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1	Characterization of combustion anomalies in a hydrogen-fueled
2	1.4 L commercial spark-ignition engine by means of in-cylinder
3	pressure, block-engine vibration, and acoustic measurements
4	
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13	
14	Abstract
15	Abnormal combustion phenomena are among the main hurdles for the introduction of
16	hydrogen in the transportation sector through the use of internal combustion engines (ICEs).
17	For that reason the challenge is to guarantee operation free from combustion anomalies at

For that reason the challenge is to guarantee operation free from combustion anomalies at conditions close to the ones giving the best engine output (maximum brake torque and power). To this end, an early and accurate detection of abnormal combustion events is decisive in order to allow the electronic control unit deciding suitable correcting actions. In this work, an automotive size 4-cylinder 1.4 L naturally aspirated port-fuel injection spark ignition Volkswagen engine adapted to run on hydrogen has been investigated. Three distinct methods (in-cylinder pressure, block-engine vibration and acoustic measurements) have been employed to detect abnormal combustion phenomena provoked through the enrichment of the

25	hydrogen-air mixture fed to the cylinders under a wide range of engine speeds (1,000		
26	5,000 rpm). It has been found that the high-frequency components of the in-cylinder pressure		
27	and block engine acceleration signals obtained after a Fourier transform analysis can be used		
28	for very sensitive detection of knocking combustion cycles. In the case of the ambient nois		
29	measurements, a spectral analysis in terms of third octave bands of the signal recorded by a		
30	microphone allowed an accurate characterization. Combustions anomalies could be detected		
31	through more intense octave bands at frequencies between 250 Hz and 4 kHz in the case of		
32	backfire and between 8 kHz and 20 kHz for knock. Computational fluid dynamics simulations		
33	performed indicated that some characteristics of the engine used such as the cylinder valves		
34	dimensions and the hydrogen flow rate delivered by the injectors play important roles		
35	conditioning the likelihood of suffering backfire events.		
36			
37	Keywords: Backfire; Hydrogen; Internal combustion engine; Knock; Noise; Pre-ignition.		
38			
39	Nomenclature		
40			
41	ABDC	after bottom dead centre	
42	ATDC	after top dead centre	
43	BDC	bottom dead centre	
44	BTDC	before top dead centre	
45	CA	crank angle (°)	
46	CFD	Computational Fluid Dynamics	
47	CR	compression ratio	

- 48 DI direct injection
- 49 EVC exhaust valve closing

50	H ₂ -ICE	hydrogen-fueled ICE	
51	ICE	internal combustion engine	
52	MAP	manifold air pressure	
53	MBP	maximum brake power (kW)	
54	MBT	maximum brake torque $(N \cdot m)$	
55	n	engine speed (rpm)	
56	NO _x	nitrogen oxides (ppm)	
57	PCC	Pearson's correlation coefficient	
58	PFI	port-fuel injection	
59	RON	Research Octane Number	
60	SA	spark advance (° BTDC)	
61	SI	spark ignition	
62	t	simulation time: time passed from the piston positioning at TDC (s)	
63	t_0	time passed between the intake valve opening and the piston reaching TDC (s)	
64	TDC	top dead centre	
65	WOT	wide open throttle	
66	Z_{iv}	intake valve positioning (m)	
67	Z_p	piston positioning (m)	
68			
69	Greek letters		
70			
71	λ	air-to-fuel ratio	
72	$\omega^{im}_{_{H_2}}$	fraction of hydrogen injected in the intake manifold after intake valve closing, %	
73			

74 **1. Introduction**

75

76 Hydrogen of renewable origin has potential to play a relevant role in a more sustainable 77 and environmental-friendly future transportation sector [1,2]. Whereas big R&D efforts are 78 being directed toward vehicles mounting electric engines fueled by fuel cells or batteries, less 79 attention is being paid to the internal combustion engines (ICEs) fueled with hydrogen or 80 mixtures of hydrogen with other fuels such as methane (natural gas or biogas) [3,4]. In spite 81 of their intrinsically low thermodynamic efficiency, ICEs fueled with hydrogen (H₂-ICEs) 82 have the appealing advantages of being very robust and of requiring relatively easy and cheap 83 modifications of the conventional gasoline-fueled ICEs running on hydrogen [5-9]. H₂-ICEs 84 would speed up, at least as a transitory technology, the incorporation of hydrogen into the 85 transportation sector.

86 Even though hydrogen exhibits some properties making it a very convenient fuel for use in ICEs such as wide range of flammability limits in air (4-75 vol. % H₂) that facilitate both 87 88 fuel-lean (in practice air-to-fuel ratios $\lambda < 4$) and fuel-rich operation, and very rapid 89 combustion rates that improve the process efficiency (*i.e.* the indicated fuel conversion 90 efficiency that can be determined from a thermodynamic analysis of the engine operating 91 cycle [10]), other characteristics have less desirable effects [11,12]. In this regard, the low 92 density of H₂, the increased NO_x emissions due to the high flame temperatures, and its 93 propensity for producing abnormal combustion phenomena are key factors that limit the power output of H₂-ICEs. The limitations introduced by the low density of H₂ can be offset 94 95 using suitable combustion mixture formation strategies such as supercharging and unthrottled 96 operation at variable λ for spark-ignition (SI) port-fuel injection (PFI), SI direct-injection (DI) 97 of H₂ in the cylinders, or even compression ignition DI. However, the strong influence of the 98 combustion mixture composition on the engine power output, NO_x emissions and combustion anomalies makes very challenging selecting the best H₂-ICE operating conditions [13,14]. Verhelst and Wallner have analyzed the possible control strategies that can be adopted for optimizing the trade-off existing between engine power output on the one hand, and NO_x emissions and combustion anomalies on the other, that hinders operating H₂-ICEs at or near stoichiometric fuel-air mixtures [15].

