CFD Analysis of Hydrogen Injection Pressure and Valve Profile Law Effects on Backfire and Pre-ignition Phenomena in Hydrogen-Diesel Dual Fuel Engine

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Abstract

This paper focuses on optimizing the hydrogen TMI (timed manifold injection) system through valve lift law and hydrogen injection parameters (pressure, injection inclination and timing) in order to prevent backfire phenomena and improve the volumetric efficiency and mixture formation quality of a dual fuel diesel engine operating at high load and high hydrogen energy share. This was achieved through a numerical simulation using CFD code ANSYS Fluent, developed for a single cylinder hydrogen-diesel dual

21 fuel engine, at constant engine speed of 1500 rpm, 90% of load and 42.5% hydrogen
22 energy share. The developed tool was validated using experimental data. As a results, the
23 operating conditions of maximum valve lift=10.60 mm and inlet valve closing=30 °CA
24 ABDC (MVL10 IVC30) prevent the engine from backfire and pre-ignition, and ensure a
25 high volumetric efficiency. Moreover, a hydrogen start of injection of 60 °CA ATDC
26 (HSOI60) is appropriate to provide a pre-cooling effect and thus, reduce the pre-ignition
27 sources and helps to quench any hot residual combustion products. While, the hydrogen
28 injection pressure of 2.7 bar and an inclination of 60°, stimulate a better quality of
29 hydrogen-air mixture. Afterwards, a comparison between combustion characteristics of
30 the optimized hydrogen-diesel dual fuel mode and the baseline (diesel mode) was
31 conducted. The result was, under dual fuel mode there is an increase in combustion
32 characteristics and NOx emissions as well as a decrease in CO2 emissions. For further
33 improvement of dual fuel mode, retarding diesel start of injection (DSOI) strategy was
34 used.

35 **Keywords:** Hydrogen-diesel dual fuel mode; Hydrogen TMI system; Hydrogen injection
36 parameters; valve lift law; CFD Analysis.

37

38   **1. Introduction**

39   Renewable hydrogen while used as fuel can help to overcome both fossil fuel depletion
40   and air pollution [1]. Indeed, hydrogen has very attractive combustion properties such as
41   high diffusivity, high flame speed and wide flammability range. These last are very
42   helpful to improve energetic and environmental engine performances. However,
43   abnormal combustion such as backfire [2,3], pre-ignition [4,5], and knock phenomenon
44   [3,4] can occur while using hydrogen in internal combustion engine. The backfire or pre-
45   ignition decreases the power output of an engine [1,6]. Moreover, the rise of the intake
46   manifold pressure resulting from backfire and pre-ignition is susceptible to harm the
47   intake system [7]. To prevent backfire, eliminating ignition source in contact with
48   hydrogen-air mixture in the intake manifold can be used. In the literature, several
49   solutions have been proposed to achieve this condition, such as (i) decreasing the overlap
50   period, (ii) retarding the timing of the inlet valve opening (iii) using leaner mixtures, (iv)
51   implementing exhaust gas recirculation and (v) intake air cooling systems [8-10]. On the
52   other hand, pre-ignition phenomena produce an increased chemical heat release rate, that
53   lead to a rapid pressure rise, acoustic oscillation and higher surface temperature. The later
54   can further advance the start of combustion, which in turn leads to a runaway effect, and
55   if left unchecked will lead to engine failure [11]. According to Verhelst et al. [7], the
56   presence of pre-ignition in internal combustion engine causes the symmetrical phasing of
57   the in-cylinder pressure, which leads to a drop of the indicated mean effective pressure

(IMEP) to almost zero. For hydrogen engines, pre-ignition is more pronounced when the hydrogen-air mixture is near the stoichiometric condition [7], and this limits the equivalence ratio for this kind of engines [11]. Pre-ignition is the result of various conditions such as an increase in the engine speed and load [7], an increase in the inlet pressure or inlet temperature and an increase in the compression ratio [11]. Numerous studies have been done to overcome pre-ignition in internal combustion engine and several strategies have been proposed to achieve this goal [9-12] among which, a use of an intake charge cooling system; a cold spark plugs and aged sodium filled valve [10] or the implementation of a variable valve timing strategy for effective scavenging of exhaust residual. The control of ignition advance and design of appropriate hydrogen induction system were also used to overcome pre-ignition [7,11]. Das et al. [12] designed a hydrogen timed manifold induction system that helps to pre-cool the charge, which leads to quench and dilute any residual combustion product that could be present in the compression space near top dead center (TDC). Thus, hydrogen induction methods can play a critical role in the development of a practical hydrogen engine [12]. In fact, with a specific design, hydrogen induction system can prevent abnormal combustion such as backfire and pre-ignition [10] and can also allow an ultra-lean combustion regime to be achieved with high volumetric efficiency, high thermal efficiency and lower NO_x emissions [10]. In practical, there are five techniques to introduce hydrogen in internal combustion engines; Carburation, Continuous Manifold Injection (CMI), Timed

78   Manifold Injection (TMI), Low Pressure Direct Injection (LPDI) and High Pressure
79   Direct Injection (HPDI) [1,10,12]. The first method is the simplest technique because it
80   does not require a major modification in the existing engine [10] and ensures a
81   homogeneous hydrogen-air mixture [4]. However, the carburation increases the risk of
82   backfire in hydrogen internal combustion engine [10] and reduced volumetric efficiency
83   and power outlet of the engine since the gas replaces some amount of intake air [4]. The
84   same problems are encountered in CMI. However using hydrogen direct injection
85   prevents pre-ignition and backfire [1,12] and induce higher volumetric efficiency
86   compared to other techniques [13]. But it requires an injector that could resist to higher
87   combustion temperature and prevent corrosion. Furthermore, a specific design of the
88   injector is necessary to ensure a better lubrication between the injector moving parts [1].
89   Another problem with direct injection is that the time allowed for mixing of hydrogen
90   and air after injection is very short [12] and this affects the combustion efficiency.

