7 to 10. In these equations, ϵ is the
458 admissible threshold for the desired response. To achieve an optimum and balanced
459 point (an operating condition with lowest possible NOx, soot, fuel consumption and the
460 highest efficiency), the minimum ϵ is found so that only one value fulfills all conditions.

$$BSNO_x < BSNO_{x_{min}}(1 + \epsilon) \quad (7)$$

$$BSSoot < BSSoot_{min}(1 + \epsilon) \quad (8)$$

$$BSFC < BSFC_{min}(1 + \epsilon) \quad (9)$$

$$GBE > GBE_{max}(1 - \epsilon) \quad (10)$$

461

462 The optimized point for each of the operating conditions can be seen in Table 10. The
 463 values from the model were later experimentally measured to verify the accuracy and
 464 precision of said model. From the optimized values, it can be mentioned that the Sol is
 465 delayed (within the specified limits) for all operating conditions, which is an injection
 466 strategy that helps in the reduction of NOx emissions. Regarding the other variables, no
 467 specific trend can be detected in terms of injection pressure, pilot injection
 468 characteristics nor air management characteristics. The table also includes the
 469 responses with their respective confidence interval for the model and the measurement
 470 error for the experimental values. From the table, good agreement between predicted
 471 and measured values can be seen. Responses are again presented as differences
 472 following Equation 4.

473 Table 10 Optimized operating conditions settings and normalized results for both
 474 modelled and experimental responses with their associated errors.

Settings				
Variable	1250 rpm @ 2 bar	1500 rpm @ 14 bar	2000 rpm @ 8 bar	2000 rpm @ 22 bar

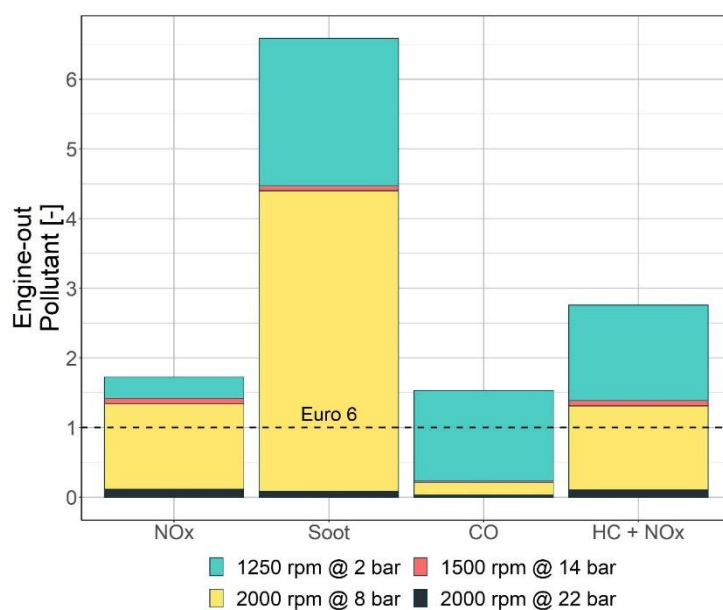
Sol [deg bTDC]		-4	2	2	5.5
Rail Pressure [bar]		290	860	940	1050
Vol. pilot 1 [mm ³]		1.9	1.0	1.8	1.2
Dwell pilot 1 [ms]		750	500	630	1000
Vol. pilot 2 [mm ³]		0.85	-	1.3	-
Dwell pilot 2 [ms]		790	-	600	-
Air [mg]		180	640	435	850
Boost pressure [kPa]		103.7	180	156	245
Responses					
Δ BSNOx [g/kWh]	Mod.	0.1±0.1	2.1±0.1	1.24±0.08	3.6±0.1
	Exp.	0.0±0.2	2.2±0.1	1.11±0.08	3.7±0.1
Δ BSSoot [g/kWh]	Mod.	0.00±0.01	0.02±0.01	0.15±0.01	0.06±0.01
	Exp.	0.03±0.05	0.03±0.07	0.21±0.06	0.09±0.03
Δ BSFC [g/kWh]	Mod.	65±2	13±4	14.0±2	0±2
	Exp.	70±7	11±2	12±2	5±2
Δ GBE [%]	Mod.	0.9±0.3	7.0±0.7	7.1±0.2	8.9±0.2
	Exp.	0.0±0.7	7.5±0.3	7.2±0.3	8.4±0.3