104 As concerns the abnormal combustion phenomena, they are, of course, not unique to H₂-105 ICEs as they are typical problems for the improvement of the thermal efficiency of 106 conventional engines running on liquid fuels [10,16-17]. Combustion anomalies can be 107 classified into three main categories: pre-ignition, backfire and knock [15], although the 108 actual situation is much more complex due to the interaction between these phenomena [10]. 109 For example, the occurrence of pre-ignition increases the likelihood of suffering backfire or 110 knock in the next combustion cycles [18]. In any case, all of them consist in unscheduled 111 combustion events that have negative effects on the engine performance. These effects can 112 vary from a big loss of power output in the case of pre-ignition to the risk of severe damage of 113 engine components in the case of backfire and knock. They can be distinguished by their 114 origin and timing within the engine operating cycle. Pre-ignition and backfire are caused by 115 hot spots inside the combustion chamber (spark plug electrodes, hot valves, oil ash, etc. [12]) 116 that ignite the fuel-air mixture before the spark plug fires in SI engines. Pre-ignition takes 117 place typically during the early stages of the compression stroke whereas backfire, also 118 known as backflash, occurs during the intake stroke of engines with external fuel-air mixture 119 formation systems. As the intake valves are still open, mixture combustion can extend to the 120 intake manifold resulting that, in addition to the loss of torque output, backfire can cause 121 strong damage of the mixture formation and fuel injection systems. The wide range of 122 flammable H₂-air mixture compositions and the low energy required to ignite these mixtures 123 that, as a matter of fact, reaches a minimum for the stoichiometric composition [12,15], are

124 the main reasons for the tendency of H_2 to suffer from pre-ignition. Backfire problems can be 125 reduced adopting fuel DI strategies; moreover, minimizing the possible causes of hot spots 126 formation will obviously help to operate an engine reasonably free from pre-ignition and 127 backfire. To this end, suitable design and maintenance of the fuel injection and engine cooling 128 systems are very important. The fact that H_2 combustion does not generate particulates is an 129 advantage in this regard.

130 In contrast to pre-ignition and backfire, knock occurs in SI engines after the spark plug 131 has fired and a flame front has been formed inside the cylinder. It takes place within the so-132 called knock window that goes from the late stages of the compression stroke when the piston 133 is very near to the top dead centre (TDC) to several crank angle (CA) degrees at the beginning 134 of the expansion stroke [19]. End-gas conditions change rapidly with flame propagation. 135 Particularly, the temperature and pressure increase markedly as a result of the heat generated 136 by the flame front and the compression due to the motion of the piston and the expansion of 137 the hot combustion products thus leading to an acceleration of the combustion reactions rate. 138 If the conditions are such that the concentration of free radical chemical species reaches 139 critical values [18], spontaneous auto-ignition of the unburned gases can take place without 140 the participation of any ignition source. This occurs at one or more points inside the end-gas 141 region (typically near the cylinder walls [10,20]) giving rise to knock. This phenomenon has 142 stochastic nature and the increase of pressure produced can reach peak values of several 143 thousands of kPa in the case of heavy knock. Moreover, high-frequency oscillating pressure 144 waves are generated that consist in acoustic vibration modes characteristic of the combustion 145 chamber geometry. These waves are transmitted through the metallic structure causing engine 146 vibration and a very characteristic sharp metallic (pinging) noise. In the event of prolonged 147 heavy knock, the strong thermal and mechanical stresses suffered by the components of the 148 combustion chamber may result in severe engine damage (piston ring sticking or breakage,

cylinder head gasket failure, cylinder head erosion, piston melting, etc. [10]). Obviously the severity of knock will be higher at high engine loads and under any operating circumstance allowing the mass of auto-ignited end-gas to be a large fraction of the fresh charge. For that reason the spark advance (SA) becomes a key operating parameter to be optimized for obtaining the maximum brake torque (MBT) possible under knock-free conditions [21]. Exhaust gas recirculation has been also identified as an effective strategy to suppress knock [22].

Knock also depends greatly on the fuel properties and combustion chemistry [23]. In this regard, the induction time is defined as the time needed for some critical chemical species to reach a given concentration that allows initiating the combustion chain reactions by autoignition [10]. It is widely accepted that when the end-gas temperature and pressure are such that the induction time becomes lower than the time required to combust the whole fresh charge by flame propagation the knock phenomenon will likely take place [24]. On the other hand, the end-gas heterogeneities are key in determining the auto-ignition mode [18].

163 There is some controversy in the literature regarding the tendency of H₂ to originate 164 knock. The very high auto-ignition temperature and combustion rate of H₂ are factors that 165 should contribute to an increased resistance to knock compared to the conventional liquid 166 fuels. However, wide variations in flame propagation rates taking place during combustion 167 when operating on pure H₂ have been considered to increase the risk of suffering from 168 combustion anomalies [23]. The debate is due in part to the very different octane numbers 169 reported for H₂ that in the case of the Research Octane Number (RON) range from 60 [25] to 170 above 120 [12]. Verhelst and Wallner have discussed on these discrepancies pointing out that 171 they are due to the experimental difficulties introduced by the high rate of H₂ combustion in 172 air under stoichiometric conditions and the strong dependence of the reaction rate on mixture 173 composition [15]. As pointed out by these authors, it is questionable using octane ratings to

174 measure the knock resistance of H₂ because these standardized methods were developed for 175 liquid fuels. Tang et al. [26] did not detect knock during an investigation carried out with an 176 automotive-size 2.0 L PFI H₂-ICE. It should be noted that this study was carried out with the 177 engine running unthrottled on lean mixtures with λ values between 1.4 and 3. The only 178 abnormal phenomenon noticed was pre-ignition that was observed when the engine was run 179 on the richest H₂-air mixture considered ($\lambda = 1.4$) at compression ratio (CR) of 14.5:1 and 180 engine speed of 3,000 rpm. However, several studies dedicated to investigate the onset 181 mechanism, detection and characterization of knock reveal that this phenomenon is an 182 important problem for H₂-ICEs fueled with stoichiometric or near-stoichiometric H₂-air 183 mixtures [23,25-33]. As a result, key parameters such as CR, λ , and SA should be carefully 184 selected in order to be able of giving the highest possible torque output at any time without 185 knocking. Unfortunately these limitations give rise to a remarkable decrease of the peak 186 power output compared to that of the operation with gasoline. In this regard, peak power 187 values up to 35 % lower at low and moderate engine speeds and up to 50 % lower at the 188 highest speeds (6,000 rpm) have been reported [5].

