1 Numerical simulation on combustion and NO_x emission characteristics of a
2 turbocharged opposed rotary piston engine fuelled with hydrogen under
3 wide open throttle conditions

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Abstract: Under the stress of environmental pollutions and fossil fuel consumption caused by on-road transport, hybrid vehicles are attracting much attention. Opposed rotary piston (ORP) engines are a promising power source for hybrid vehicles, due to their compact designs and high power density. In this paper, combustion and emission characteristics of a turbocharged ORP engine fuelled with hydrogen were investigated to evaluate the overall performance of this engine. The results indicated that volumetric efficiency of this ORP engine was higher than 89.0% for all the given cases. Peak in-cylinder pressure was in the range of 51.0~69.0 bar; and 4000 RPM scenario had the maximum value, being benefitted from high intake temperature and pressure, and high volumetric efficiency. Combustion duration of this engine ranged 27~43 °crank angle (CA), and combustion phase happened at 7.5~13 °CA after top dead centre (TDC). Peak nitrogen monoxide (NO) formation rates were corresponding to 5~13 °CA after TDC; accumulated NO decreased slightly after reaching the peak value for low engine speed conditions. Discharge pressure at the start of the exhaust stroke was higher than 6.0 bar, especially for 5000 RPM case whose value was approximately 11.0 bar. This ORP engine presented excellent torque characteristics, and the maximum indicated power density was approximately 104.0 kW L⁻¹ which was much higher than turbocharged four-stroke reciprocating engines fuelled with gasoline.

Keywords: Hybrid vehicles; opposed rotary piston engines; turbocharger systems; hydrogen; combustion characteristics; NO_x emission

1. Introduction

With the rapid development of hybrid vehicles and range extender electric vehicles, high power density internal combustion (IC) engines are attracting considerable attention, such as two stroke engines [1, 2] and Wankel engines [3-5]. Performance of two-stroke engines and Wankel engines has been widely researched. For example, Ning et al. [6] investigated the effect of fuel injection

45 timing and compression ratio on the performance of a naturally aspirated two-stroke spark ignition
46 engine. Its power density was approximately 30 kW L^{-1} under the conditions of 3000 RPM engine
47 speed, wide open throttle, compression ratio of 7.2, and fuel injection timing of 240° crank angle
48 (CA) before top dead centre (TDC). However, maximum brake thermal efficiency was lower than
49 27.0% caused by lower compression ratio and higher unburned fuel fraction than four-stroke
50 reciprocating engines [6]. Carbon dioxide (CO) and hydrocarbon (HC) emission factors of
51 two-stroke engines were much higher than those of four-stroke reciprocating engines [7], especially
52 under idle conditions due to serious incomplete fuel combustion and large overlaps of intake and
53 exhaust valves opening. Peden et al. [8] compared the performance of a reciprocating engine and a
54 Wankel engine using a 1D simulation method. Wankel engines had a higher ratio of cylinder
55 surface/volume (caused by narrow and long combustion chambers) and presented higher leakages
56 than reciprocating engines [8], resulting in lower brake thermal efficiency despite of higher power
57 density. Chen et al. [9] investigated stratified charge combustion in a natural gas-diesel fuelled
58 Wankel engine to improve the engine performance. The results indicated that diesel flame
59 propagation was enhanced by blending natural gas, contributing to higher combustion rates. The
60 peak in-cylinder pressure increased by 24.17% when the natural gas blend ratio increased to 20.0%;
61 soot and CO emissions decreased significantly as well, but it led to an increase of NO_x emission.

62 Apart from Wankel engines and two-stroke engines, opposed rotary piston (ORP) engines (or
63 twin-rotor piston engines) have few moving parts and compact designs, and can deliver high power
64 density. Dent [10], Zhang [11], and Chen [12] put forward a twin-rotor piston engine whose cyclic
65 period (if four cylinders) was half of four-cylinder reciprocating engines. Piston movements and
66 operation theory of this engine were analysed using mathematical equations [11, 12]. Further, Zou
67 et al. [13] estimated the power density, with the maximum value of approximately 78 kW L^{-1} under