475

476 **5 Application of simplified WLTC cycle for the evaluation of an LCF blend**

477 After the optimization of the operating conditions in section 4, the simplified driving
478 cycle shown in section 3 is applied to first estimate the potential of the LCF to be able to
479 fulfill Euro 6 emissions and to calculate the potential CO₂ reductions that can be
480 achieved by the use of a fuel with 33% volumetric renewable content. Figure 11 shows

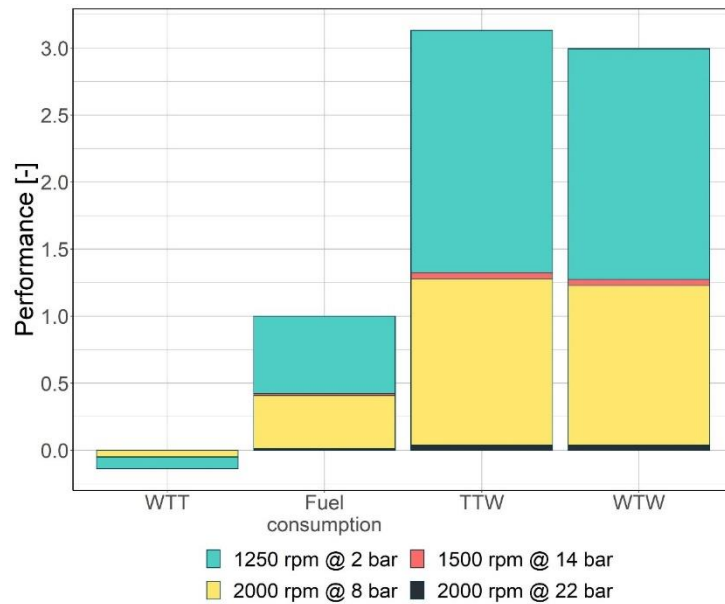
481 the main pollutants divided by their Euro 6 limits. In the figure it should be highlighted
 482 that Euro 6 limits are not fulfilled. For the case of NO_x, the cycle emissions with the LCF
 483 are around 1.75 times the Euro 6 limit. On the other side, soot emissions are over 6
 484 times the admissible limit. Regarding the products of incomplete combustion (HC and
 485 CO) the Euro 6 limit is exceeded by 1.5 and 2.8 times respectively. Although emissions
 486 are not fulfilled, is important to remember that the values here presented correspond
 487 to engine-out values, thus some improvement regarding emissions can be achieved if an
 488 aftertreatment system were to be considered. In the case of soot particulates, it has
 489 been reported that diesel particulate filters (DPF) can have efficiencies beyond 95% [34].
 490 A DOC in turn would oxidize big part of CO and HC reported efficiencies of 90% [24].
 491 Assessing these aftertreatment scenarios it is feasible to consider that emissions can be
 492 fit into Euro 6, although further dedicated testing is desired to confirm this hypothesis.
 493 Additionally, it is worth considering that high soot levels would require some
 494 maintenance for the DOC at more frequent intervals than with the current baseline
 495 calibration.