189 Most studies on knock occurrence in H₂-ICEs have been performed using single-cylinder 190 research engines at moderate or low speeds [23,27-30]. On the other hand, investigations 191 carried out on automotive-sized H₂-ICEs did not observe knock [26,33] or focused on 192 recording the in-cylinder pressure trace for detecting knock [25] or studying the distinctive 193 characteristics of knock produced by H_2 auto-ignition [31,32]. In this context, a commercial 194 SI Volkswagen engine adapted to run on hydrogen (PFI) has been employed in this work to 195 investigate H₂ combustion anomalies. Three techniques based on the in-cylinder pressure, 196 block engine vibration and ambient acoustic measurements have been employed. The data 197 obtained have been analyzed to detect and characterize abnormal combustion events under a 198 wide range of engine speeds. To our knowledge, there is no previous study similar to this one

199 performed on automotive-size H₂-ICEs, especially as concerns noise measurements. Finally, 200 computational fluid dynamics (CFD) simulations have been performed in order to assess to 201 what extent the characteristics of the adapted commercial engine used can influence on some 202 of the abnormal combustion phenomena detected, particularly backfire.

203

204 **2. Engine characteristics, experimental setup and methods**

205

206 The engine and test facility used in this study were described in detail elsewhere [4,6]. 207 Briefly, a Volkswagen 4-cylinder 1.4 L naturally aspirated PFI SI engine with a CR of 10.5:1 208 was employed. It gave maximum brake power (MBP) and MBT of 59 kW at 5,000 rpm and 209 132 N·m at 3,800 rpm, respectively, when fueled with gasoline. The engine was adapted to 210 run on H₂ resulting in a significant performance reduction (MBP of 32 kW at 5,000 rpm and 211 MBT of 63 N·m at 3,800 rpm) due in great part to the conservative operating conditions 212 employed. As concerns the test bed cell, it consisted of an eddy current dynamometer AVL 80 213 [4,6]. Hydrogen and air flow rates were determined using mass-flow meters (Bronkhorst) with 214 a precision of ± 0.5 %. Pressure and temperature in the intake manifold were recorded with a 215 Bosch 03C.906.051 apparatus. The CA and pressure in cylinder number 1 were measured 216 with Kistler 2613B1 ($\pm 0.02^{\circ}$) and 6117B ($\pm 0.6^{\circ}$) sensors, respectively. The exhaust gases 217 were analyzed with a Horiba MEXA-720NOx analyzer for NO_x determination with an 218 accuracy of \pm 30 ppm.

As for the block engine vibrations produced by abnormal combustion events they were measured using an accelerometer [34-36]. As a matter of fact this type of sensors are typically mounted on the commercial automotive engines fabricated in series. Whereas in-cylinder pressure measurements are typical at the laboratory scale, this technique is too costly to be implemented in commercial vehicles [27]. In this work, a Bruel & Kjaer 4504 tri-axial piezoelectric CCLD accelerometer (range: 1-10,000 Hz; sensitivity: $10 \pm 20 \%$ mV/g) was used and placed near the head of the cylinder in which the combustion anomalies were recorded. Preliminary experiments showed an excellent agreement between the responses of the original accelerometer and the one mounted on the engine-block. The most intense signals were obtained in the direction parallel to the axis of the cylinders. Only the data recorded in that direction will be presented.

One of the main novelties of this work is that ambient sound measurements have been also performed to characterize abnormal combustion events. The acoustic measurements were conducted in the engine test bed cell that behaved as an almost semi-anechoic room. Sound pressure was recorded using a G.R.A.S. 40AC high-precision condenser microphone (up to 40 kHz with a sensitivity of 12.5 mV/Pa) placed 1 m from the engine.

235 After starting up the engine using an initial λ of 1.7, it was let idle for a few minutes for 236 suitable warming. The experiments were performed in such a way that the H₂-air mixture fed 237 to cylinder number 1 was enriched in the fuel (decreasing values of λ) by increasing the H₂ 238 injection pulse width stepwise until that combustion anomalies appeared. In most of the 239 experiments, only one cylinder was fed with the enriched mixture in order to prevent the 240 engine from suffering severe damage. The process was repeated at engine speeds ranging 241 from 1,000 rpm to 5,000 rpm and full load (wide open throttle, WOT). SA was set at 242 10 ° BTDC whereas the exhaust valves closed at CA of 3 ° after top dead centre (ATDC) and 243 the H₂ injection started at CA of 22 ° ATDC during the intake stroke. SA value was selected 244 according to our previous experience with the engine that showed that 10 ° BTDC constitutes a trade-off between satisfactory engine performance and combustion anomalies [4,6,8]. 245 246 Abnormal combustion occurrence could be detected by a characteristic pinging noise 247 followed by a strong bass noise accompanied by a great decrease of the brake torque. Once 248 that point was reached the engine was shut off.

249 To guarantee a correct characterization free from unwanted signals, data used for 250 abnormal combustion events detection (in-cylinder pressure, accelerometer and microphone 251 signals) were recorded with a sufficiently high frequency of 100 kHz. On the other hand, the 252 parameters related with the engine operation (engine speed, λ , intake manifold temperature and pressure, injection pulse width and NO_x concentration in the exhaust gases) were 253 254 registered with a frequency of 10 Hz. Another important aspect is the number of engine cycles 255 analyzed. Brunt et al. recommended a sample of at least 1,000 cycles for a suitable 256 determination of the intensity of the combustion events on a Ford Zetec 2.0 L 4-cylinder 257 engine fueled with gasoline [37]. In our case the samples ranged from 1,224 cycles at engine 258 speed of 1,000 rpm to 3,275 at 3,000 rpm and 2,725 cycles at engine speed of 5,000 rpm. This 259 resulted in experiments lengths ranging from 147.2 s at 1,000 rpm to 65.6 s at 5,000 rpm.