91   The fourth technique which is TMI is the most efficient technique to introduce the
92   hydrogen in the internal combustion engine. Indeed, an appropriately designed TMI
93   system can eliminate undesirable combustion phenomena such as backfire and pre-
94   ignition, increase engine performance and decrease pollutants emission levels [1,5,12,14].
95   Moreover, this technique does not require any radical modifications in the existing
96   system [14], and it has the capacity to start fuel delivery at a timing position sometimes
97   after the beginning of intake stroke [5]. Consequently, the TMI embodies the advantages

98 of direct injection technique and carburetor one i.e. it eliminates both pre-ignition and
99 backfire phenomena and ensures a homogenous hydrogen air mixture in the combustion
100 chamber.

101 For engines implemented with TMI system, hydrogen injection parameters such as the
102 injection pressure and timing, injection position, injection nozzle area (diameter), and
103 injector inclination, have a significant effect on combustion performance, emissions and
104 abnormal combustion [15,16]. Through the literature, different studies have been
105 performed to identify the effect of these parameters on engine performances. Wang et al.
106 [16] have established a 3D simulation model for a port fuel injection hydrogen internal
107 combustion engine using AVL Fire software to investigate the quality of the hydrogen air
108 mixture formation and the combustion characteristics of the hydrogen fueled engine
109 under different hydrogen injection timings, nozzle hole positions and nozzle hole
110 diameter. According to their results, an optimum choice of the hydrogen injection
111 parameters is required to improve the uniformity of the hydrogen-air mixing in the
112 cylinder and the combustion characteristics. Chintala et al. [17] have used a CFD
113 software to investigate the effect of the gas injector angle and location on gas (CNG or
114 H_2) - air mixture formation, backfiring and thermal efficiency at different injection
115 pressure and engine speed. They observed that the mixture velocity and engine speed are
116 the key parameters for the optimization of the critical distance of the gas injector between
117 the injector mounting point and inlet valve axis in intake manifold of a dual-fuel engine.

118 According to their results, the critical distance decreases with increasing engine speed at
119 a constant injection pressure while it increases with increasing injection pressure at a
120 constant engine speed. They also conclude that the gas injector for CNG and H₂ fuel
121 needs to be mounted on intake manifold within the critical distance in order to avoid fuel
122 accumulation and backfiring. In addition, they observed that mixing rate of gaseous fuel
123 with air increases with increasing gas injection pressure. On the other hand, Liu et al. [6]
124 numerically investigated the effect of injection timing on hydrogen-air mixture formation
125 at different engine speeds and equivalence ratio of a hydrogen internal combustion
126 engine. They conclude that the backfire event is mainly related to the concentration of
127 hydrogen residual at the intake ports in the manifold injection, thus, the leaner the
128 concentration of the residual, the lower possibility of the backfire event. Moreover,
129 according to this research, a limited injection end timing is required to prevent backfiring
130 risk. Cheng et al. [18] evaluated the effect of hydrogen injection timing on mixture
131 formation, power output, thermal efficiency, cycle-to-cycle variation and backfiring at
132 different engine speeds and loads. They could evaluate an optimized hydrogen injection
133 timing for various engine speeds and loads. Yang et al. [19] studied the effect of natural
134 gas injection timing on the performance and emission of a turbocharged dual fuel
135 common rail engine under different pilot injection timing and pressure at low load. They
136 reported that retarded natural gas injection timing could achieve a stratified-like air–fuel
137 mixture in the cylinder under different pilot injection conditions. This provided a method

138 to improve combustion performance and exhaust emissions at low loads. Saravanan et al.
139 [20] experimentally studied the effects of the hydrogen injection timing and duration on
140 performance and emissions of a DI diesel engine at various loads. They could define
141 optimum operating conditions for which an increased thermal efficiency and reduced
142 azote oxide (NO_x), carbon monoxide (CO), carbon dioxide (CO₂) and unburned
143 hydrocarbon (HC) emissions were observed. Yang et al. [21] numerically investigated the
144 effects of three hydrogen injection modes and nozzle diameter on mixture formation and
145 combustion performance at different equivalence ratio and engine speed in a hydrogen
146 fueled spark ignition engine with port fuel injection. They found that using spaced dual
147 injection improves hydrogen-air mixture uniformity and combustion velocity, increases
148 NO_x emission and reduces the probability of backfire. They also reported that the
149 uniformity coefficient decreases gradually and the indicated power and indicated thermal
150 efficiency increased first and then decreased with increasing the nozzle diameter.
151 Chintala et al. [22] numerically investigated the effect of water injection on the maximum
152 hydrogen share limited by mixture auto-ignition and knocking problem in hydrogen
153 based dual fuel engine. They observed that it could be increased from 18.8% with
154 conventional dual fuel engine to 60.7% with water injection at 100% full load. Salvi et al.
155 [23] experimentally studied the effect of volumetric compression ratio, spark timing and
156 exhaust gas recirculation (EGR) on engine performance, emission characteristics and
157 backfire occurrence in a hydrogen fuelled spark ignition engine. They found that with an

158 optimum choice of compression ratio, EGR and spark timing, the thermal efficiency and
159 NO_x emission are improved and the risk of backfire occurrence is reduced. Tsujimura et
160 al. [24] modified a diesel engine to work on direct injection hydrogen engine with EGR
161 and supercharging. They experimentally studied the effect of various operating
162 parameters such as: hydrogen injection timing, pressure injection, spark ignition timing,
163 intake oxygen concentration and equivalence ratio, on NO_x emission and thermal
164 efficiency. Moreover, they studied the effect of intake and exhaust valve closing timing.
165 They found a significant decrease of NO_x emission (100 ppm) and increase of indicated
166 thermal efficiency (+50%) for optimal values of the previous operating parameters.
167 Dhyani et al. [25] experimentally analyzed the effect of knocking on backfire in a multi-
168 cylinder hydrogen engine. They investigated its control by varying spark timing and
169 hydrogen injection timing. They found that knocking combustion can be linked with
170 backfire, as probability of backfire occurrence decreases with the reduction in knocking
171 risk. In addition, they reported that retarded spark timing and delayed hydrogen injection
172 timing reduce the risk of backfire occurrence. Dhyani et al. examined, in another
173 experimental study [26], the effect of cooled EGR and water injection strategies on the
174 possibility of backfire occurrence, NO_x emission and performance of a multi-cylinder
175 hydrogen engine. They found a reduction of backfire occurrence probability and NO_x
176 emissions using both strategies without affecting brake thermal efficiency. They also

177 reported that water injection strategy is more efficient as compared to cooled EGR to
178 control backfire occurrence with ultra-low (near zero) NO_x emission.

