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Additional Information

1	Intelligent charge compression ignition combustion for range
2	extender Medium Duty Applications
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20	Abstract

21 Electrified powertrains have been growth in the last few years due to the increase in 22 powertrain efficiency. However, for heavy-duty vehicles the right choice it is not clear. 23 The long-routes and large number of daily kilometres makes that current battery 24 technology it is not prepared to cover the minimum requirements. A mid-term solution 25 is hybrid powertrains. The mix between pure electric range and range extender mode in 26 liquid fuels make perfect to complete a large distance. However, tailpipe pollutant and 27 CO<sub>2</sub> emissions are still a disadvantage against pure electric powertrain. This study 28 analyses the potential of hybrid powertrains running in an advanced combustion mode 29 as Intelligent Charge Compression Ignition. Due to the flexibility of the combustion mode 30 different renewable energy fuels are tested: Butanol, Methanol and Biodiesel. The work 31 is focused in urban buses due to the potential of electrified powertrains in this context 32 and the large number of vehicles concentrated in cities. The results show that pure 33 electric bus reduce 54% the CO<sub>2</sub> emissions at LCA level. Meanwhile the Intelligent Charge Compression Ignition allows to 32% with one renewable fuel (Diesel-Butanol) 34 35 and 66% with two renewable fuels (Biodiesel-Methanol) with respect to the non-hybrid diesel reference. 36

## 37 Keywords

Renewable Energy; Advanced Combustion Mode; Electrified Powertrain; Life CycleAnalysis

#### 41 **1. Introduction**

Heavy-duty vehicles including buses, delivery and other utility trucks, are the new focus of research because are usually operated based on defined daily routes and have large emissions due to the total weight [1]. Therefore, a number of cities are already paying attention on cleaner public transport, while many bus operators are renewing their fleet or deploying low-emission vehicles. Options as Battery Electric Vehicles (BEV), Plug-In Hybrid Electric Vehicles (PHEV), Full Hybrid Electric Vehicles (FHEV) and Mild Hybrid Electric Vehicles (MHEV) are appear in the recent years [2].

49 Inside hybrid vehicles exist a large offer of powertrain architectures. Hybrid urban buses are considered as one such option, with the main reduction in costs expected from 50 51 a decreased fuel consumption (FC) over conventional buses. Powertrain simulation 52 results indicate that both parallel and series hybrid systems can offer fuel economy 53 benefits up to 45% over conventional buses [3][4]. Results from experimental 54 assessments vary. Gerbec et al. [5] found that the FC of a hybrid-diesel bus was 15–18% 55 lower than a corresponding conventional one, depending on traffic conditions in the city of Poznan, Poland. Hallmark et al. [6] reported an average 11.8% higher fuel economy 56 of three hybrid buses than two conventional ones in Iowa, USA. Hu et al. [7] observed a 57 58 30% fuel savings potential, after examining the results of one hybrid bus over a 59 conventional one in Sakarya, Turkey. Guo et al. [8] also reported significant fuel benefits 60 from two parallel hybrid buses over conventional ones, but the variability in driving conditions did not make possible to precisely quantify the improvement. Zhang et al. [9] 61 62 analysed on-road emissions of 75 Euro II to Euro V transit buses in Beijing, China, including two Euro IV single deck hybrid-diesel buses. Hybrid-diesel buses were found 63 64 to consume 29% less fuel compared to conventional ones. Moreover, Range Extender Vehicles (REV) use an onboard electricity generator to provide additional energy if the 65 66 battery is depleted during operation [10]. This allows to reduce the battery pack size compared to BEV. REV can be PHEV or FHEV depends if is added an external connection 67 68 for grid charging during parking. However, the optimal component selection when is 69 combined elements of conventional powertrain and BEV is not trivial. In addition, the 70 control system of this components increases in complexity. The right selection is crucial to find the optimal trade-off between fuel economy, drivability, and vehicle cost [11]. 71 72 Therefore, multiple performance objectives are the best option [12]. Depends on the 73 vehicle use segment, public transports or trucks for parcel delivery, the same powertrain 74 may not be optimal in all situations [13]. Therefore, is extensively used the numerical 75 evaluation for vehicle evaluation for powertrain sizing under driving scenarios 76 representing realistic driving missions [14]. Compared to parallel and power-split hybrid 77 vehicle architectures, which have less battery capacity, REVs reduce the transient 78 behaviour of the internal combustion engine (ICE) because the wheels are uncoupled 79 for the ICE and electric machine (EM) generator. This allows to operate the engine along the optimal operation line at desired rotational speed [10]. This make a new scenario 80 81 for the application of advanced combustion modes [15].

82 Several technologies are available for emissions control in diesel engines. The 83 current emissions control systems used to meet the European Union (EU VI) limits rely in passive actions as selective catalytic reduction (SCR) for NOx emissions control. To 84 85 comply with the 10-ppm ammonia limit, averaged over the World Harmonized Transient Cycle, ammonia slip catalysts (ASC) are widely used. For particle control, diesel 86 87 particulate filters (DPF) are present in all EU VI compliant systems, heavily relying on a 88 diesel oxidization catalyst (DOC) for passive and active regeneration [16]. This means a 89 large and expensive aftertreatment system to mitigate the emissions generated in the combustion chamber. In the EU VI normative this is enough but beyond 2025 is expected 90 91 to be introduced EU VII [17]. This new restriction will have 90% lower NOx than EU VI 92 [18]. Also, modification of the on-road test used in type-approval, in-service conformity, 93 and market surveillance is expected, with an emphasis on shorter trips, low-load, and 94 cold-start operation. Similar to Europe, China is in the preparatory groundwork to 95 develop China VII standards to be applied beyond 2025. Therefore, reducing engine-out 96 emissions is crucial nowadays. Low temperature combustion modes as homogeneous 97 controlled compression ignition (HCCI) [19] and premixed charged compression ignition 98 (PCCI) [20] have been studied in the last years. Low emissions and high efficiency were 99 expected to be simultaneously achieved if combustion takes place under homogeneous or slightly stratified conditions in advanced combustion modes. Main barriers that 100 101 obstruct these modes is the absent of direct methods to control the ignition timing 102 (mainly in HCCI). Therefore, it is seen high-pressure rising rate under higher engine load 103 and misfire under lower engine load (mainly in PCCI). To overcome this issue, some 104 researches has proposed the Reactivity Controlled Compression Ignition (RCCI) 105 combustion mode [21] that enables a higher control of the combustion process by the 106 use of two fuels with different reactivity. This allows to create a mixture stratification among the temperature stratification seen in HCCI. The high reactivity fuel (Diesel, 107 108 dimethyl ether DME, oxymethylene dimethyl ethers OMEx) is injected directly in the 109 combustion chamber (DI) and the low reactivity fuel (Gasoline, Ethanol, Methanol) in 110 the port fuel injector (PFI). This combustion concept is applied in Compression Ignition (CI) engines. The main advantage is that combines elements seen in conventional 111 112 combustion modes commercially available (CI Diesel and Spark Ignited (SI) Gasoline). 113 The main drawback is that the port injection might cause rich fuel areas and fuels being 114 trapped in crevice regions. This increase HC and CO emissions even higher than SI mode 115 because of the large crevices of CI engines. To improve even more the combustion concept a new dual-fuel combustion mode appears in the recent years called: Intelligent 116 Charge Compression Ignition (ICCI) combustion mode [22]. The main advantage is the 117 flexibility to inject the Low Reactivity Fuel (LRF) in both DI and PFI. This allows a better 118 119 stratification by selecting the best reactivity gradient according to engine operating 120 condition. In the ICCI mode, most of low-reactivity fuel is directly injected during the 121 intake stroke with single or multiple stage split injection [23]. Then, the rest of lowreactivity fuel and high-reactivity fuel are directly injected in succession to establish 122 crossed stratifications of the equivalence ratio and reactivity in the cylinder. Under the 123 124 various engine loads, ICCI mode can form flexible stratifications to control the heat release by adjusting injection parameters such as injection timings, stages of split injection, and energy ratios of fuels, etc [24].