260

- 261 **3. Results and discussion**
- 262

263 3.1. Abnormal combustion characterization

264

265 In contrast to block-engine vibration and sound measurements, the in-cylinder pressure 266 values give a direct measure of the dynamics of the combustion process. Fig. 1 shows an 267 example comparing the characteristics of normal and abnormal combustion cycles recorded at 268 the highest engine speed (5,000 rpm) and $\lambda = 1.52$. The graph shows the evolution with CA of 269 the pressure (gauge) in cylinder number 1. Note that the origin of the CA axis is situated at 270 spark time (350 °= 10 ° BTDC). Data along a CA period of 50 ° characterized by the highest 271 in-cylinder pressures are provided. This CA window is slightly higher than the range of 40 ° 272 from TDC recommended by Brunt et al. in a study performed with an automotive-sized engine [37]. As can be seen, during the normal combustion cycle the in-cylinder pressure 273

274 increases gradually after the spark plug fires until reaching a maximum value of about 53 bar 275 at TDC. The cycle showing knock is characterized by high-frequency pressure oscillations 276 with a maximum amplitude of about 20 bar leading to a peak pressure close to 84 bar also at 277 TDC. This almost doubles the pressure rise rate of 1.0 MPa/CA considered as the lower limit 278 for heavy knock [24]. The amplitude of the pressure oscillations decreases progressively 279 ATDC although the oscillations are still present at CA of 40 ° ATDC during the expansion 280 stroke. It can be observed that during the knocking cycle the in-cylinder pressure rises more 281 rapidly than during the normal combustion cycle in accordance with Li and Karim [23]. 282 Presumably this lowers the induction or delay time leading to the occurrence of a spontaneous 283 auto-ignition of the end-gas [24]. Cycle-to-cycle combustion variations and flame instabilities 284 may also result in a temperature increase and thermal inhomogeneity that facilitate reaching 285 the critical conditions that provoke knock [24,32]. According to Li et al. [38] the energy 286 density and heat release rate in hot spots play critical roles in determining knock intensity. In 287 the case of backfire the in-cylinder pressure is very low and shows a very smooth decrease 288 during the expansion stroke. This is due to the fact that the fuel has been already burned 289 during the previous intake stroke.



Fig. 1. Evolution of the in-cylinder pressure with CA at engine speed of 5,000 rpm for the following cycles: normal cycle, knocking cycle, and backfiring cycle.

293 A more complete characterization of the abnormal combustion phenomena is given in 294 what follows taking as base case the experiments performed at an intermediate engine speed 295 of 2,000 rpm. Fig. 2 shows the evolution along time of the in-cylinder pressure, accelerometer 296 and microphone signals and the temperature in the intake manifold. On the other hand, Fig. 3 297 depicts the evolution of the parameters characterizing the engine performance for the same 298 experiments. The width of the hydrogen injection pulse was increased from its initial value of 299 6.2 ms ($\lambda = 1.7$) resulting in a progressive decrease of the λ value. After 100 s the pulse width 300 was about 6.9 ms ($\lambda = 1.45$) and the brake torque reached an almost steady value of 57 N·m. 301 The NO_x concentration and in-cylinder pressure also increased reaching 430 ppm and 60 bar, 302 respectively. On the other hand, the accelerometer and microphone recorded normal signals of 303 \pm 15 g and \pm 5 Pa, respectively.



304

Fig. 2. Evolution with time of the parameters used for the characterization of abnormal combustion phenomena at engine speed of 2,000 rpm. From top to bottom: in-cylinder pressure, accelerometer signal, microphone signal, and intake air temperature.



Fig. 3. Evolution with time of the performance parameters at engine speed of 2,000 rpm. From top to bottom: brake torque, NO_x concentration in the exhaust gases, air-to-fuel ratio (λ) and H₂ injection pulse width.

312 As can be seen in Fig. 2, the first knock event was registered after 107 s, when strong 313 signals of ± 160 g and 75 bar, were recorded by the accelerometer and the pressure sensor, 314 respectively. This event was audible and it was decided to maintain constant the hydrogen 315 injection pulse width; however, the microphone did not register any clear signal 316 distinguishable from the background noise. At this point the engine entered a 40 s period 317 characterized by strong vibrations reaching an amplitude of up to +300 g, and pressure peaks 318 of up to above 80 bar; a characteristic pinging noise could also be heard. During this period the brake torque showed a very slight tendency to decrease whereas the NO_x emissions 319 320 remained essentially unchanged (see Fig. 3). After 155 s a strong hoarse noise was produced 321 that could be recorded by the microphone (amplitude of up to + 10 Pa). This was followed by 322 an abrupt decrease of the in-cylinder pressure and the brake torque and erratic readings of the 323 exhaust NO_x concentration. This last event consisted in backfire as deduced from the intense 324 increase of the intake air temperature produced. At that moment the engine was switched off.

325 Similar results (not shown) were observed at 1,000 rpm, 4,000 rpm and 5,000 rpm, 326 whereas at 3,000 rpm no knock was detected by the sensors and the engine passed directly 327 from normal running to backfire. However, by increasing the spark advance from 10 ° BTDC 328 to 20° and 30° BTDC knock was detected before backfire also at 3,000 rpm. It should be 329 noted that if ignition is started far from TDC there is a higher likelihood of suffering knock 330 and of producing more intense pressure oscillations [23]. Moreover, spark advance becomes 331 critical in the case of engine operation under lean-burn conditions due to more pronounced 332 cycle-to-cycle combustion variations that also contribute to increase knock likelihood [39].

334 3.2. Knocking combustion cycles: analysis of the in-cylinder pressure and accelerometer335 signals

336

As shown in the previous section, knock could be identified by means of the abrupt variations of the readings recorded by the in-cylinder pressure transducer and the block engine accelerometer. Now the correlation between these two signals is analyzed.

340 Mass-elastic systems show natural vibration frequencies so that for a given frequency the 341 system vibrates according to characteristic amplitude and phase which is known as a vibration 342 mode. Only some of the lowest order frequencies are of practical interest because the high-343 order ones are generally significantly damped. In the case of ICEs, combustion (both normal 344 and abnormal) and motion of engine components cause vibrations that are transmitted through 345 the engine structure. Of course, the intense in-cylinder pressure oscillations associated to 346 knock provoke stronger vibrations that can be detected with an accelerometer. This is the 347 reason why commercial engines mount these simple sensors for knock detection and engine 348 operation control and management instead of the much more expensive and complex in-349 cylinder pressure transducers and optical sensors [35,36].