the condition of wide open throttle, naturally aspirated, and an equivalent ratio of 0.8. Gao et al. [14] explored the power output of an ORP engine, using 1D simulation approaches over various engine speeds and loads. It indicated that brake thermal efficiency of this ORP engine was at a similar level to reciprocating engines; meantime, the rated power output was approximately 40 kW at 5000 RPM engine speed (0.55 L displacement) for naturally aspirated conditions. The power density was almost twice of the naturally aspirated reciprocating engines, and was even higher than Wankel engines. Further, pumping losses in the intake stroke of this ORP engine were analysed [15] using a 3D numerical simulation approach. It was demonstrated that pumping losses of this ORP engine were higher than reciprocating engines, due to the short duration of intake and discharge process, and no early opening and late closing for intake and exhaust ports. Additionally, the combustion and emission characteristics of the ORP engine fuelled with hydrogen were explored using 3D simulation method [16] that the NO_x emissions were significantly dependent on engine speed.

Since the concerns on the environmental problems caused by on-road transport emissions increase, clean fuels such as hydrogen [17-19] and natural gas [20-22] are attracting much attention, especially for hydrogen fuel. Combustion process of hydrogen is free of the formations in particulate matters (PM), greenhouse gas (CO_2), CO, and HC. Additionally, flam propagation speed of hydrogen combustion is much higher than other types of fuels. The merits mentioned above make hydrogen as an excellent fuel for IC engine applications. Many researchers [23-26] were devoted to investigating and exploring high performance IC engines fuelled with hydrogen or its blends. Ganesh [27] compared the performance of a single cylinder reciprocating engine fuelled with gasoline and hydrogen. It indicated that brake thermal efficiency of this engine fuelled with hydrogen was approximately 2% higher than that of gasoline; however, the maximum NO_x concentration of hydrogen fuel combustion was more than four times higher than that of gasoline,

caused by high in-cylinder temperature. Açıkgöz et al. [28] also demonstrated that hydrogen additions effectively increased the brake thermal efficiency of IC engines and decreased CO₂, HC, and CO emissions [28], which was consistent with other researches [29-31].

Compared to reciprocating engines, hydrogen fuel will be benefitted more for Wankel engines and ORP engines. Because hydrogen fuel can ease many disadvantages caused by narrow and long combustion chambers of Wankel engines; it will also be much helpful for the ORP engines due to their short cyclic period. Ozcanli et al. [32] reviewed recent studies on the hydrogen usage in spark ignition Wankel engines, the conclusions were drawn that hydrogen fuel and its blends were effective to drop brake specific fuel consumption and carbon dioxide (CO₂) emission; and it worked well to avoid abnormal combustion. Many researches have been done for the applications of various hydrogen blends to Wankel engines, such as gasoline/hydrogen [33], ethanol/hydrogen [34], natural gas/hydrogen [35], and n-butanol/hydrogen [36]. Due to low mass fraction of hydrogen in air/fuel mixture, power density of IC engines fuelled with hydrogen is usually lower than other types of fuel.

Turbocharger systems are a perfect technology to compensate for power losses of IC engines [37]. Luo et al. [38] investigated combustion and emission characteristics of a turbocharged spark ignition engine fuelled with pure hydrogen. Maximum in-cylinder pressure ranged from 35.0 to 60.0 bar for the engine speed range of 1500~4000 RPM under wide open throttle conditions. NO_x concentration in the above scenarios ranged from 300 to 1200 ppm; additionally, the concentration increased with engine loads under the conditions of 2500 RPM engine speed and an equivalence ratio of 0.55. Further, the effect of equivalence ratio on turbocharged engine power output and NO_x emission at low engine speed conditions were investigated [39]. The maximum brake thermal efficiency was approximately 30%; and NO_x concentration reached 7000 ppm when equivalence ratio was 0.8 for 1500 and 2000 RPM engine speeds. Turbocharger systems significantly increased

114 NO_x emission although the power losses caused by hydrogen applications were effectively
115 compensated. Effective technologies could be used to decrease the NO_x emissions, such as
116 permanent/electromagnet-based fuel reforming system [40], exhaust gas recirculation [41],
117 lean-burn [42], and selective catalytic reduction [43, 44]. During hydrogen combustion, only
118 thermal NO_x was formed due to a lack of nitrogen and carbon elements in hydrogen [45]. In
119 addition, the formation process of thermal NO_x was much slower than prompt NO_x [46].
120 Combustion duration in time of ORP engines was much shorter than four-cylinder reciprocating
121 engines, which can prevent the formations of thermal NO_x to some extent, especially for high
122 engine speed conditions.