127 In this work, the powertrain design of an urban bus is considered. The bus has a 128 series hybrid powertrain with an internal combustion engine as range extender where the correct sizing and emissions reduction potential are explored. The powertrain is 129 130 optimized for different driving cycles to analyse how the driving mission and passengers affects the selected powertrain. A simulation model of the powertrain is developed and 131 optimization strategies are used to compute the optimal battery and engine sizing. 132 133 Later, a novelty combustion concept is tested with conventional and renewable energy 134 fuels as Bio-Diesel, Methanol and Butanol. The dual-fuel concept shows great potential 135 to mitigate the high-volume consumption of these low heating value fuels. In addition, the stratified temperature and reactivity help to strongly reduce the engine-out 136 emissions. The results are compared against conventional powertrains and pure electric 137 138 bus in an life cycle analysis (LCA) basis. Therefore, the main novelty of this work is a new 139 methodology to optimize hybrid range extender buses based in real driving cycles. In addition, this work presents results for a standard bus in different powertrain 140 technologies analysed in European and Asia context. Emissions as CO<sub>2</sub> in different basis 141 142 as well as NOx, HC and CO are presented for different fuels. This add interesting 143 information that can not be found in the bibliography up to the knowledge of the 144 authors.

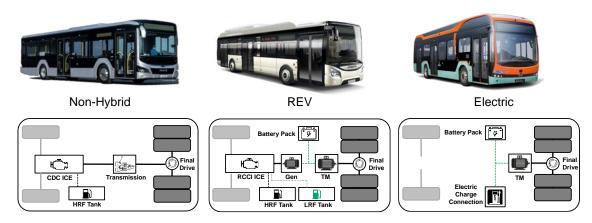
## 145 2. Methodology

146 In this section is presented the methodology used for the study of ICCI combustion 147 mode in a REV. The bus vehicle model, driving cycles used to test the concept under 148 transient conditions, powertrain design, combustion experimental data and life cycle 149 analysis approach is presented.

## 150 2.1. Vehicle Model

Three powertrains are studied in this work, including a non-hybrid powertrain 151 operating with diesel (representative of the most used current system in the market 152 [25]), REV operating under a low temperature combustion mode with two fuels and a 153 pure battery electric bus (representative of zero tailpipe emissions vehicle available in 154 155 the market [26]). The work will be focus in optimize the REV and compare with the 156 baseline non-hybrid and pure electric buses. The base of the REV truck is based in a IVECO Urbanway series hybrid [27]. Figure 1 show the vehicles used and a scheme of the 157 components layout that are simulated in the OD vehicle model. The vehicles are model 158 in GT-Suite V2021 (Gamma Technologies) and the main components specification for 159 160 the baseline cases (Non-hybrid and Electric) are taken from manufacturer publications. 161 The powertrain validation was done by the authors in previous manuscript with a Volvo 162 FL 18-tons medium duty truck [28]. This vehicle has the same engine and powertrain 163 components that the Volvo 7900 (equivalent to the MAN Lion City). The results show a 164 difference below 2% in fuel consumption with a good agreement in terms of power and torque prediction. The REV is designed in current work to efficiently work under ICCI 165

166 combustion mode. Therefore, ICE and battery size are optimized by a Design of167 Experiments (DoE).



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Figure 1 – Bus Models used to evaluate a conventional powertrain (non-hybrid CI Diesel), range extender vehicle (REV with dual fuel ICCI concept) and pure electric bus BEV). The model are created using GT-Suite 2021 from Gamma Technologies<sup>®</sup>.

172 Table 1 shows the main bus specifications. The battery pack is simulated by a stack 173 of series and parallel cylindrical cells (3.3 V and 2.5 Ah from A123 Lithium-Ion phosphate 174 LFP [29]). The electric machine is model by JMAG software using the rated power and torque specifications [30]. The efficiency map obtained is introduced in the GT-SUITE 175 176 electric machine model. Transmission components are simulated with average efficiency of 0.97. Lastly, the ICE is simulated with experimental engine test bed 177 178 stationary maps. This method allows to an accurate and fast simulation of the fuel 179 consumption and engine-out emissions.

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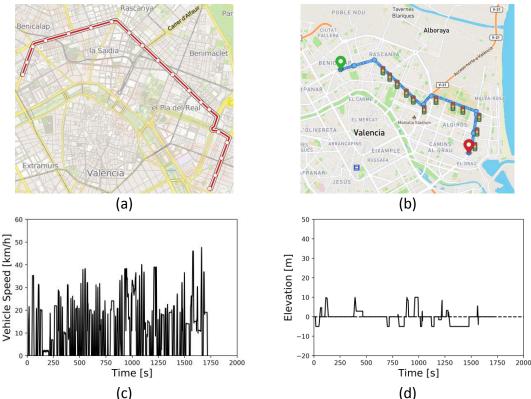
Table 1. Bus specifications by type: Non-Hybrid, REV and Electric.

Parameter	Non-Hybrid	REV	Electric	
Model Name	MAN Lion's City	Prototype	BYD 12m eBus	
Engine Type	Diesel, EUVI compliant with ATS, CI engine	Dual-Fuel ICCI, CI engine	-	
Maximum Passenger Capacity		70		
Gross Weight (Kg)	19000 19500		20000	
Rated Power - Engine/Motor (kW)	265 / -	To be designed	- /150 x 2	
Maximum Torque – Engine/Motor (Nm)	1600 /	To be designed	/ 550x2	
Battery Capacity (kWh)	-	To be designed	348	
Length (mm)	12000			
Width (mm)	2550			
Height (mm)	3060	3280	3370	

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# 182 **2.2. Bus Routes**

The vehicles are simulated in transient conditions representatives of real routes in two different scenarios. It was selected Europe (Valencia, Spain) and Asia (Shanghai, China) due to the different vehicle use (city population, geography and traffic) and electric mix (Europe based in Renewable energy 38% and Fossil 35% [31] meanwhile China mainly Fossil 65% and Renewable energy 27% [32]). This will allow to compare the non-hybrid, REV and Electric performance and total emissions in two drastically different scenarios. To obtain the routes, an online driving cycle generator is used called GT- 190 RealDrive. This plugin of GT-SUITE allows in real time using MapBox tools [33] to obtain 191 the vehicle speed and elevation profile against the distance travelled. After simulate the 192 route with the 0D vehicle model is possible to obtain the real speed profile against time depends on the vehicle performance. This will guarantee a correct vehicle sizing testing 193 194 environment. Figure 2 shows the driving cycle methodology scheme in an example case 195 of one-line bus in Valencia, Spain. First the route is taken from the city bus company 196 with the trajectory and stops. Later, the start and end of the route is inserted in GT-RealDrive with the via points marked as the stops. In each stop, the vehicle stays 30 197 198 seconds, representative of an average bus stop. The speed profile and altitude are 199 obtained against time. It is important that traffic level and signals are considering in the 200 route generation.