350 In this work, distinction between high and low frequencies has been made taking as 351 reference the values above and below 20 times the engine speed, respectively. According to 352 this criterion, Fig. 4 and Fig. 5 show typical readings of the in-cylinder pressure transducer 353 and the accelerometer, respectively, for normal and knocking combustion cycles. Signals 354 were decomposed into their low- and high-frequency components by means of Fourier 355 transform (FT) analysis. In both cases the engine speed was 2,000 rpm and the signals 356 corresponded to the values recorded within spark time (10 ° BTDC) and 40 ° ATDC. It can be 357 seen that for the normal combustion cycles the pressure signal coincides with the low-358 frequency component whereas the accelerometer signal is very weak and indistinguishable

from the low- and high-frequency components. In the case of the knocking cycles, the pressure signal is dominated by the low-frequency component whereas the oscillations are well represented by the high-frequency component. In contrast, the accelerometer signal is dominated by the high-frequency component as can be seen in Fig. 5.

363 It can be then concluded that the high-frequency component of the in-cylinder pressure 364 and block engine acceleration signals obtained after a FT analysis can be used for very 365 sensitive detection of knock events in H₂-ICEs of automotive size. Making the distinction 366 between low and high frequency on the basis of the engine speed is useful to take into account 367 at every moment the influence of this key parameter on the engine vibration characteristics 368 because other factors such as the engine geometry, the speed of sound, etc. will not change 369 significantly. A value of 20 times the engine speed was adopted after a preliminary screening. 370 The exact value of this reference is not very critical provided it is relatively close to the 371 engine speed which seems reasonable.



Fig. 4. Evolution of the in-cylinder pressure with CA at engine speed of 2,000 rpm for typical
normal (left) and knocking (right) combustion cycles showing the in-cylinder transducer raw
signal and its low-frequency and high-frequency components.



Fig. 5. Evolution of the acceleration with CA at engine speed of 2,000 rpm for typical normal
(left) and knocking (right) combustion cycles showing the accelerometer raw signal and its
low-frequency and high-frequency components.

380 A further analysis of the sensors signals has been performed through the study of the 381 evolution of the integral average of the high-frequency components' modulus. This is shown 382 in Fig. 6 and Fig.7 for the readings from the accelerometer mounted on the block engine and 383 the in-cylinder pressure transducer, respectively. For each engine speed considered, the 384 possible linear correlation between the accelerometer and the pressure transducer signals has 385 been assessed through the values of the Pearson's correlation coefficient (PCC). In these 386 experiments, the air-to-fuel ratio (λ) of the mixture decreases from cycle to cycle due to a 387 gradual increase of the H₂ injection pulse width. The high values of the integral averages 388 observed after about 2,000 cycles indicated the appearance of knock events. When the 389 complete datasets are considered, the PCC values obtained at 2,000 rpm, 4,000 rpm and 390 5,000 rpm are 0.701, 0.613 and 0.699, respectively, that, given the large size of the samples, 391 indicate a high degree of linear correlation. It should be noted that no knocking cycles were 392 detected at 3,000 rpm so data corresponding to that engine speed were not considered. In 393 contrast, the PCC at engine speed of 1,000 rpm was only 0.200 thus revealing lack of linear 394 correlation between the signals. This is a low speed regime for an automotive size engine, 395 close to idling. This is a fluctuating regime showing speed oscillations around the set point 396 that provoke in-cylinder pressure instabilities. This can be appreciated in Fig. 7 where at 397 1,000 rpm the in-cylinder pressure changes gradually during the first combustion cycles until 398 the reading is stabilized. These relatively smooth pressure changes do not translate to the 399 acceleration signal due to its inertial character that results in remarkable damping. If the 400 cycles preceding the 220 one at 1,000 rpm are discarded the PCC increases from 0.200 to 401 0.819 showing strong liner correlation also at this speed.



403 Fig. 6. Evolution of the integral average of the high-frequency components' modulus of the
404 accelerometer signal for each of the combustion cycles indicated at engine speeds of (from
405 bottom to top): 1,000 rpm, 2,000 rpm, 4,000 rpm and 5,000 rpm.



Fig. 7. Evolution of the integral average of the high-frequency components' modulus of the
in-cylinder pressure signal for each of the combustion cycles indicated at engine speeds of
(from bottom to top): 1,000 rpm, 2,000 rpm, 4,000 rpm and 5,000 rpm.

410 A more detailed observation of Fig. 7 suggests that knocking combustion cycles are 411 characterized by values of the integral average of the high-frequency components' modulus of 412 the in-cylinder pressure signal above 0.5. From the 2,500 combustion cycles shown in Fig. 7 413 at engine speed of 2,000 rpm only 39 cycles fulfill this criterion. The PCC for the high-414 frequency components of the accelerometer and the pressure transducer signals during these 415 cycles is 0.584 thus indicating a practically linear correlation. On the other hand, at engine 416 speed of 5,000 rpm only 9 cycles seemed to present knocking events but in this case the PCC 417 was - 0.294 which indicates that the correlation between the signals losses relevance at high

418 engine speeds. The reason could be the inertial nature of the vibrations leading to the signal 419 captured by the accelerometer. Knock generates vibrations that require time to be completely 420 damped, especially the low-frequency vibration modes. Therefore, normal combustion cycles 421 can be mistakenly identified as knocking ones if one or several of the preceding cycles 422 suffered from abnormal combustion events. As the engine speed increases this possibility is 423 more likely because the time interval available for vibrations damping among consecutive 424 combustion cycles decreases. In this regard, if the correlation investigated is among the 425 integral average values of the high-frequency components' modulus of the in-cylinder 426 pressure signal of the 9 knocking cycles and those of the accelerometer signal for the cycles 427 just following the knocking ones [27], the PCC reaches a much higher value of 0.537. The 428 silentblocks incorporated into the commercial engines for absorbing vibrations and reducing 429 noise introduce non-linearity among the in-cylinder pressure and engine block acceleration 430 thus complicating the rapid identification of knock. As a result, the criteria used to identify 431 knock with accelerometers mounted on the block engine should be more restrictive and be 432 adapted to the engine speed. From the results shown in Fig. 6 it can be suggested that whereas 433 integral average values of the high-frequency components' modulus of the accelerometer 434 signal above 15 can be used at engine speeds below 2,000 rpm, this limit has to be increased 435 to about 30 for higher speeds.