123 In summary, many researches have been done to investigate the hydrogen applications to Wankel
124 engines and reciprocating engines. However, to the authors' knowledge, few studies are available to
125 date about hydrogen applications to turbocharged ORP engines although they present many
126 advantages for hybrid vehicles and range extender electric vehicles' applications. In this paper, the
127 authors investigated combustion and emission characteristics of a turbocharged ORP engine fuelled
128 with hydrogen over various engine speeds using a 3D numerical simulation method. In-cylinder
129 pressure evolutions, heat release rates, combustion durations, and NO_x formation during engine
130 operation were addressed.

131 **2. Materials and methods**

132 In this section, ORP engine structures, engine operation theory, numerical simulation method, and
133 simulation model descriptions are conducted.

134 **2.1 Configurations of the opposed rotary piston engine**

135 As the power density drop of IC engines fuelled with hydrogen, turbocharger systems should be
136 adopted to compensate the power losses. Table 1 shows the technical specifications of the

137 turbocharged ORP engine. It is a small scale, four-cylinder, and turbocharged spark ignition engine;
 138 it has a displacement of 0.5468 L and a compression ratio of 9.73. There are two engine blocks, two
 139 shafts, two spark plugs, three intake ports and one exhaust port. Cyclic period of this ORP engine is
 140 360 °crank angle (CA), with each stroke lasting 90 °CA; and the geometrical angle was 120 °for
 141 each stroke. Similar to Wankel engines, combustion chambers of this engine always rotate during
 142 operations.

143 Table 1 Technical specifications of the opposed rotary piston engine

Specifications	Values
Ignition method	Spark ignition
Stroke number	4
Cylinder number	4
Spark plug number	2
Shaft number	2
Compression ratio	9.73
Displacement/ L	0.5468
Intake system	Turbocharged
Fuel type	Hydrogen
Fuel injection type	Port fuel injection
Crank angle per stroke/ °CA	90
Intake port number	3
Exhaust port number	1

144 ORP engines are free of connecting rod mechanism and have few moving parts; the configurations
 145 are presented in Figure 1. Piston 1 and piston 3 are connected with shaft 1, and these two pistons are
 146 opposed positioned. It is the same for piston 2, piston 4, and shaft 2. These two shafts are coaxial
 147 and are fixed using bearings (not shown in the figure) on the engine blocks. Gaps between the end
 148 faces of the two shafts may lead to serious leakage, which can worsen the engine performance.
 149 Additionally, the sealing approach will be different from reciprocating engines and Wankel engines.

150 There are four bowls in each piston, which makes it possible to adjust spark timing for achieving
 151 excellent engine performance. The combustion chambers are composed of inner faces of two engine
 152 blocks, end faces of adjacent pistons, and faces of bowls. It should be noted that piston positions in
 153 Figure 1 (d) should be adjusted to be consistent with valve timing. In addition, there are two spark
 154 plugs oppositely positioned on the two engine blocks, and the bowls in pistons pass that area during
 155 engine rotations, as presented in Figure 1 (d). More details about the engine configurations were
 156 presented in the authors' previous work [15]. Being superior to reciprocating engines whose layouts
 157 of intake and exhaust ports are limited by spark plugs and cylinder head size, intake ports, exhaust
 158 ports, and spark plugs of the ORP engine are located at different positions of engine blocks.

159 Figure 1 Structures of the opposed rotary piston engine

160 2.2 Operation descriptions of the opposed rotary piston engine

161 As pistons rotate all the time during engine operations, crank angle definitions in this work are
 162 different from reciprocating engines and Wankel engines. Crank angle of this ORP engine is defined

163 as the positions of cylinder centre; top dead centres (TDCs) and bottom dead centres (BTCs) are
 164 corresponding to the positions where cylinder volumes are the minimum value and maximum value
 165 respectively, as indicated in Figure 2. So there are two TDCs and two BTCs in this engine. “TDC 1”
 166 and “BDC 1” are corresponding to 0 °CA and 90 °CA, respectively. Fluid domains of the numerical
 167 model in this paper are presented in Figure 2(b), which includes three intake pipe domains, one
 168 exhaust pipe domain, four combustion chamber domains, and two spark plug domains in total.