179 Other parameters, like valve lift law, inlet valve close (IVC) timing, inlet valve open
180 (IVO) timing and maximum valve lift, may also have a great importance in the control of
181 abnormal combustion, volumetric efficiency, engine performance and exhaust emissions
182 of an engine equipped with TMI system. Some researchers focused on these parameters
183 to improve engine efficiency. Jia et al. [27] numerically investigated the effect of IVC
184 timing and Start of Injection (SOI) on combustion performance and emissions of a diesel
185 premixed charge compression ignition (PCCI) engine. They found out that IVC timing
186 and SOI affect the ignition timing, combustion temperature and effective compression
187 ratio. They concluded that adjusting IVC and SOI can optimize engine emissions, fuel
188 economy and ringing intensity. Moreover, Zhang et al. [28] experimentally evaluated the
189 influence of the late inlet valve closing (LIVC) and the rebreathing valve strategies of
190 inlet and exhaust valve (second opening of inlet/exhaust valves) on combustion
191 characteristics and exhaust emissions of a diesel engine at low loads. They have
192 suggested using the rebreathing valve strategies at lower engine loads, and the standard
193 and late IVC strategies at higher loads to improve emission and combustion
194 characteristics. Xu et al. [29] used an electromagnetic inlet valve train (EMIV) to regulate
195 the inlet valve control parameters in order to improve the performance of a gasoline
196 engine. They could analyze the influence of inlet valve train on the intake charging,

197 power consumption and pumping loss of a gasoline engine. They found out that with an
198 optimized valve law, the intake charging can be improved and power consumption
199 reduced, therefore they conclude that the application of EMIV is an effective system to
200 improve the performance of the engine. Li et al. [30] numerically investigated the
201 influence of intake backflow on the in-cylinder situation and auto ignition of a gasoline
202 engine. They observed a decrease of the mean temperature with increasing the intake
203 backflow. Moreover, they found out that the auto ignition timing first delayed, then,
204 advanced as the intake backflow increased. Çinar et al. [31] experimentally studied the
205 impact of the valve lift on in-cylinder pressure, heat release rate, engine performance and
206 exhaust emissions of a Homogeneous Charge Compression Ignition (HCCI) gasoline
207 engine. They observed an improvement in engine performance, reduction in exhaust
208 emissions with extended range of engine operation without knock when using a low valve
209 lift. Finally, Verhelst et al. [32] while investigating the impact of variable valve timing on
210 power, emissions and backfire of a bi-fuel hydrogen/gasoline engine, found that variable
211 valve timing is a way to improve power output, reduce NO_x emission and avoid
212 backfiring risk.

213 Through the literature, it can be seen that few researches focus simultaneously on the
214 effect of injection parameters and valve lift law on backfiring, intake charging and
215 mixture formation of a dual fuel hydrogen-diesel engine. Therefore, there is a crucial
216 need to conduct the related study. The aim of this work is to optimize a hydrogen TMI

217 system through valve lift law (maximum valve lift and IVC timing) and hydrogen
218 injection parameters (pressure, inclination and injection timing) in order to prevent
219 backfire phenomena, improve volumetric efficiency and mixture formation quality of a
220 dual-fuel diesel engine. To achieve this goal, a numerical simulation using CFD code
221 ANSYS Fluent was developed and validated with experimental data.

222

223 **2. Numerical approach**

224 **2. 1. Geometric configuration and mesh generation**

225 The engine simulated is a Lister Petter TS1 mono cylinder, four strokes direct injection
226 diesel engine with a displacement of 0.63 liters. The engine and diesel fuel injector
227 characteristics are given in Table 1. For dual fuel mode, hydrogen is injected in the intake
228 manifold. The inlet and exhaust duct geometry with gas injector position is shown in Fig.
229 1. The distance between the hydrogen injector and intake valve ($P_0 - P_1$) is set to 150
230 (mm), the hydrogen injector prototype chosen for this study is DYMCO Corp/GISM-
231 i1000, the characteristics of the injector are summarized in Table 2.

232 Because the number of cases to investigate is significant, the 3D simulation requires an
233 excessive calculation time. For this reason, 2D approach has been first adopted to the
234 choice of intake valve law (MVL and IVC). Then, the results of this approach have been

235 compared to 3D ones and validated using experimental data [33]. Afterwards, 3D
236 simulation approach was used to select the hydrogen injector parameters (hydrogen start
237 of injection, hydrogen injection pressure and hydrogen injector inclination). Finally, these
238 results were used for the full cycle simulation.

239 For 2D and 3D geometry, the computational domain was divided into sub-volume (multi-
240 block methods). In 2D geometry, the structured mesh is used with a quadrilaterals cell
241 shape for the totally sub-volume. In 3D geometry, the structured mesh is used with a
242 hexahedral cell shape for all sub-volume except for the intake port, exhaust port and the
243 contact region between injector and intake manifold that have an unstructured mesh with
244 a tetrahedral cell shape as it is shown in Fig. 2.

245 The main challenge to simulate a three-dimensional internal combustion engine is the
246 dynamic mesh due to moving boundaries such as cylinder, valves and piston head [34].
247 Three methods exist to update the mesh of a moving boundary project: smoothing, re-
248 meshing and layering [35]. In our case the layering method has been adopted, Fig. 2
249 shows the engine mesh at TDC and BDC. The intake and exhaust valve dynamic mesh is
250 assumed by a valve profile using a user defined function (UDF). Fig. 3 shows the valve
251 lifts profiles for various IVC and MVL; the law of valve lift is given by following
252 equation [33]:

$$l_v = \frac{MVL}{2} \left[1 - \cos \left(\frac{2\pi\theta + C + AO}{AO + RC + 180} \right) \right]$$

253 MVL : Maximum Valve Lift (mm)

254 θ : Crank Angle Degree (°CA)