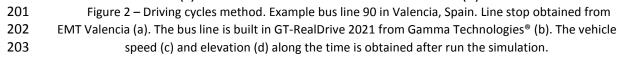
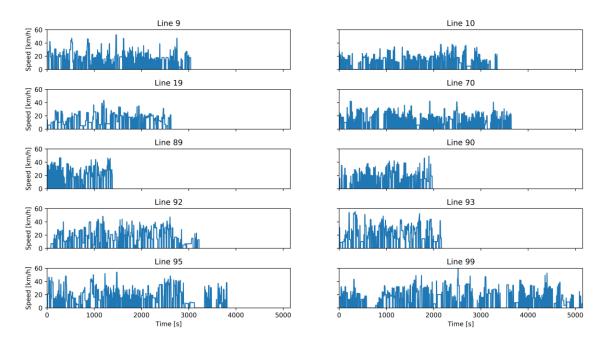


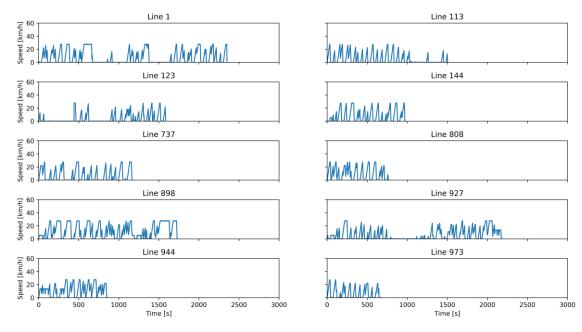
Figure 3 and Figure 4 shows ten driving cycles representative of the most used routes in Valencia and Shanghai, respectively. It is possible to see that the total time that a bus needs to complete the route goes between 30 minutes to 85 minutes. The maximum speed not exceed the 60 km/h in any case with some flat vehicle phases representative of traffic jams.





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Figure 3 – Ten main bus lines in Valencia: 9, 10, 19, 70, 89, 90, 92, 93, 95, 99. The driving cycles are representative of Europe conditions and used to evaluate the different buses configurations.



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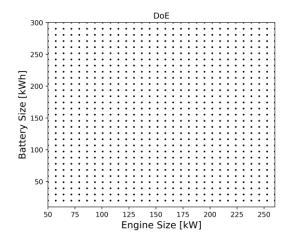
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Figure 4 – Ten main bus lines in Shanghai: 1, 113, 123, 144, 737, 808, 898, 927, 944 and 973. The driving cycles are representative of Asia conditions and used to evaluate the different buses configurations.

For the vehicle simulations, the mass of a passenger was defined as 68 kg. This is used in the Federal Transit Administration (FTA) bus testing regulations [34]. Several cases will be tested ranging from empty bus up to 70 passenger (max passenger capacity) that represents 4760 kg.

# 220 **2.3. Optimization and Performance Procedure**

To correctly size the REV, the battery and internal combustion engine energy capacity and power are studies, respectively. An optimization with a DoE of 400 cases is 223 used with a range between 20 (minimum to feed the EM) to 300 kWh (representative of 224 a pure electric bus) for the battery and 50 to 280 kW of engine size (see Figure 5). The battery is scaled by a Thevenin equivalent cell model, adding cells in parallel 225 226 configuration. The battery pack is maintained in 600V representative of current vehicles in the market. In the case of the ICE, it is supposed a fixed brake thermal efficiency (BTE) 227 228 of 40% for this first optimization approach. As the ICE operates in a generator mode with 229 a specific operating condition this assumption is conservative. For a conventional diesel 230 combustion, the maximum BTE can achieve 43% and above BTE of 40% in medium to 231 high engine load [26]. For advanced combustion modes the values can be even higher, 232 as will be demonstrated later in the manuscript. Despite is a strong hypothesis, it is 233 useful to size the engine and battery with a simple DoE approach. The assumption 234 cannot be done if the operating condition is three time lower than the maximum engine size. Summarizing, for a selected driving cycle a DoE is run to obtain the final fuel 235 236 consumption. The total vehicle fuel consumption for different battery size and engine 237 power is obtained. The minimum fuel consumption case is taken as optimum. Therefore, 238 for this section of the work is supposed to work with pure diesel with a BTE of 40%. 239 Later, the ICCI with different fuel will be evaluated. Figure 5 shows the DoE test matrix. 240 Full factorial with 20 levels is used to a deep space search.



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- 242 243

Figure 5 – DoE space search for battery and internal combustion engine sizing.

To preliminary evaluate the bus in a well-known driving cycle, Manhattan Bus Cycle (MBC) is used [35]. The Manhattan cycle was developed based on actual observed driving patterns of urban transit buses in the Manhattan core of New York City. The cycle is characterized by frequent stops and very low speed. Later in the manuscript Valencia and Shanghai cycle will be used. This MBC cycle is useful for bibliography comparison of the results.

Figure 6 shows the DoE results for MBC driving cycle with different passenger load. It was tested from 0, 35 and 70 passengers. For empty and medium load cases the optimum is found at 60 kW of ICE power and 64 kWh of battery size. The full bus case increases to 94 kW of ICE power and 79 kWh energy capacity. In spite of the change in ICE power, low battery size (< 50 kWh) increases the fuel consumption. The isolines of fuel consumption are almost linear for different ICE power for a battery size. Therefore, the battery size is seen as a more critical parameter. In addition, from Figure 6 it is possible to understand the passenger effect between
empty bus to full bus. The fuel consumption increases 20% in the optimum case. If
compare the optimum case for empty truck (same as 35 passenger, 60 kW ICE and
64 kWh battery) at 70 passenger loads, the case increases 1% with respect to the
optimum (94 kW ICE and 79 kWh battery). Therefore, as the idea is to reduce sources
the lower component size is the best selection in this case.

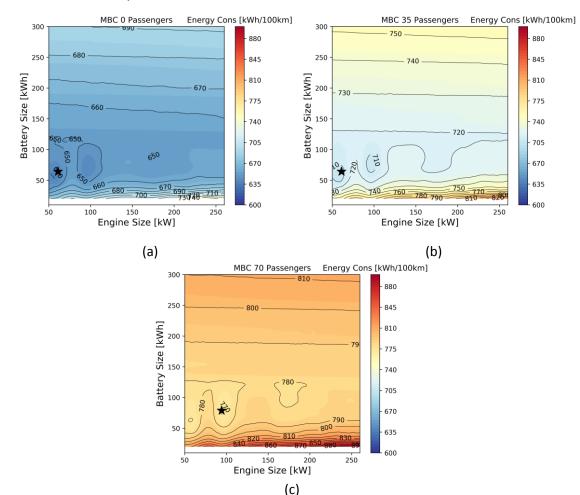


Figure 6 – Bus passenger influence with 0 (a), 35 (b) and 70 (c) with a SOC to charge of 0.45 in the
 Manhattan Bus Cycle.