436

437 *3.3. Engine noise analysis*

438

As already mentioned, one of the main novelties of this work is the use of ambient noise measurements to identify abnormal combustion events. It is well known that phenomena such as knock is accompanied by a characteristic pinging noise so it is interesting to explore the possibility of using acoustic measurements for the detection of abnormal combustion. Fuel combustion produces the so-called combustion noise, which is the most important source of
noise in an ICE. Combustion noise is a complex phenomenon affected by the characteristics
of the fuel as well as that of the engine and its operating conditions [40].

Returning to the results shown in Fig. 2 and corresponding to an engine speed of 2,000 rpm, Fig. 8 and Fig. 9 show the instantaneous values of the in-cylinder and acoustic pressures for a series of normal and knocking combustion cycles, respectively.



450 Fig. 8. Evolution with time of the in-cylinder (blue signal) and acoustic (red signal) pressures451 for a series of normal combustion cycles at engine speed of 2,000 rpm.

449

It can be seen that normal combustion cycles show in-cylinder peak pressures of about 55 bar and acoustic pressures oscillating within \pm 3.5 Pa. In Fig. 9, three knocking combustion cycles can be clearly identified by peak in-cylinder pressures above 70 bar the (1st, 3rd and 7th cycles). In contrast, the acoustic pressure for these abnormal cycles show only slightly higher amplitudes (within \pm 5 Pa) compared to those of the normal combustion cycles.



458 Fig. 9. Evolution with time of the in-cylinder (blue signal) and acoustic (red signal) pressures459 for a series of normal and abnormal combustion cycles at engine speed of 2,000 rpm.

A more in-depth characterization of the acoustic properties of a pair of normal and knocking combustion cycles is shown in Fig. 10 which presents a spectral analysis in terms of third octave bands. Octave-band analysis is incorporated by the most usual methods regarding the assessment of sound perception [41].





466 It can be seen that both cycles can be distinguished by means of the highest frequency 467 bands (between 8 kHz and 20 kHz) which are around 8-10 dB more intense in the case of the 468 knocking cycle than for the normal combustion. Furthermore, the spectral analysis is also 469 useful to identify abnormal combustion phenomena associated to backfire. As mentioned in 470 section 3.1. backfire was characterized by an abrupt increase of the intake air temperature 471 accompanied by a strong hoarse noise. Fig. 11 shows the spectral power of a normal 472 combustion cycle and two anomalous cycles consisting in knock and backfire, respectively. 473 The number above the bars indicate the power change (in dB) with respect to the normal 474 combustion cycle. It can be seen that backfire shows octave bands more intense by 7-16 dB in 475 the range of frequencies comprised between 250 Hz and 4 kHz in comparison with the other 476 combustion cycles.



478 Fig. 11. Spectral analysis of typical normal, knocking and backfiring cycles at engine speed of479 2,000 rpm.

480

481 **4.** Computational Fluid Dynamics (CFD) simulation of the engine performance

482

483 *4.1. Aim and scope*

484

In this work, a commercial Volkswagen 4-cylinder 1.4 L originally designed to be fed with gasoline and adapted to run on hydrogen has been used. One of the most important modifications performed consisted in the implementation of the hydrogen feeding system. In this regard, the original inlet manifold was replaced by another one made in metal for safer operation in the event of backfire. In addition, the gasoline injectors were replaced by gas injectors that were fixed to the inlet manifold by means of a metallic support and connected to a hydrogen accumulator through stainless steel tubing. The accumulator was necessary in 492 order to guarantee that the injectors were supplied with hydrogen at a constant and suitably493 low pressure compared to the one in the gas cylinders that stored the fuel (200 bar).

494 Injection system configuration and its operating parameters such as injection timing and 495 pulse width duration may have strong influence on the local fuel/air composition inside the 496 intake manifold and cylinder. It was observed during the experiments that knock did not 497 appear immediately after increasing the injection pulse width duration but it occurred some 498 time after that, which suggested that hydrogen could be accumulating inside the manifold. To 499 check this possibility, a computational fluid dynamics (CFD) study was conducted to simulate 500 the performance of the hydrogen injection system used in this work. Simulations were accomplished using ANSYS-CFX[®] 15.0 software. The physical model consisted in the intake 501 502 manifold, cylinder head and hydrogen injector geometries shown in Fig. 12.



503

504 Fig. 12. Physical CFD model of the intake manifold, fuel injector and cylinder head.

505

506 4.2. Simulation conditions

507

508 Simulations were performed under transitory regime being TDC and the intake valve 509 closing the initial and final instants, respectively. The following simplifying assumptions 510 were adopted: hydrogen injection was considered isothermal at 25 °C and buoyancy 511 phenomena were neglected as transport was dominated by convective effects. On the other 512 hand, the side of the intake manifold opposite to the cylinder was modeled as an open surface 513 at constant manifold air pressure (MAP) allowing the entry of air due to the suction associated 514 to the piston motion. MAP value was set at 0.92 bar according to the values recorded by the 515 electronic control unit during the experiments performed at WOT. As concerns turbulence the 516 k-ɛ model was adopted. After a preliminary study on grid independence of the solution, a 517 moving grid with *ca.* 250,000 volume elements was adopted to describe the piston and valves 518 motion.

The gas injectors used provided hydrogen at constant mass flow rate of 0.31 mg/ms during the pulse, being 1.2 ms and 0.2 ms the time required for the injector opening and closing, respectively. Injection timing was initially set at CA of 22 ° ATDC. It should be noted that exhaust valve closing (EVC) timing was established at CA of 15.3 ° in order to allow suitable cooling to reduce the likelihood of backfire.