255 AO: Advance Opening (°CA)

256 RC: Retard Closing (°CA)

257 C: Constant (=180 (°CA) for exhaust and 360 (°CA) for intake).

258 **2. 2. Numerical modeling procedure and validation**

259 The CFD code used in this study is ANSYS Fluent v16.0. Pressure based solver and
 260 coupled scheme for pressure-velocity coupling were used. The second order implicit
 261 scheme was chosen for temporal discretization. For spatial discretization, the second
 262 order scheme was chosen for pressure and second order upwind for density, momentum
 263 and turbulent kinetic energy. In this work, the residual is set to 10^{-6} . The energy equation
 264 is solved for all cases to calculate the temperature evolution. In order to relate the
 265 pressure with temperature and density the state equation is also used, the charge (air,
 266 mixing gas) was assumed as ideal gas [21, 38]. The turbulent flow was modeled using the
 267 k- ϵ RNG model [40, 41]. The "discrete phase" model available in ANSYS Fluent makes
 268 it possible to simulate the two-phase jet in the combustion chamber. This model uses
 269 several sub-models that can define; droplet size, velocity distribution, sprays angle,

270 particle trajectory, spray breakup, collision, coalescence and particle evaporation. For
271 breakup of the jet, the wave model of Reitz was used. This model considers that the
272 breakup of the liquid jet is due to the relative velocity difference between the liquid phase
273 and the gaseous phase, this model is the most popular used for high injection pressure
274 [38,39]. The combustion model chosen for this study is laminar finite rate/eddy
275 dissipation scheme [22,39,40], with one reaction for diesel and one reaction for hydrogen.
276 The reaction rate is equal to the minimum of the laminar finite rate or eddy dissipation
277 scheme. For the ignition delay, the Hardenberg & Hase (H&H) correlation is chosen [40,
278 42]. The ignition is ensured by the diesel fuel in dual fuel engine mode; therefore, the
279 ignition delay correlation was applied to the diesel fuel. NO_x considered in this study are
280 thermal and prompt [36, 42]. The extended Zeldovich mechanism is used for thermal
281 NO_x formation and Fenimore mechanism for prompt NO_x [36].

282 Boundary conditions chosen for this study are the atmospheric pressure for air inlet and
283 gaseous mixture outlet, and a fixed temperature for inlet and outlet. The values are taken
284 from experimental measurements. For hydrogen inlet boundary condition, mass flow rate
285 type was selected and applied at the inlet area of the injector (fig. 2). For this, an UDF is
286 developed to introduce the mass flow rate as a function of crank angle for each
287 corresponding hydrogen injection pressure at a fixed energy share and engine speed,
288 taking in consideration the opening and closing time and the injection duration.

289 The wall heat transfer losses are estimated by Hohenberg correlation. To introduce the
290 empirical heat transfer correlation, a user defined function is developed and implemented
291 successfully. The Hohenberg model performs best comparing with the others correlations
292 [41]. Two full cycles were realized in a single simulation. Each simulation was initiated
293 at Top Dead Center (TDC) during the intake stroke. For the first cycle, the hybrid
294 initialization provided by ANSYS Fluent is used. In the second cycle, the initial values of
295 the parameters are obtained from the results of the first cycle. This second cycle is the
296 cycle considered in all our investigations.

297 **2.3. Grid sensitivity study**

298 Mesh generation is a critical step to build multi-dimensional CFD engine model because
299 the mesh quality has a significant impact on the numerical stability of the CFD solver and
300 the mesh density which can affect the simulation results [36]. Several grids were created
301 and examined. Table 3 shows the number of cells at TDC and BDC.

302 Fig. 4 (a) shows the in-cylinder mass evolution under different mesh refinement. It can be
303 seen that no significant difference was observed with mesh refinement. The maximum
304 deviation is less than 0.25 % in the 2D approach and less than 0.06 % in the 3D
305 simulation. Considering both computational time and the quality of results, case 7 is
306 chosen for the 2D mesh and the case 5 for the 3D simulation (Table 3).

307 **2.4. Time step sensitivity study**

308 For the study of the time step sensitivity, the in-cylinder mass evolution is used in such a
309 way that when the two valves are closed, the mass in the combustion chamber is constant.
310 Fig. 4 (b) shows the evolution of in-cylinder mass for different crank angle step size in
311 cases of 2D and 3D simulations. For the 2D simulation, 0.1 and 0.05 ($^{\circ}\text{CA}$) verified mass
312 conservation, therefore, the time step chosen is 0.05 ($^{\circ}\text{CA}$). For 3D simulation 0.1 ($^{\circ}\text{CA}$)
313 time steps is chosen. These choices take in consideration simulation time.

314 **2.5. Comparison between 2D and 3D simulations**

315 For 2D approach, the geometry was modified in order to verify the volumetric
316 compression ratio, a constant depth was introduced, the bowl was removed and the squish
317 clearance was adjusted accordingly (see Fig.2).

318 Fig. 5 shows the in-cylinder volume and mass profiles with the 2D and 3D simulations.
319 For the in-cylinder volume profiles, the two curves are almost similar. However, there is
320 a slight difference during intake stroke that can be caused essentially by the depth value
321 of valve. For the in-cylinder mass profiles, a small difference exists between the 2D and
322 3D simulations; this difference is probably due to the inlet valve reference flow area and
323 discharge coefficient. The error in in-cylinder mass is less than 4.0 %. Therefore, it can
324 be concluded that the 2D approach reproduces the 3D simulations.

325 **2.6. 2D - 3D validation**

Fig. 6 shows the comparison of in-cylinder pressure profiles of a cold flow between the experimental results [33] and 2D and 3D numerical results. The numerical and experimental results are in good agreement. However, a slight difference was noticed, and the error in the maximum pressure is 0.88 (bar) (1.68%) in 3D simulation and 1.75 (bar) (3.6%) in 2D simulation. The 2D and 3D simulations are therefore validated.

In this study, first, the intake valve lift law (MVL and IVC) is optimized using 2D approach. The results of the optimal intake valve lift law are then confirmed with a 3D simulation. Then, hydrogen injector parameters (HSOI, hydrogen injection pressure and injector inclination angle) are optimized with 3D simulation. Afterwards, the engine performance of both diesel and dual fuel modes are analyzed, and finally the diesel start of injection (DSOI) is optimized for dual fuel mode. The method of step by step is adopted to optimize each considered parameter. When the effect of one parameters on dual-fuel diesel engine operating mode is studied, the others parameters were kept at a fixed value, then, the fixed value is replaced by the optimal value for each investigated parameter successively.