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265 Figure 7 shows the DoE results for MBC driving cycle at different battery 266 management strategy. The battery value evaluated is the state of charge (SOC) at 267 which the battery changes from pure electric mode to battery charge mode (the ICE 268 is turn on to return the energy to the battery up to the initial level 0.6). Three SOC charge values are analysed at: 0.55 (Figure 7a), 0.45 (Figure 6b) and 0.30 (Figure 7b). 269 The last value is selected close to the minimum recommendable of 0.25 for the type 270 271 of cell used in the current study. The results show that for the optimum selection it has a low influence in the results with the optimum at 0.55. The 0.45 and 0.30 gives 272 an increase of 0.5% and 1.5% at the optimum. It is remarkable from the results that 273 274 0.55 gives worst values at high battery capacity due to the excess of weight in the 275 bus and the no use of the battery energy due to the narrow range of the operative 276 SOC.

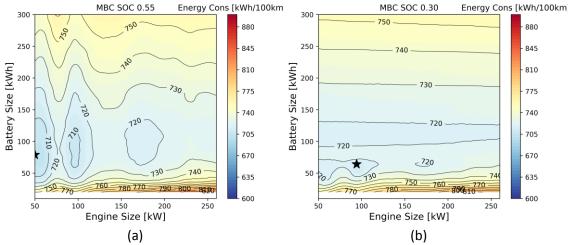


Figure 7 – Bus SOC influence at 0.55 (a), and 0.30 (b) with a passenger load of 35 in the Manhattan Bus
 Cycle .

Figure 8Figure 7 shows the DoE results for driving cycles in Valencia and Shanghai. Also, this result can be compared with Figure 6b. It possible to see that the cycle has a strong impact in the final fuel consumption results. Valencia cycle has 24% of less fuel consumption. Mainly this depends on the regenerating braking and the amount of start of stops of the cycle. On the other hand, for the same passenger load the optimum for the ICE and battery size are the same. This is a strong point of the powertrain due to the flexibility to apply in different cycles.

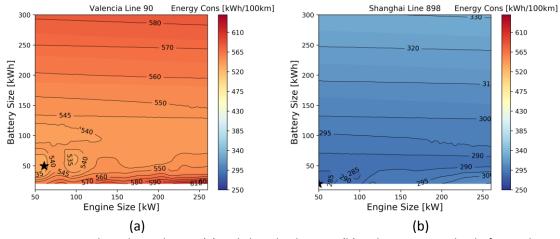


Figure 8 – Bus in the Valencia line 90 (a) and Shanghai line 898 (b) with a passenger load of 35 and SOC
 of 0.45.

288 Figure 9Figure 7 shows the DoE results for MBC cycle but at different driving length. One MBC takes 1089 s (18.2 min), so the cycle was repeated up to complete 289 1, 5 and 15 hours. The results can be compared with Figure 6b. The fuel consumption 290 291 is close between cycles. The unique differences are at high battery size were the 292 pure electric mode has larger effect when increase the driving distance. However, as 293 the battery need to be recharged by the ICE the efficiency of the powertrain not has 294 large improvements. It is important to note that the cases with high duration implies high computational cost. Therefore, from this analysis can be obtained that one MBC 295 is enough to have an accuracy fuel consumption value for a daily bus operation. 296

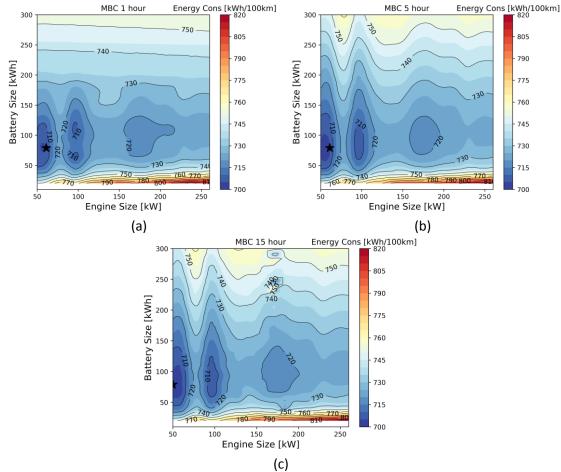




Figure 9 – Bus operational time 1 hour (a), 5 hours (b), and 15 hours (c).

299 In spite of the DoE optimization for a particular daily driving cycle, the OEM and 300 costumers want that the bus can operate also in extreme conditions. To analyse this, 301 a performance vehicle analysis is the right tools. By a MATLAB vehicle model code, 302 the maximum wheel force depends on the REV mode is shown in Figure 10. For 303 comparison the six gear non-hybrid bus is plotted. The EV mode of the REV represent the condition of a battery enough charged to deliver all the required power to feed 304 305 the EM. On the other hand, the hybrid charge sustaining (HEV CS) represents the 306 condition of the battery depleted and the ICE delivering the required power. Three different conditions are tested representing an ICE maximum power of: 50 kW, 100 307 kW and 150 kW. It is possible to see that in EV mode the wheel force is higher than 308 309 Non-hybrid bus until 15 km/h. Above 20 km/h the non-hybrid has large power due 310 to a more powerful ICE than the REV TM. In spite of the lower wheel force, both 311 vehicles achieve 120 km/h and allows uphill higher than 20% grade with vehicle 312 speed at least of 25 km/h. It is important to note that this study is performed with 313 the bus totally loaded. When the ICE in the REV is turn on and the battery is totally depleted the REV maximum wheel force decrease. With 50 kW of ICE the bus cannot 314 perform uphill higher than 15% and uphill of 5% only up to 20 km/h. When increase 315 to 100 kW the capabilities increase up to 30% and 40 km/h, respectively. Lastly, the 316 150 kW achieves 45% and 55 km/h. Analysing the road inclination of different 317

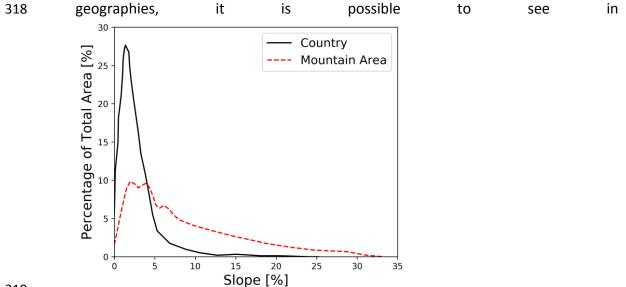




Figure 11 that is not common to find road grade higher than 20% and negligible cases more than 30%. Therefore, from a performance perspective the ICE need at least 100 kW to have an acceptable performance in extreme conditions.