As concerns the piston positioning, a value of 0 was assigned to TDC whereas the piston displacement adopted negative values given by the following expression obtained after considering the slider-crank engine geometry:

527
$$Z_p = -0.00402 + 0.0378 \cdot \cos\left[\left(\frac{2\pi}{60} \cdot n\right) \cdot t\right] + 0.0024 \cdot \cos\left[\left(\frac{4\pi}{60} \cdot n\right) \cdot t\right]$$
(1)

where Z_p (m) is the piston positioning, *n* (rpm) is the engine speed and *t* (s) is the time passed from the piston positioning at TDC. On the other hand, the positioning of the intake valve (Z_{iv}) was – 1.56 mm at TDC and was given (in m) by:

531
$$Z_{iv} = -0.0037 \cdot \left(\cos \left[\left(\frac{2\pi}{60} \cdot n \right) \cdot \frac{360}{214} \cdot t_0 \right] - \cos \left[\left(\frac{4\pi}{60} \cdot n \right) \cdot \frac{360}{214} \cdot \left(t + t_0 \right) \right] \right)$$
(2)

where t_0 (s) is the time passed between the start of the intake valve opening and the instant when the piston reaches TDC (*i.e.* the time required to turn the 19° of crank angle corresponding to the intake valve opening advance).

535

536 4.3. Simulation results

537

538 Fig. 13 A-D includes a sequence of images showing the contour maps of hydrogen molar 539 fraction in the intake manifold and cylinder during the intake stroke obtained from the CFD 540 simulations of the engine running at 2,000 rpm. Hydrogen injection started at 22 ° ATDC and 541 the injection pulse width was 6 ms. Fig. 13 A shows that after 3.3 ms (40 ° ATDC) when the injection is close to ending, the hydrogen concentrates near the injector. After 7.5 ms (Fig. 542 543 13 B, 90 ° ATDC) the injection has finished and it can be seen that hydrogen has spread 544 within the intake manifold whereas there is almost no hydrogen in the cylinder. Fig. 13 C shows that after 12.5 ms, at 150 ° ATDC the great majority of hydrogen has entered the 545 546 cylinder by the suction caused by the piston displacement. Finally, when the intake valve 547 closes at 195 ° ATDC (16.25 ms) some hydrogen still remains within the intake manifold as 548 shown in Fig. 13 D. Depending on the evolution of the situation during the subsequent 549 combustion cycles it is possible that an accumulation of hydrogen within the intake manifold 550 takes place. In that case the mixture entering the cylinder will be richer than expected so the 551 likelihood of knock will increase even maintaining constant the injector pulse width. As 552 hydrogen is present within the intake manifold the risk of suffering from backfire during 553 engine operation is evident; as a matter of fact, the backfire events detected in this work were 554 preceded by knocking combustion cycles as explained in section 3.1. The results suggest that 555 the temperature increase provoked by knock, together the presence of hydrogen in the intake 556 manifold lead to combustion while the intake valve is open.



Fig. 13. Hydrogen molar fraction in the intake manifold and cylinder at CA values ATDC of:
A) 40 °; B) 90 °; C) 150 ° and D) 195 ° (engine running at 2,000 rpm).

The problem of hydrogen accumulation could be due to the fact that the engine was designed to run on gasoline, that is, a liquid fuel with a density much higher than that of hydrogen. For that reason, the valves dimensions, which are suitable for gasoline PFI seem to be not so large as to guarantee a sufficiently high hydrogen volumetric flow rate. In this regard, Fig. 14 shows the evolution of the amounts of hydrogen and air that have entered the cylinder during the intake stroke according to the CFD simulations.



Fig. 14. CFD simulation results corresponding to the hydrogen (blue line) and air (red line)
amounts in the cylinder during the intake stroke (engine running at 2,000 rpm).

568 It can be seen that the mass of air within the cylinder increases gradually until reaching 569 bottom dead centre (BDC) at CA of 180°. In contrast, the mass of hydrogen inside the 570 cylinder increases sharply within a relatively narrow range of CA values between about 100 ° 571 and 140° ATDC; afterwards, the amount of hydrogen remains almost constant. This is 572 because the hydrogen injection is significantly retarded (22 ° ATDC) in order to allow the 573 cooling of the exhaust valve after closing. The very small decrease of the amount of gases 574 observed ABDC may be due the pressure increase due to the beginning of the compression 575 stroke and/or to a dragging effect associated to the intake valve closing.

The preceding results suggest that a possible solution would be advancing the injection time although the risk exists that the exhaust valve is still excessively hot. However, taking into account that the simulations were performed at an intermediate engine speed of 2,000 rpm and that running at higher speeds has to be feasible, advancing the injection time should be considered as a realistic option in order to attend the requirements of engine operation at highly demanding conditions. To investigate the effect of advancing the injection 582 timing a series of CFD simulations were performed at injection times of 1 ° and 22 ° BTDC,

583 injection pulse widths of 4 ms and 6 ms and engine speeds of 2,000 rpm and 4,000 rpm.

Engine speed	Injection pulse	Injection advance	$\omega_{_{H_2}}^{im}$ (%)
(rpm)	width (ms)	(° BTDC)	
2,000	4	1	5
2,000	4	22	6
2,000	6	1	5
2,000	6	22	9
4,000	4	1	30
4,000	4	22	48
4,000	6	1	50
4,000	6	22	62

584 Table 1. Results of the CFD simulations performed at various H₂ injection conditions.

585

586 Table 1 shows the mass fraction of the hydrogen injected that remained in the intake manifold ($\omega_{H_2}^{im}$) after the intake valve closing. As expected, advancing the injection time has a 587 588 positive effect on the introduction of hydrogen into the cylinder; however, the phenomenon is 589 largely dominated by the engine speed. This is because the timing window available for 590 injection decreases as the engine speed increases. So even greatly advancing the injection 591 time (1 ° BTDC) and reducing the injection pulse width (4 ms) the fraction of hydrogen that 592 cannot enter the cylinder at 4,000 rpm is as high as 30 %. As a matter of fact, the majority of 593 hydrogen (62%) remained in the intake manifold at 4,000 rpm if the injection time is

594 maintained at 22 ° BTDC. Moreover, if the injection pulse width is relatively large, hydrogen 595 would be injected at crank angles well above 160 ° BTDC when the suction capacity of the 596 cylinder is very limited. If this situation is maintained from cycle to cycle a non-steady 597 situation is established leading to an accumulation of hydrogen that can provoke abnormal 598 combustion events. Therefore, in addition to a suitable dimensioning of the valves, the design 599 of the hydrogen injectors is another key factor. Indeed, as already mentioned, the injectors 600 mounted deliver hydrogen at a mass flow rate of 0.31 mg/ms which seems to be insufficient 601 for guaranteeing an operation free from backfire at high engine speeds.