3. Results and discussion

3. 1. Valve lift law

344 The selection of the valve lift law has been done by analyzing the in-cylinder mass,
345 backflow mass, maximum pressure and aspiration work using a 2D approach for the cold
346 airflow case. To achieve this goal, three maximum valve lift (MVL10.6, MVL8.0 and
347 MVL6.0 mm) combined with three intake valve closing (IVC70, IVC50 and IVC30 °CA
348 ABDC) for seven engine speeds (from 1000 to 2500 rpm), were examined. This
349 represents 63 cases.

350 The in-cylinder mass is the value of mass evolution inside the cylinder after the intake
351 valve close. Fig. 7 (a) shows the effect of MVL and IVC on the in-cylinder mass for
352 different engine speeds. At early IVC (IVC30), the in-cylinder mass decreases with speed
353 for all cases. While at IVC50, the variation of the in-cylinder mass still slightly
354 decreasing with speed for MVL6.00 however, it was almost negligible for the other cases.
355 At late IVC (IVC70), the in-cylinder mass increases lightly with the speed for all MVL
356 investigated. These results can be explained by the fact that the time allowed to the
357 airflow is more significant in late IVC at high speeds. Jiangtao Xu et al [29] indicated that
358 the volumetric efficiency increases for early IVC at low speeds and decreases at high
359 speeds. Therefore, for late IVC, the volumetric efficiency decreases at low speeds and
360 increases at high speeds. Our results are in concordance with those finding.

361 For early IVC, the intake charge increases with the increase of MVL, especially at high
362 speeds. On the other hand, for late IVC, the intake charge decreases when increasing the

363 MVL. These results are in agreement with those find by J. Xu et al. [29] in case of early
364 IVC, and Clenci et al. [37] in case of late IVC.

365 The backflow mass is the difference between the maximum in-cylinder mass during the
366 intake stroke and the in-cylinder mass after the intake valve close. According to Fig. 7
367 (b), the backflow mass decreases almost in all cases with increasing the engine speed for
368 all valve lift law, and it decreases with decreasing the MVL. This can be attributed to the
369 fact that the airflow inertia increases with increasing engine speed which can justify the
370 decrease of backflow mass with engine speed. The effect of IVC on the backflow mass is
371 more significant than the effect of MVL. It can be noted that the backflow mass is
372 significant at ICV70, and very low (insignificant) at IVC30. This is because late IVC
373 could help to expel a portion of in-cylinder charge in the intake port.

374 The aspiration work is a representative of pumping losses; it was calculated through the
375 integral of the in-cylinder pressure from IVO to IVC. Fig. 7 (c) shows the effect of MVL
376 and IVC on the aspiration work for different engine speeds. As seen in Fig. 7 (c),
377 regardless of the IVC, decreasing MVL increases the aspiration work. This can be
378 explained by the fact that lowering MVL decreases the effective flow area. Moreover,
379 increasing engine speed also increases the pumping losses. Similar results were found by
380 J. Xu et al [29].

Fig. 7 (d) shows the effect of IVC and MVL on the maximum pressure (at TDC in case of cold airflow) for various engine speeds. In almost all cases, at Early IVC (IVC30), the in-cylinder peak pressure decreases with speed, except for MVL10.6. However, for all MVL, the in-cylinder peak pressure increases slightly with the speed at IVC50, while it increases considerably at Late IVC (IVC70). Therefore, we can consider that, for most cases, Early IVC increases the in-cylinder peak pressure, and Late IVC decreases the in-cylinder peak pressure. This is in concordance with the results of Jia et al [27] and Zhang et al [28]. Moreover, for Early IVC, the in-cylinder peak pressure increases with increasing MVL, in particular at high speeds, which is in agreement with Clenci et al [37] findings. Our results show that adjusting the IVC and varying the MVL can be a way to control the effective compression ratio. Consequently, as the valve lift law changes, it is recommended to adjust the diesel start of injection, to obtain a better thermal efficiency and thus lower fuel consumption, lower pressure rise rate and reduced exhaust emissions [27]. Indeed, according to Jia et al [27], the ignition timing is controlled by IVC timing, the reduced ignition delay result in advancing the start of combustion, which increases the pressure rise rate and NO_x emissions.

Based on previous results, the MVL10 IVC30 (MVL = 10.60 mm and IVC30 °CA ABDC) valve lift law prevents the engine from backfire (backflow very low), allows high volumetric efficiency, high maximum pressure and low pumping losses. Therefore, for the upcoming study, the valve lift law with MVL10 IVC30 is chosen.

401 To confirm if the valve lift law MVL10 IVC30 chosen with 2D simulations in case of
402 cold airflow, was also valid for the 3D simulations at engine run conditions chosen for
403 this study which are fixed to 90% load, 1500 rpm and 42.5% hydrogen energy share. The
404 existing and recommended valve lift law (IVC70 and IVC30) with Maximum Valve
405 Lift=10.60 mm was used to simulate the cylinder mass and backflow mass with 3D
406 approach for various engine speed, then the results were compared with the 2D
407 simulations ones. Fig. 8 shows the profile of in-cylinder mass and backflow mass for the
408 valve lift law MVL10 IVC70 and MVL10 IVC30 at 90% of load and 42.5% hydrogen
409 energy share using 3D simulation. According to Fig. 8, the 3D results confirm the 2D
410 ones, except for engine speed greater than 2000 rpm. Indeed, unlike the 2D simulations,
411 in 3D ones, the in-cylinder mass is greater in case of IVC70 compared to IVC30 for the
412 engine speed greater than 2000 rpm. However, the backflow mass is very low in case of
413 IV30 for all the engine speed range. This has no effect on the choice of valve lift for this
414 study. This is because, except for engine speed higher than 2000 rpm, the IVC30 case
415 ensures a greater intake charge and there is negligible backflow mass, which prevent the
416 engine from backfiring. Therefore, it can be concluded that 3D simulations confirm the
417 2D approach at speeds lower than 2000 rpm. In fact, as it was noted by Xu et al [29], the
418 volumetric efficiency increases with the late IVC at high engine speed. On the other
419 hand, it increases with the Early IVC at low engine speed. Our results for 3D simulation
420 are in good agreement with those findings.