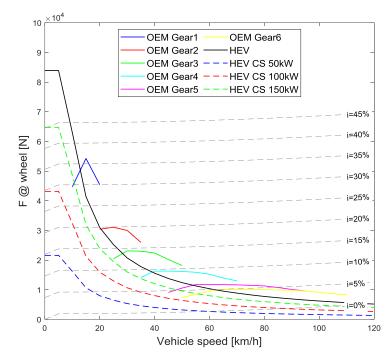


Figure 10 – Performance Analysis for REV and conventional non-hybrid powertrain in terms of wheel force for different vehicle speed and road grades.

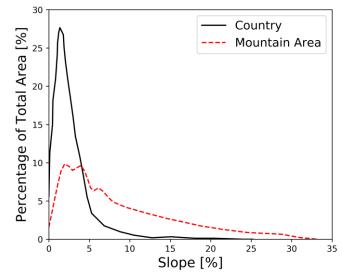


Figure 11 – Slope gradient analysis of urban expansion in China [36]. Representative of extreme normal and extreme condition that the buses can be used.

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### 2.4. Combustion Concept

Having the right size of the battery package and ICE, now it is time to select the engine to apply the low temperature combustion mode. In this work, an Intelligent Charge Compression Ignition combustion mode in a 4-cylinder 5 L engine originally designed to operate under CDC was taken. Modification as additional DI and PFI for LRF is done. Main engine specification are shown in Table 2 and calibration strategy can be found in [24].

339 The main benefits of the ICCI with respect to RCCI are the possibility of direct injection of the LRF as well as the HRF. In RCCI the port injection with the fixed inlet 340 341 angle might cause rich fuel areas and fuels being trapped in crevice regions, both of 342 which would increase emissions of HC and CO emissions. In addition, the ICCI 343 improves the LRF stratification in the combustion chamber due to the injection 344 timing change during compression stroke. The ICE calibration at different rotational speeds and loads was performed with flexible stratifications to control the heat 345 release by adjusting injection parameters such as injection timings, stages of split 346 347 injection, and energy ratios of fuels, among others. High reactivity fuel and low 348 reactivity fuel were directly injected with a pressure of 140 MPa and 30 MPa, 349 respectively. The temperature of lubricating oil and coolant were maintained within 85±2°C and 80±2°C for all operation conditions. 350

351

#### Table 2. ICE main specifications.

Engine Parameters	Value
Bore [mm]	114
Stroke [mm]	130
Number of Cylinder [-]	4
Total Volume [L]	5.3
Compression ratio [-]	18:1
EGR loop	High-Pressure
Boost method	Mechanical Turbocompounding
Direct Injection [-]	Eight injectors for HRF and LRF
Number of holes for DI [-]	Six holes injector
Piston geometry [-]	Conventional re-entrant bowl
Port fuel Injection [-]	Four injectors for LRF

353 Conventional fuels (Diesel, Gasoline) and renewable energy fuels (Biodiesel, 354 Methanol and Butanol) are tested in stationary conditions. Main fuel specification is shown in Table 3. Table 3. Fuels specifications. Biodiesel is regarded as a promising alternative 355 due to its similar properties with diesel and good performance in CI engines. Methanol 356 357 has a low carbon content and a high oxygen content, potential to reduce soot, CO and 358 HC. Lastly, Butanol compared to methanol and ethanol, has a lower vapor pressure, better blending ability, and greater energy density when used in ICE. All of the previous 359 mentioned renewable energy fuels have the capability to reduce the well to wheel 360 361 (WTW) CO<sub>2</sub> emissions due to the ultra-low well to tank (WTT) CO<sub>2</sub> values.

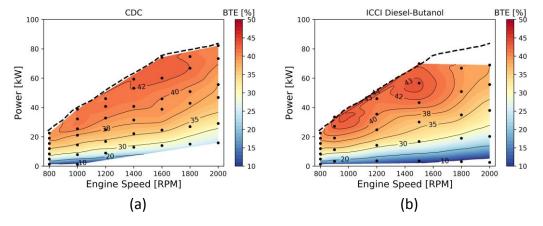
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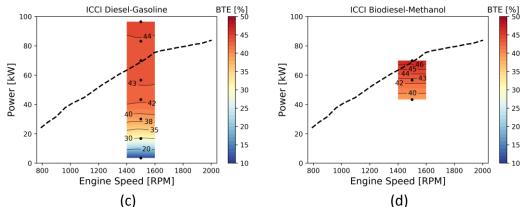
Table 3. Fuels specifications.

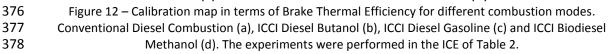
Fuel Parameters	Diesel	Gasoline	Biodiesel	Methanol	Butanol
Type of fuel [-]	HRF	LRF	HRF	LRF	LRF
Cetane Number [-]	53	-	53	5	25
Research Octane Number [-]	-	95	-	106	96
Lower heating Value [MJ/kg]	42.7	42.6	37.1	19.9	33.2
Flash Point [ºC]	74	18	225	11	35
Density [g/L @20ºC]	831	750	880	790	809
CO <sub>2</sub> ratio [gCO <sub>2</sub> /gfuel]	3.17	3.09	3.17	1.38	2.38
CO <sub>2</sub> TTW [gCO <sub>2</sub> /MJfuel]	74.2	72.5	85.4	69.3	69.2

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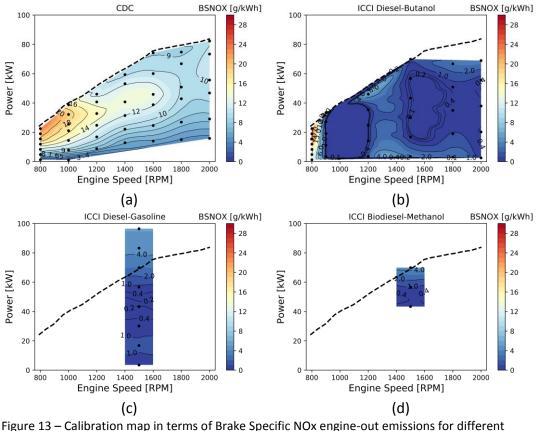
Figure 12 shows the brake thermal efficiency values for the calibrated points in 364 365 CDC and ICCI mode. The original equipment manufacturer (OEM) diesel calibration achieves 42% of BTE at 60 kW and 1400 rpm. The ICCI Diesel-Butanol was calibrated 366 367 in 26 operative conditions, with a maximum BTE of 43% at 55 kW and 1500 rpm. Due 368 to the good performance of the ICE in this engine speed the other fuels in ICCI mode 369 are calibrated in that region to reduce calibration cost. As the REV has an operation 370 in particular engine points, it is not necessary an all calibration map. The ICCI with 371 Diesel-Gasoline achieves 44% of BTE above 60 kW. In the case of Biodiesel-Methanol 372 it was possible to achieve the highest BTE around 46%. The calibration setting as 373 injection timing, fuel injected, EGR rate can be found in previous research group publications [22][23][24]. As change for each fuel, cannot be showed in the current 374 375 manuscript for brevity reasons.