496

497 Figure 11 Cycle engine-out criteria pollutants normalized by the Euro 6 regulation
498 limits

499 In Figure 12 the fuel consumption can be seen with a value of 1 as the results are
500 normalized for that response. However, when applying Equation 1, the fuel
501 consumption of the LCF can be evaluated with a correlation to commercial diesel, finding
502 that the studied LCF has only 0.54% higher fuel consumption than diesel if both
503 contained the same amount of energy by mass. Another important result that can be
504 obtained with the simplified WLTC are the fuel consumption and CO₂ emissions
505 including Well-to-Tank (WTT), Tank-to-Wheel (TTW) and Well-to-Wheel (WTW). The
506 studied fuel is carbon negative due to its 33% volumetric renewable content, and thus
507 the equivalent WTT CO₂ has a negative value. This implies that the fuel production
508 removes more CO₂ from the atmosphere than it emits. On the other hand, the TTW
509 emissions are 3.13 the fuel mass which is directly extracted from the coefficient shown
510 in Table 3. Finally, in terms of WTW a slight reduction can be appreciated compared to
511 TTW due to the added effect of the negative WTT value, however this reduction
512 corresponds only to 4.8% reduction in the total equivalent CO₂.



513

514 Figure 12 Fuel consumption and CO₂ equivalent emissions normalized by the fuel
 515 consumption of the engine

516 **6 Summary and conclusions**

517 This study compiled the description of a simplified driving cycle methodology to evaluate
 518 the performance of a given engine using only a few experimental conditions and the
 519 calibration of such operating conditions using polynomial models and statistical analysis.
 520 From the combination of both methodologies the optimization and assessment of an
 521 LCF blend was possible within a commercially available Diesel engine. The main
 522 attractive for the use of a simplified methodology to evaluate a driving cycle is the
 523 avoidance of the calibration of the complete engine map (in favor of the calibration of
 524 only a few selected conditions), which can be a costly and time extensive procedure; in
 525 particular, when evaluating LCFs whose operation and characteristics have to be
 526 explored in a more intensive manner and for which large quantities are difficult to
 527 procure due to their experimental nature.

528 Regarding the optimization process, it was confirmed that the engine operation can be
529 refined to fulfill specific constraints with a DoE with variation of defined parameters,
530 and subsequent statistical modelling. In particular, is possible to comply with the
531 limitation of NO_x and soot emissions, which are two of the main pollutants in CI engines.
532 Finally, an optimization function is presented that sought to find the most balanced
533 operating condition in terms of NO_x, soot, BSFC and GBE.

534 From the results obtained in this study, it can be highlighted that:

- 535 • The simplified WLTC methodology shows good agreement with OEM reported
536 fuel consumption and GT-Power model driving cycle simulations (around 5% of
537 deviation).
- 538 • The created models and experimental values are very close in terms of BSFC,
539 BSNO_x, BSSoot, BSHC and BSCO. Additionally, is observed how the confidence
540 interval of the models overlaps with experimental values when considering
541 experimental error
- 542 • Although engine-out Euro 6 main criteria pollutant emissions are not compliant,
543 the application of an aftertreatment system will let the emissions fulfill Euro 6.
- 544 • Using an LCF with 33% renewable content, and properties similar to diesel fuel,
545 a reduction of 4.8% equivalent WTW CO₂ can be obtained, when compared with
546 TTW emissions due to the use of atmospheric CO₂ during the fuel production
547 process, which is reflected with a negative WTT CO₂ value.

548 **Acknowledgments**

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552

553

554 **Abbreviations**

BMEP	Brake mean effective pressure
CI	Compression ignition
DOC	Diesel oxidation catalyst

DOE	Design of experiments
DPF	Diesel particulate filter
EV	Electric vehicle
FAME	Fatty acid methyl esters
GBE	Gross brake efficiency
HC	hydrocarbons
HVO	Hydrogenated vegetable oil
ICE	Internal combustion engine
LCF	Low carbon fuel
LHV	Lower heating value
OEM	Original equipment manufacturer
PM	Particulate matter
PRR	Pressure rise rate
SI	Spark ignition
SOI	Start of injection
TTW	Tank-to-wheel
WLTC	World harmonized Light vehicle Test Cycle
WLTP	World harmonized Light vehicle Test Procedure
WTT	Well-to-tank
WTW	Well-to-wheel