421 **3. 2. Hydrogen injector parameters**

422 The aim of this section is to optimize hydrogen injection parameters such as the injection
423 pressure, injector inclination and start of injection. The engine operation conditions were
424 fixed to 90% load, 1500 rpm with hydrogen energy share of 42.5%.

425 **3. 2. 1. Hydrogen injection pressure**

426 To select the hydrogen injection pressure, six hydrogen injection pressures (1.2, 1.7, 2.2,
427 2.7, 3.7 and 4.5 bar) were examined for the existing and recommended valve lift law and
428 two hydrogen start of injection, therefore, the cases IVC70 HSOI60, IVC30-HSOI60 and
429 IVC30-HSOI43 were considered. To achieve this goal, the hydrogen mass fraction
430 distribution in the air before the intake valve closing was quantified to identify the risk of
431 the flammability of hydrogen in the air, and thus the risk of backfiring for each case.

432 The injector characteristics curve shown in Fig. 9 is used to determine the hydrogen mass
433 flow and the injection duration corresponding to the provided hydrogen injection
434 pressure.

435 Fig. 10 shows the profiles of the average hydrogen mass fraction in the intake manifold
436 volume for the valve lift law IVC70-HSOI60, IVC30-HSOI43 and IVC30-HSOI60. In the
437 case IVC70-HSOI60, hydrogen-air mixture is repressed to the intake port for all
438 hydrogen injection pressures before the intake valve closing as seen in Fig. 10 (a). This

439 means that the mass fraction of hydrogen after intake valve closing is significant and
440 thus, the risk of backfiring is high.

441 For IVC30, it can be seen from Fig. 10 (b) and (c) that for hydrogen injection pressure of
442 1.2 bar at both HSOI43 and HSOI60 and hydrogen injection pressure of 1.7 bar at
443 HSOI60, high hydrogen fractions were accumulated in the intake manifold at the intake
444 valve closing. This can be attributed to the high injection duration and the low mass flow
445 rate (see Fig. 9). Which means that, after hydrogen injection ends, the time available for
446 hydrogen to reach the combustion chamber is smaller than the required time [17]. As a
447 result, hydrogen injection pressure of 1.7 bar for HSOI43 and 1.2 bar for both HSOI43
448 and HSOI60 cannot be used due to the high risk of backfiring.

449 In the case IVC30-HSOI43, the hydrogen mass fraction is almost zero at the intake
450 manifold after intake valve closing for hydrogen injection pressure of 2.2, 2.7, 3.7 and 4.5
451 bar, except for hydrogen injection pressure of 1.7 bar, which means that the hydrogen
452 does not completely reach the combustion chamber. In the case IVC30-HSOI60, the
453 hydrogen mass fraction is also almost zero in intake manifold for the hydrogen injection
454 pressure of 2.7, 3.7 and 4.5 bar, but it is not the case for hydrogen injection pressure of
455 2.2 bar. For those two cases, the hydrogen fraction is too low; therefore, the occurrence of
456 pre-ignition cannot be verified. Consequently, various engine speeds were examined to
457 verify the backfiring risk at these cases.

Fig. 11 shows the distributions of hydrogen mass fraction for different engine speeds at hydrogen injection pressure of 1.7 bar in case IVC30-HSOI43, and 2.2 bar in case IVC30-HSOI60 at intake valve closing. The low flammability limit is $\varphi = 0.1$ (fuel-air equivalence ratio) [7], which corresponds to 0.3% mass fraction in hydrogen-air mixture. According to Fig. 11, in the case HSOI43 with $P = 1.7$ bar, there is a little accumulation of hydrogen in intake port and the fraction reaches the flammability limit only in specific zones at 1000, 1500 and 2500 rpm. In the case HSOI60 with $P = 2.2$ bar, the accumulation of hydrogen in intake port is significant and the fraction reaches the flammability limit therefore the risk of backfire is greater.

As a result, for a fixed injection position and induced hydrogen mass per cycle, the possible hydrogen injection pressures to be used without having the accumulation of hydrogen in intake port and thus the backfiring risk are: 2.2, 2.7, 3.7 and 4.5 bar for IVC30 HSOI43 °CA ATDC and 2.7, 3.7 and 4.5 bar for IVC30-HSOI60 °CA ATDC.

3. 2. 2. Hydrogen start of injection (HSOI)

Fig. 12 shows the profiles of the average in-cylinder temperature as function of the hydrogen injection pressure at 90% load and 1500 rpm for two hydrogen start of injection (HSOI43 and HSOI60 °CA ATDC) and a fixed total injected hydrogen mass (42.5% energy share). Two hydrogen mass fractions have been considered for this study. The first one is 0.001% represented in Fig. 12 (a) which shows that the hydrogen begin

reaching the combustion chamber. The second value is 0.3% (Fig. 12 (b)) which corresponds to the lower flammability limit of the hydrogen-air mixture. Fig. 12 (c) is an example (HSOI43 and 2.7 bar hydrogen injection pressure) which explains how the in-cylinder temperature corresponding to a given in-cylinder hydrogen mass fraction during the intake stroke, is determined. Each point in fig. 12 (a) and (b) is obtained basing on a figure similar to Fig. 12 (c). According to Fig. 12 (a) and (b), the in-cylinder temperature increases with increasing hydrogen injection pressure. This is because hydrogen velocity increases proportionally to the injection pressure which reduces the time taken to reach the combustion chamber. Moreover, the in-cylinder temperature for a constant hydrogen mass fraction is higher at HSOI43 compared to HSOI60. Therefore, HSOI60 is more able to provide a pre-cooling effect and thus, decrease the chance of pre-ignition sources presence and helps to quench any hot residual combustion products. This leads to prevent the engine from backfire and pre-ignition risk [6,8,14]. Thus, for the remaining study, the HSOI60 was chosen.

3. 2. 3. Effect of hydrogen injection pressure and hydrogen injector inclination on mixture quality

A heterogeneous mixture can contribute to deteriorate the engine performance [10,17], and increasing pollutant emissions. It can also increase the risk of pre-ignition and knock. In this section, mixture quality is examined when varying hydrogen injection pressure

496 and hydrogen injector inclination. Fig. 13 shows the hydrogen mass fraction distribution
497 for two hydrogen injector inclinations (45° and 60°) combined with three hydrogen
498 injection pressures (2.7, 3.7 and 4.5 bar), at a constant engine speed of 1500 rpm and
499 various crank angle positions.