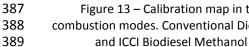






379 The main advantage of ICCI is the possibility to reduce NOx emissions due to the 380 low combustion chamber temperature. The brake specific NOx map is shown in 381 Figure 13. It possible to note the high improvements with respect to the CDC, around one order of magnitude. In addition, the NOx is below 0.4 g/kWh, current EUVI and 382 383 China VI emissions limit. This means that it has potential to remove Selective 384 Catalytic Reduction (SCR), Ammonia Slip Catalyst (ASC) and Urea injection. Diesel-Butanol under ICCI combustion shows the largest improvements in terms of NOx 385 followed by the Diesel-Gasoline. 386





combustion modes. Conventional Diesel Combustion (a), ICCI Diesel Butanol (b), ICCI Diesel Gasoline (c) and ICCI Biodiesel Methanol (d). The experiments were performed in the ICE of Table 2.

### 390 2.5. Life Cycle Analysis

To have a global analysis of each powertrain potential an LCA is included considering Well to Tank, Tank to Wheel and vehicle fabrication, maintenance, and disposal CO<sub>2</sub> generation. The CO<sub>2</sub> computation is done by a deep research bibliography in order to analyse component environmental impact in two scenarios (Europe and Asia) when is possible. The values taken for this study are depicted in Table 4. The reference source is added.

397

Table 4. CO<sub>2</sub> impact by fuel production, component production, maintenance and disposal.

Component	CO <sub>2</sub> Europe	CO <sub>2</sub> Asia		
Diesel WTT [g <sub>CO2</sub> /MJ <sub>Fuel</sub> ]	15.9 [31]	18.0 [37]		
Gasoline WTT [g <sub>CO2</sub> /MJ <sub>Fuel</sub> ]	13.1 [31]	16.5 [37]		
Butanol WTT [g <sub>CO2</sub> /MJ <sub>Fuel</sub> ]	-31.6	[38]		
Methanol WTT [g <sub>CO2</sub> /MJ <sub>Fuel</sub> ]	-42.0 [39]			
Biodiesel WTT [g <sub>CO2</sub> /MJ <sub>Fuel</sub> ]	-27.3	[40]		
Electricity WTT [g <sub>CO2</sub> /MJ <sub>Fuel</sub> ]	88 [41]	166 [32]		
Battery Manufacturing [kg <sub>c02</sub> /kWh]	75 [42]	110 [42]		
Conventional Powertrain [tonco2/Vehicle]	9.9	[43]		
Hybrid Powertrain [ton <sub>co2</sub> / Vehicle]	16.7	[43]		
Electric Powertrain [tonco2/ Vehicle]	9.8 [43]			
Bus body [tonco2/ Vehicle]	45.1 [43]			
Chassis [ton <sub>co2</sub> / Vehicle]	45.4	45.4 [43]		
Conventional End of Life [tonco2/Vehicle]	12.2	[43]		
Hybrid End of Life [tonco2/ Vehicle]	11.9	[43]		
Electric End of Life [tonco2/ Vehicle]	13.7	[43]		
Tires [kg <sub>c02</sub> /unit]	600	[44]		
Water Cooling [g <sub>CO2</sub> /lt]	1600 [45]			
Oil Lubricant [g <sub>CO2</sub> /lt]	2714 [45]			
Transmission Lubricant [g <sub>CO2</sub> /lt]	2140	[45]		

398 The drop-in fuels (Diesel and Gasoline) are slightly higher in Asia than Europe due to 399 higher transportation cost. China imported a little more than two thirds of its petroleum for domestic consumption and the percent of import will most definitely grow with time. 400 About 90% of imported crude was shipped from overseas, primarily from the Middle 401 402 East and Africa. The delivery of gasoline and diesel in China is primarily accomplished by 403 rail and by ship along the coast and major rivers. Road delivery is used as supplements 404 and for short-range distribution purposes. Pipeline delivery of gasoline and diesel 405 remains rather limited presently.

406 On the other hand, the renewable energy fuels were taken the same values for both 407 scenarios due to the uncertainties of the production conditions of these fuels. A range 408 of minimum and maximum estimated in the bibliography are taken. The electricity mix 409 is well tracked by several studies. As over 60% of total electricity in China is from coal 410 firing and low renewable energy, it generates more GHG emissions than it does in the 411 Europe. Electricity grid transmission and distribution losses are applied to each country 412 based on International Energy Agency (IEA) statistics. On average at EU level 413 transmission and distribution losses increase the carbon intensity of the grid by about 414 7%. On top of this, 10% efficiency losses were added: 5% from the charger equipment and 5% from the battery charging efficiency. Therefore, the value of Table 5 is multiplied 415 416 by 1.07 and then by 1.10 for each country.

Battery manufacturing is a crucial aspect in this work to a fair comparison between non-hybrid, REV and BEV. The research bibliography of [42] is taken as reference due to the deep analysis in different scenarios. In china the battery production will generate 420 more CO<sub>2</sub> emissions due to the energy mix. It is important to note that it is supposed 421 that the battery will be produced in Europe. If this scenario changes and the battery is 422 produced in China and send to Europe the trend will be revert. However, it was 423 preferred to supposed that the battery is produced in each continent.

The vehicle life was estimated in 16 years that is equivalent to 800,000 km. Vehicle maintenance is separated into maintenance of the vehicle and tire replacement. It is estimated 50 lt/year of oil lubricant, 150 lt/year refrigerant liquid and 13 lt/year transmission lubricant. The tires are replaced each year (50,000 km) with six tires per bus. The bus production and disposal are taken from [43] because analyse the vehicle CO<sub>2</sub> impact for similar buses than are studied in the current work.

## 430 **3. Results**

## 431 **3.1. ICCI performance and emissions**

432 This section presents the performance and engine-out emissions of the ICCI REV bus 433 concept in Valencia and Shanghai driving cycles. The CDC non-hybrid and EV commercial 434 buses are included for comparison as well as the CDC REV. The model is based in map-435 based approach where the power request to the engine and electric motors is calculated 436 in each instant based on the powertrain forces and the energy management strategy. Therefore, the CDC and ICCI modes are changed by modify the engine map in the ICE 437 sub model. The calculus is based in the operation in steady state conditions. The 438 439 transient effect is considered negligible for this concept. This is in line with the results showed by the authors in previous publications [13][46][47]. 440

The following figures show a Notched box plot. This type of graph depicts the 441 442 median, minimum, maximum and confidence interval. For this case 10/90 percentile is 443 used. The data groups the results for each combustion concept and fuels in the case of 444 three passenger load (0, 35 and 70 passengers) and ten driving cycles. Figure 14 shows 445 the energy consumption for all vehicles. In both scenarios the EV is the most efficiently 446 followed by the REV. As the maximum BTE of all fuels combinations is similar, the ICCI in 447 the hybrid vehicle has similar energy reductions. The Biodiesel-methanol case shows slightly improvements due to the 45% of BTE. The absence of the ICE makes the BEV 448 449 80% more efficiently than the non-hybrid. The hybrid was close to 30% of energy 450 reductions thanks to the higher ICE efficiently and regenerative braking. The avoid of 451 idle phase also allows to energy saving. For all cases Valencia cycles presents higher 452 energy consumption due to higher vehicle speed than in Shanghai.