Finally, suitable manifold design should take into account the speed of sound for proper tuning of the pressure waves and injector opening (intake manifold resonance charging). That speed is different for hydrogen-air mixtures than for the gasoline-air ones, which can also contribute to the accumulation of hydrogen.

606

607 **5. Best engine performance**

608

609 Taking into account the engine limitations some final experiments were carried out in 610 order to determine its best possible output at conditions free from abnormal combustion 611 events. To that end, after an initial warming-up period the hydrogen-air mixture fed to the 612 four cylinders was progressively fuel-enriched by increasing the injection pulse width. The 613 engine was operated at different speeds and the highest values of the brake torque and power 614 that could be achieved in the absence of abnormal combustion events were determined in each 615 case. The results are compiled in Table 2 where the values of injection pulse width and the 616 air-to-fuel ratio have been also included.

617 It can be seen that the hydrogen-air mixture providing the best output becomes leaner 618 (higher λ) as the engine speed increases. This could be due to the fact that at higher engine

619 speeds the amount of hydrogen injected also increases as well as the fraction of the hydrogen 620 that remained in the intake manifold, thus increasing the likelihood of provoking abnormal 621 combustion events.

Whereas the highest value of the brake power (33.5 kW) was obtained at the maximum engine speed considered (5,000 rpm), the highest brake torque (67.2 N·m) resulted at 4,000 rpm. On comparing these values with the best engine performance achieved when gasoline is used as fuel (59 kW at 5,000 rpm and 132 N·m at 3,800 rpm) [6], it is clear that an output loss of about 50 % results when replacing gasoline by hydrogen. This is due to a great extent by the propensity of hydrogen to suffer from abnormal combustion phenomena which remarks the importance of their early and accurate detection.

Engine speed	Injection pulse	Air-to-fuel	Brake torque	Brake power
(rpm)	width (ms)	ratio (λ)	(N·m)	(kW)
1,000	7.59	1.30	50.3	5.27
2,000	7.85	1.35	63.5	13.3
3,000	7.92	1.42	65.4	20.5
4,000	8.42	1.49	67.2	28.1
5,000	8.76	1.52	64.0	33.5

629 Table 2. Best engine output at the speeds indicated and normal combustion conditions.

630

631 **6.** Conclusions

A good correlation between in-cylinder pressure and block-engine acceleration
 measurements has been found regarding the detection of knocking combustion cycles in a
 port-fuel injection spark ignition internal combustion engine of automotive size fueled with

635 hydrogen-air mixtures. To improve the accuracy, signals were decomposed into their low- and 636 high-frequency components by means of conventional Fourier transform analysis. High and 637 low frequencies were distinguished as the values above and below 20 times the engine speed, 638 respectively. Knock events were very well described by the high-frequency components of the 639 pressure and acceleration signals which showed changes associated to the abnormal 640 combustion event of up to about 20 bar and 250 g, respectively. The adopted criterion, based 641 on the engine speed, has the advantage of taking into account the important effects introduced 642 by the engine speed in conditioning the likelihood of suffering abnormal combustion events.

643 To the best of our knowledge, in this work the in-cylinder pressure and block-engine 644 vibration measurements are carried out simultaneously together with ambient noise recording 645 for the first time. The raw signal recorded by the microphone allowed to detect the strong 646 hoarse noise associated to backfire but it did not allow distinguishing knock from the 647 background signal in spite of the characteristic pinging noise that could be heard during some 648 combustion cycles. However, a spectral analysis of the raw signal in terms of third octave 649 bands greatly improved the sensitivity. In this regard, a typical knocking cycle could be 650 distinguished from a normal combustion cycle through the highest frequency bands (between 651 8 kHz and 20 kHz) which were ca. 8-10 dB more intense. As concerns backfire, this anomaly 652 could be associated to more intense octave bands at the lowest frequencies (between 250 Hz 653 and 4 kHz). These results indicate that detection of abnormal combustion events is possible 654 through acoustic measurements. An optimization of the experimental conditions, particularly 655 microphone location, will surely provide a much more accurate detection results that the ones 656 achieved in this work. Therefore there is great potential for the development of acoustic 657 sensors for abnormal combustion detection in automotive engines.

658 CFD simulations performed with a physical model that reproduced the engine systems for 659 mixture formation and fuel injection revealed that combustion anomalies can arise as a result

660 of the fact that the engine was originally designed to run on gasoline, a fuel much more dense 661 than hydrogen. It has been found that a fraction of the hydrogen injected still remains in the 662 intake manifold after the intake valve has closed. This fraction increases with the increase of 663 the injection pulse width to obtain richer mixtures and especially when the engine speed rises 664 (e.g. from 5-9 % at 2,000 rpm to 30-62 % at 4,000 rpm) due to the reduced time window 665 available for fuel injection. The accumulation of hydrogen that takes place increases the risk 666 of backfire which in turn increases the likelihood of suffering from knock events in the 667 subsequent combustion cycles. The simulation results indicated that the dimension of the 668 valves and the hydrogen flow rate delivered by the injectors were not sufficiently large as to 669 assure that all the injected hydrogen enters the cylinders. The conclusion is that although the 670 adaptation of gasoline engines to run on hydrogen is obviously feasible, a dedicated design is 671 highly recommended when the engine will be fueled with hydrogen in order to avoid the 672 problems associated to abnormal combustion phenomena.

673

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675

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