500 As already seen in Fig. 10 (b), hydrogen injection ends at 175.6, 152.7 and 143.2 °CA
501 ATDC for hydrogen injection pressure of 2.7, 3.7 and 4.5 bar, respectively. The hydrogen
502 injection finished early before IVC for hydrogen injection pressure of 3.7 and 4.5. This
503 means that a considerable amount of air was introduced in intake manifold without
504 mixing with hydrogen (see Fig. 13 (a)). This is explained by the fact that increasing
505 hydrogen injection pressure, increases mass flow rate and thus decreases the injection
506 duration, as already seen in Fig. 9. When the injection pressure is greater than 2.7 bar (3.7
507 and 4.5 bar), the time available for hydrogen to reach the combustion chamber is more
508 significant compared to the time taken after the end of hydrogen injection. On the other
509 hand, according to Fig. 13 (b), during the end of compression stroke, 150 and 165 °CA
510 ABDC, the hydrogen concentrations are high at the exhaust valve sideway and low at the
511 intake valve sideway for injection pressures 3.7 and 4.5 bar. In addition, the hydrogen
512 injection pressure 2.7 bar was able to enhance the hydrogen-air mixture quality compared
513 to the other tested pressures. This is clearly visible at the 150 and 165 ° CA ABDC as
514 shown in Fig. 13 (b).

515 The inclination of 60° gives a better mixing quality of hydrogen-air mixture compared to
516 that of 45° . This was observed at the compression stroke (Fig. 13 (b)), where the
517 concentration of hydrogen is higher at exhaust valve sideway and lower at intake valve
518 sideway for hydrogen injector inclination of 45° .

519 As results, the hydrogen injection pressure 2.7 bar and the injector inclination of 60°
520 allow a good homogeneity of hydrogen-air mixture.

521 **3. 3. Engine Performance**

522 Fig. 14 shows the engine combustion performances, such as in-cylinder pressure and
523 temperature, heat release rate, rate of pressure rise and the exhaust emissions of NO_x and
524 CO₂ of the standard diesel mode (D IVC70), and the optimized hydrogen-diesel dual fuel
525 mode (DF IVC30) for hydrogen injection pressure $p=2.7$ (bar), at an engine speed of
526 1500 rpm.

527 An increase of peak in-cylinder pressure, rate of pressure rise, in-cylinder temperature
528 and heat release rate with dual fuel mode, is observed from Fig. 14. This is due to the
529 higher burning velocity and diffusivity of hydrogen [2,13] that speeds up the initiation of
530 the premixed combustion and help to achieve the complete and almost instantaneous
531 combustion of the air-fuel mixture.

532 Moreover, the concentration of CO₂ emissions is lower in hydrogen-diesel dual fuel
533 engine compared to conventional diesel engine. This is due to the use of hydrogen which

534 is a free carbon fuel, and the improvement of the combustion efficiency with hydrogen
535 addition.

536 However, the NO_x specific emissions were higher with hydrogen-diesel dual fuel mode
537 compared to the conventional diesel engine in these operating conditions. The increase of
538 these emissions is mainly due to the rise of in-cylinder temperature [2,15] and high
539 residence time of the high temperature gases in the cylinder [43].

540 **3. 4. Effect of diesel SOI**

541 While investigating the hydrogen-diesel dual fuel engine combustion characteristics, it is
542 crucial to investigate the diesel start of injection (DSOI) timing. Therefore, Fig. 15 shows
543 the effect of retarding DSOI by 0, 3, 5, 8, 10 and 12 °CA compared to baseline case, on
544 combustion characteristics and exhaust emissions of NO_x and CO_2 . It can be observed
545 from Fig. 15 that retarding DSOI to values higher than 8 °CA, decreases the peak in-
546 cylinder pressure, in-cylinder temperature and the rate of pressure rise. However, it has
547 not a great effect on the rate of heat release (HRR). A decrease of CO_2 emissions with
548 increasing DSOI delay was also observed. Furthermore, according to Fig. 15, NO_x
549 specific emissions decreased while retarding DSOI to values higher than 8 °CA. This is
550 because decreasing the in-cylinder temperature helps to reduce thermal NO_x formation.

551

552 **4. Conclusion**

553 Numerical 2D and 3D dynamic simulations using CFD code ANSYS Fluent was
554 performed for a single cylinder hydrogen-diesel dual fuel engine. An attempt to optimize
555 the hydrogen TMI system through valve lift law (maximum valve lift and IVC timing)
556 and hydrogen injection parameters (pressure, inclination and injection timing) was
557 performed, in order to prevent the backfire phenomena, improve the volumetric
558 efficiency and the mixture formation quality of a hydrogen-diesel dual-fuel engine. The
559 following results were obtained:

- 560 1. The valve lift law MVL10.6 IVC30 (MVL=10.60 (mm) and IVC=30 (°CA
561 ABDC)) is the optimum choice because it reduces the risk of backfire and pre-
562 ignition while ensuring a high volumetric efficiency.
- 563 2. The HSOI60 (°CA ATDC) is able to provide a pre-cooling effect and thus, could
564 reduce the pre-ignition sources and helps to quench any hot residual combustion
565 product.
- 566 3. The hydrogen injection pressure of 2.7 (bar) and an inclination of 60° helps to
567 improve the quality of hydrogen-air mixture.
- 568 4. The optimized hydrogen-diesel dual fuel mode shows an increase of the peak in-
569 cylinder pressure, in-cylinder temperature, heat release rate, rate of pressure rise,

and NO_x specific emissions comparing to the diesel engine. However, a decrease of the concentration of CO₂ emissions was observed for the dual fuel mode.

5. For values of DSOI retard higher than 8 (°CA), the peak in-cylinder pressure, in-cylinder temperature, the rate of pressure rise and NO_x emissions are similar or lower for hydrogen-diesel dual fuel engine compared with diesel engine.