The fuel volume consumption (see Figure 15) evidence the effect of lower hearting value of the renewable energy fuels. The worst case is the Biodiesel-Methanol due to the 53% of lower LHV of methanol with respect to diesel (see Table 3). Secondly the Diesel-Butanol due to the 20% lower LHV of butanol than diesel. However, for this case the average fuel consumption is lower than the non-hybrid diesel. Both, Valencia and Shanghai cycles presents similar trends with the REV pure diesel the best case between the concepts that have liquid fuel consumption.

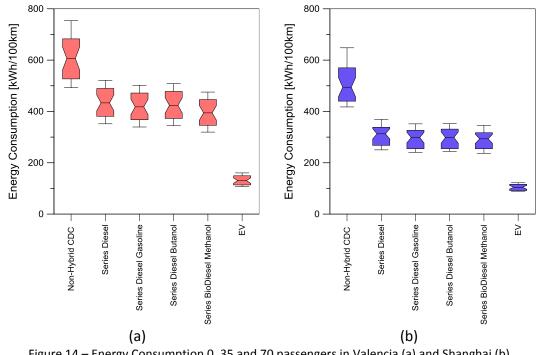




Figure 14 – Energy Consumption 0, 35 and 70 passengers in Valencia (a) and Shanghai (b).



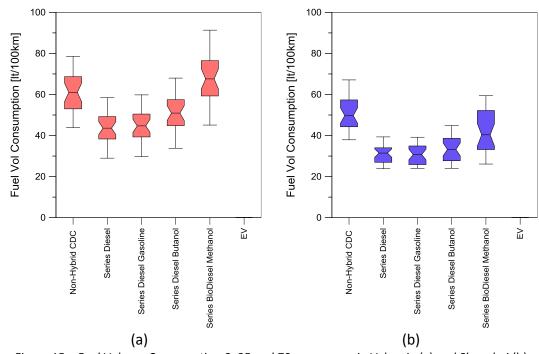




Figure 15 – Fuel Volume Consumption 0, 35 and 70 passengers in Valencia (a) and Shanghai (b).

Engine-out emissions are an important task to understand the possibility of LTC to 463 achieve EUVI or China VI emissions without ATS. Also, it is possible to understand if it is 464 possible to achieve ultra-low value thinking in current ATS for EUVII and China VII. Figure 465 16 shows the improvements of the ICCI concept with different fuels in terms of NOx 466 467 emissions. The use of a REV in diesel increase the NOx emissions. This is a disadvantage 468 that will produce higher Urea consumption to mitigate the higher NOx emissions than 469 the non-hybrid. The lowest value was achieved with Diesel-Butanol thanks to the 0.2 470 g/kWh obtained in the engine calibration process. The main advantage of the EV is the 471 absence of tailpipe emissions.

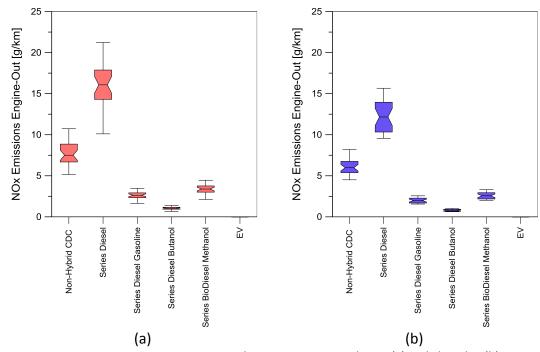
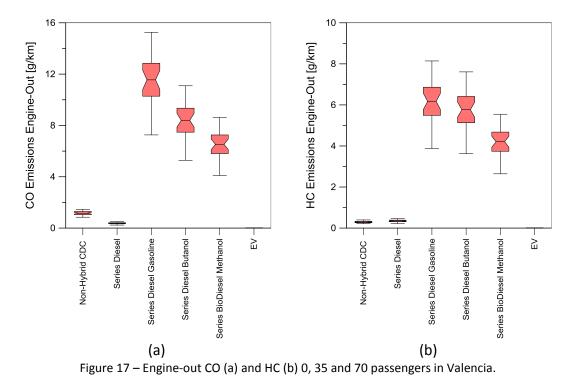




Figure 16 – NOx Engine-out 0, 35 and 70 passengers in Valencia (a) and Shanghai (b).

473 The main disadvantage of ICCI concept is the higher CO and HC engine-out emissions. 474 The indirect injection of the second fuel (Gasoline, Butanol or Methanol) make the 475 trapped fuel in the crevices produces large pollutant emissions as was seen in 476 commercial application for gasoline engines. Figure 17 shows the average values in 477 Valencia driving cycles. Shanghai present similar trends and is avoid to include the graph 478 for brevity of the manuscript. The values are one order of magnitude higher than Diesel 479 operating in non-hybrid and REV mode. These values are important to obtain to future 480 oxidation catalyst evaluations [46]. The CO emissions are higher than HC. However, EU VI is stricter in the last parameter. Therefore, HC emissions need to be studied in the 481 482 future for this type of combustion concept. The Biodiesel-Methanol was the best dual 483 fuel case with 7 g/km instead of 11.5 g/km of the Diesel-Gasoline.





## 3.2. Life Cycle Analysis

In terms of CO<sub>2</sub> emissions, a WTW and LCA analysis is done. Figure 18 shows the 486 487 WTW after including the TTW CO<sub>2</sub> emissions calculated with vehicle model simulations 488 and WTT CO<sub>2</sub> emissions from Table 4. The REV in drop-in fuels as Diesel and Gasoline 489 shows around 30% of WTW emissions reduction with respect to CDC non-hybrid in 490 Valencia and 40% in Shanghai. This is a large fuel saving if consider that only a series 491 hybrid hybridization is applied. Using renewable energy fuels, the gains increase to 65% 492 with Diesel-butanol and 75% with Biodiesel-Methanol in average for Valencia and Shanghai. The results for EV are comparable with the REV Biodiesel-Methanol thanks to 493 494 the ultra-low WTT of the renewable energy fuels (see Table 4). The results for the EV 495 bus are better for Valencia than Shanghai due to the high carbon content of the China 496 electricity mix. In both cases the EV is also a good choice with improvements around 497 75% of WTW CO<sub>2</sub> emissions with respect to non-hybrid bus.

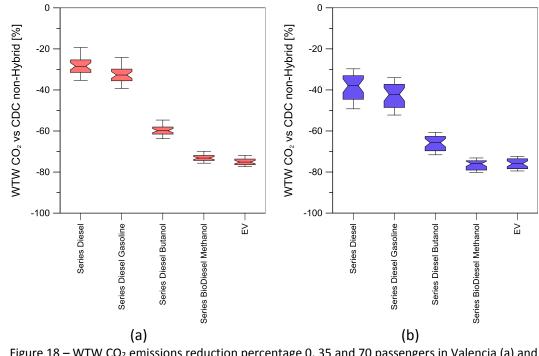
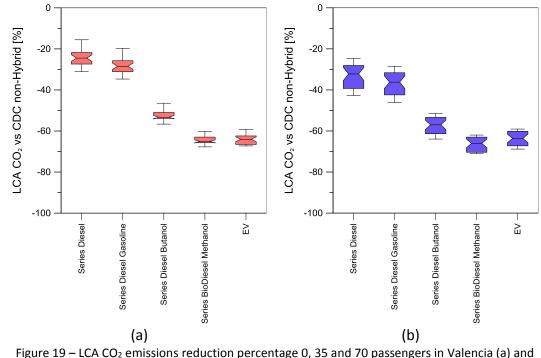
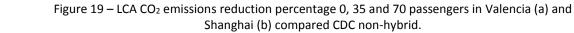




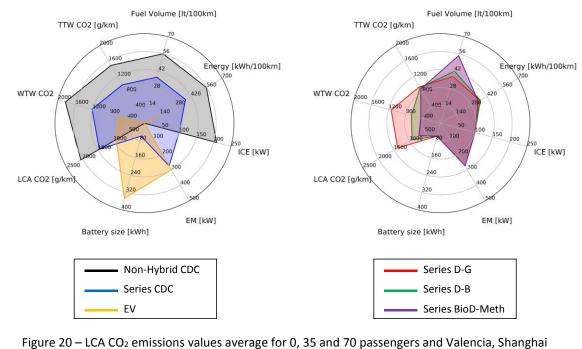
Figure 18 – WTW CO<sub>2</sub> emissions reduction percentage 0, 35 and 70 passengers in Valencia (a) and Shanghai (b) compared CDC non-hybrid.

500 When considering bus production, battery manufacturing, maintenance, and end of 501 life the results have small variations seen in the LCA (see Figure 19). The main change is 502 that the REV with two renewable energy fuels increase the CO<sub>2</sub> reduction with respect 503 to the BEV case. This is due to the high CO<sub>2</sub> emissions during the battery production. The 504 results are even improved in China scenario due to the higher carbon content of the 505 electricity mix during battery production (see Table 4). A summary of the absolute values 506 for 20 driving cycles (10 in Valencia and 10 in Shanghai) is presented in Figure 20. The 507 baseline cases are showed in the spider graph Figure 20. It is possible to see an energy 508 consumption of 117 kWh/100km instead of 560 kWh/100km of the non-hybrid. The REV 509 was in 370 kWh/100km, 35% lower than the non-hybrid. The REV with renewable energy 510 fuels shows similar energy consumption but low WTW and LCA CO<sub>2</sub> emissions. Other 511 improvements are the smaller ICE than the non-hybrid and lower battery size than the 512 pure BEV. The main disadvantage is the higher fuel volume consumption. For the large ICCI renewable energy fuel application it is necessary to produce the Butanol and 513 Methanol at lower price than the Diesel or Gasoline. 514









cycles.

### 522 4. Conclusions

523 The manuscript presents novelty results in the area of renewable energy fuels 524 and electrification. The bus numerical models show the main advantages and drawbacks 525 of using a low temperature combustion concept in a series hybrid REV. The results are 526 presented against the most common commercial vehicles. Non-hybrid series and pure 527 electric bus are included. All cases are studied in two different scenarios: Europe and 528 Asia. The driving cycles were generated in Valencia and Shanghai. The LCA values are 529 taken from continent statistics from the bibliography.

- 530 The main findings of this work are:
- The REV allows 38% of energy saving with respect to the non-hybrid concept.
   The most efficiently is the EV bus with 79% of energy reduction due to the
   higher EM operation efficiency than the ICE even in dual fuel ICCI mode.
- The series hybrid operation allows to the REV in LTC to reduce 53% the engineout NOx emissions with Diesel-Gasoline with respect of the non-hybrid diesel.
   The results are even better for Diesel-Butanol with 63% of reduction. This is mainly due to the ultra-low NOx emissions at 1500 rpm and 60 kW in the calibration process. The REV with CDC increase the NOx engine-out emissions in 35% with respect to the same combustion concept in non-hybrid.
- The WTW and LCA are favourable for electrified powertrains with 30% for REV without renewable fuels. The use of one renewable fuel (Diesel-Butanol) allows to increase the LCA saving in 55%. The inclusion of a second biofuel (Biodiesel-Methanol) allows 66% of LCA CO<sub>2</sub> reduction. These values are even higher than the EV baseline that was 54% with respect to the non-hybrid.

545 Summarizing, the use of EV is a good way to reduce CO<sub>2</sub> impact. However, the consideration of REV with biofuels is also a good solution for minimizing CO<sub>2</sub> impact in 546 547 the transportation sector. The ICCI combustion concept in this type of stationary 548 operation is ideal to also reduce engine-out emissions as NOx. Next steps in the investigation will be to go a step forward in terms of concept application. Experimental 549 550 engine real driving cycles will be performed with the data obtained in the current manuscript in terms of engine load and speed request. In addition, efforts will be applied 551 552 to understand the potential of current commercial oxidation catalyst to achieve Euro 553 legislation for the dual fuel concept.

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560 Abbreviations

ASC	Ammonia slip catalysts	HRF	High reactivity fuel Intelligent charge compression
ATS	Aftertreatment systems	ICCI	ignition
BEV	Battery electric vehicles	ICE	Internal Combustion Engine
BMEP	Brake mean effective pressure	LCA	Life cycle analysis
BSCO	Brake specific CO emissions	LHV	Low heating value
BSCO <sub>2</sub>	Brake specific CO <sub>2</sub> emissions	LI-Ion	Litium Ion batteries
BSFC	Brake specific fuel consumption	LRF	Low reactivity fuel
BSHC	Brake specific HC emissions	LTC	Low temperature combustion
BSNOx	Brake specific NOx emissions	MBC	Manhattan bus cycle
BSSoot	Brake specific soot emissions	MHEV	Mild hybrid electric vehicle
BTE	Brake thermal efficiency	NOx	Nitrogen Oxides
			Original equipment
CDC	Conventional diesel combustion	OEM	manufacturer
	China six emission legislation for		
China VI	Heavy Duty vehicles	OMEx	Oxymethylene dimethyl ether
			Belt alternator starter hybrid
CI	Compression Ignition	P0	powertrain
60	Caula an Managuida	D1	Parallel hybrid electric vehicle
CO	Carbon Monoxide	P1	without clutch Parallel hybrid electric vehicle
CO2	Carbone dioxide	P2	pre transmission
002		12	Parallel hybrid electric vehicle
CR	Compression ratio	Р3	pos transmission
			Premixed charge compression
DI	Direct Injection	PCCI	ignition
DME	Dimethyl ether	PFI	Port fuel injection
DOC	Diesel Oxidation Catalyst	PHEV	Plug in electric vehicle
			Reactivity Controlled
DoE	Design of experiments	RCCI	Compression Ignition
DPF	Diesel particle filter	REV	Range extender vehicle
EM	Electric machine	SCR	Selective catalytic reduction
	Euro six emission legislation for		
EUVI	Heavy Duty vehicles	SI	Spark Ignition
			State of the charge of the
FHEV	Full hybrid electric vehicle	SOC	battery
GCI	Gasoline compression ignition	TM	Traction motor
Gen	Generation motor	TTW	Tank to wheel
	Homogeneous charge compression		
HCCI	ignition	WTT	Well to tank
HEV	Hybrid electric vehicle	WTW	Well to wheel

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