576   **Nomenclature**

577	ABDC	After Bottom Dead Center
578	ATDC	After Top Dead Center
579	BDC	Bottom Dead Center
580	BTDC	Before Top Dead Center
581	CA	Crank Angle
582	CFD	Computational Fluid Dynamics
583	CMI	Continuous Manifold Injection
584	CNG	Compressed Natural Gas
585	CO	Carbon Monoxide (%)
586	CO ₂	Carbon Dioxide (%)
587	D	Diesel engine
588	DF	Dual Fuel engine
589	DSOI	Diesel Start Of Injection (°CA)
590	EMIV	Electromagnetic Intake Valve Train
591	HC	Unburned Hydrocarbon

592	HSOI	Hydrogen Start Of Injection (°CA)
593	HSOI43	Hydrogen Start Of Injection at 43 (°CA)
594	HSOI60	Hydrogen Start Of Injection at 60 (°CA)
595	HRR	Heat Release Rate (J/ °CA)
596	IVC	Inlet Valve Closing (°CA)
597	IVC30	Intake valve is closed at 30 °CA ABDC
598	IVC50	Intake valve is closed at 50 °CA ABDC
599	IVC70	Intake valve is closed at 70 °CA ABDC
600	IVO	Intake Valve Open (°CA)
601	MVL	Maximum Valve Lift (mm)
602	NOx	oxides of nitrogen (ppm)
603	Rpm	Rotation per minutes
604	TDC	Top Dead Center
605	TMI	Timed Manifold Injection
606	SOI	Start Of Injection (°CA)
607	UDF	User Defined Function

608   Y_{H_2} , Y_{CO_2} ,   mass fraction of H_2 (%), CO_2 (%) respectively

609   Y_{NO_x} mass fraction of NO_x (ppm)

610   θ Crank Angle Degree ($^{\circ}CA$)

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738   **Table captions**

739   Table 1. Engine and diesel fuel injector characteristics

740   Table 2. Gas injector characteristics

741   Table 3. Number of Cells for tested meshes

742

743

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Table 1. Engine and diesel fuel injector characteristics

Description	Parameter value
type	Lister petter TS1
No. of cylinders	1
Displacement volume (cm ³)	630
Rated output (kw)	4.5 at 1500 rpm
Rated Speed (rpm)	1500
Bore × Stroke (mm)	95.3 × 88.9
Compression ratio	18.0 :1
Connecting rood length (mm)	165.3
Intake valve opening and closing	36 (°CA BTDC) , 69 (°CA ABDC)
Exhaust valve opening and closing	76 (°CA BTDC) and 32 (°CA ABDC)
Diesel start of injection	15 (°CA BTDC)
Injection pressure (bar)	250
Number of holes	4

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Table 2. Gas injector characteristics

Description	Parameter value
Gas injector	DYMCO Corp/GISM-i1000
Approval Pressure (bar)	1.2 ± 0.1
Operating Temperature Range (°C)	-40 ~ +120
Operating Voltage Range (V)	DC 6~ DC 18
Operating working pressure, relative, (bar)	0.2 to 4.2
Maximum working pressure, relative, (bar)	4.5
Opening time (ms)	3.00
Closing time (ms)	1.00
Injector hole diameter (mm)	1.8

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Table 3. Number of Cells for tested meshes

		Case1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7
3D	TDC	305,331	315,831	337,848	380,978	444,665	457,265	474,065
	BDC	810,771	1,057,271	1,072,888	1,114,578	1,180,745	1,421,805	1,908,305
2D	TDC	4,636	5,028	6,146	6,709	12,258	12,694	17,472
	BDC	15,667	18,646	23,946	32,929	38,490	47,602	82,880

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758

759 **Figure captions**

760 Fig. 1. Inlet and exhaust duct geometry with gas injector position

761 Fig. 2. 2D and 3D mesh at (a) TDC, (b) BDC with geometry decomposition

762 Fig. 3. Intake valve profiles

763 Fig. 4. (a) Grid and (b) time step sensitivity for 2D and 3D mesh

764 Fig. 5. In-cylinder volume and mass evolution in the 2D and 3D approaches

765 Fig. 6. Validation of the 2D and 3D simulations

766 Fig. 7. (a) In-cylinder mass, (b) Backflow mass, (c) Pumping loss work and (d)
767 Maximum pressure for different IVC and MVL under various speeds

768 Fig. 8. In-cylinder mass and backflow mass under different engine speed

769 Fig. 9. Characteristics curve of the hydrogen injector

770 Fig. 10. Hydrogen mass fraction in intake manifold

771 Fig. 11. Hydrogen mass fraction distribution in case HSOI43 $P=1.7$ and HSOI60 $P=2.2$ at
772 various engine speed

773 Fig. 12. In-cylinder temperature of hydrogen-air mixture at a specific mass fraction of
774 hydrogen

775 Fig. 13. Hydrogen mass fraction distribution at different pressure injection and inclination
776 for $N=1500$ rpm, HSOI60 and IVC30

777 Fig. 14. Combustion characteristics and exhaust emissions of diesel (DF IVC70) and dual
778 fuel (D IVC30)

779 Fig. 15. Effect of retarding the diesel start of injection in combustion characteristics and
780 exhaust emissions

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Fig. 1. Inlet and exhaust duct geometry with gas injector position

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Fig. 2. 2D and 3D mesh at (a) TDC, (b) BDC with geometry decomposition

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Fig. 9. Characteristics curve of the hydrogen injector

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Fig. 10. Hydrogen mass fraction in intake manifold

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846 Fig. 11. Hydrogen mass fraction distribution in case HSOI43 P=1.7 and HSOI60 P=2.2 at

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various engine speed

Fig. 12. In-cylinder temperature of hydrogen-air mixture

at a specific mass fraction of hydrogen

(a) Intake stroke

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.00 (%)

(b) Compression stroke

0.6 0.62 0.64 0.66 0.68 0.7 0.72 0.74 0.76 0.78 0.8 (%)

Fig. 13. Hydrogen mass fraction distribution at different pressure injection and

inclination for N=1500 rpm, HSOI60 and IVC30

Fig. 14. Combustion characteristics and exhaust emissions of diesel (D IVC70) and dual fuel (DF IVC30)

Fig. 15. Effect of retarding the diesel start of injection in combustion characteristics and exhaust emissions