Figure 2 TDCs and BDCs of this ORP engine

171 Operation processes of this engine include intake stroke, compression stroke, expansion stroke, and
 172 exhaust stroke; additionally, each stroke lasts 90 °CA. Different from reciprocating engines and
 173 Wankel engines, there are not any overlaps for the intake and exhaust ports opening. Early opening
 174 and late closing of intake and exhaust ports do not happen during engine operations, resulting in
 175 more exhaust gas remaining in combustion chambers. Maximum and minimum geometrical angles
 176 of the cylinder domains in the movement process were 65.23 ° (at BTC) and 2.77 ° (at TDC),
 177 respectively. Pistons pass exhaust port and intake ports sequentially during engine operations, and at
 178 most two intake ports can work simultaneously, as shown in Figure 3 and Video 1. During the
 179 operation process, volume evolutions of cylinders 1 and 3 are the same, while they are the same for
 180 cylinders 2 and 4.

Figure 3 Operation processes of opposed rotary piston engine

2.3 Numerical simulation model

In this paper, FLUENT software [47] was used to perform the simulations of unsteady flow. In the numerical simulation model, hexahedral meshes were applied to all the fluid domains. Mesh numbers of all the fluid domains are shown in Table 2, the corresponding cylinder position is in Figure 4. Mesh numbers of four bowls in the same cylinder are slightly different, and Table 2 only presents one of them. The minimum orthogonal, maximum ortho skew, and maximum aspect ratio were 0.337, 0.663 and 16.726, respectively for the initial state of simulation. Sensitivity analysis of mesh number (mesh size) and residual setting (Table 3) was discussed in authors' previous work [15], where grid number 779324 and residual 10^{-6} are chosen. Due to the changes of combustion chamber volume during operations, dynamic meshes were used in engine simulation model. In this model, k-epsilon Re-Normalisation Group (RNG) viscous, species transport model, finite-rate /Eddy-dissipation models were chosen in different setting categories. Thermal NO_x model was activated for estimating NO_x emissions. For the hydrogen/air mixture ignition in this simulation model, high temperature zones (2073 K) were patched in the zones of spark plugs to ignite hydrogen/air mixture. Similar to the spark plug energy, the patched temperature also affected the

197 in-cylinder combustion to some extent. The effect of patched temperature on in-cylinder pressure
 198 evolutions was indicated in the authors' previous work [16].

199 Table 2 Mesh numbers of fluid domains and overall mesh quality

Sub-domain	Elements
Intake pipe 1	12210
Intake pipe 2	12210
Intake pipe 3	16632
Exhaust pipe	40664
Spark plug (each one)	18202
Bowl (each one)	37718
Cylinder (initial stage)	53376
Minimum orthogonal	0.337
Maximum ortho skew	0.663
Maximum aspect ratio	16.726

200
 201 Figure 4 Numerical simulation model meshes

202 Table 3 Sensitivity analysis of mesh number (mesh size) and residual setting [15]

Mesh number	Residuals	Average in-cylinder pressure at the end of intake process/ Pa
593246	10^{-6}	99599
	5×10^{-6}	99595
779324	10^{-6}	99593
	0.3×10^{-6}	99591
102672	10^{-6}	99597

203

204 **2.4 Boundary conditions of simulation scenarios**

205 The purpose of this paper focuses on the combustion and emission (NO_x) characteristics under
 206 various engine speeds and wide open throttle conditions when turbocharger systems are applied to
 207 this ORP engine fuelled with hydrogen. Table 4 shows boundary conditions of simulation scenarios.
 208 Each cycle includes one thousand time steps for all the scenarios. Boundary conditions (intake
 209 pressure, temperature and outlet pressure) of the 3D numerical simulations are from experimental
 210 results of a 1.8 L turbocharged four-cylinder reciprocating engine. So the overall performances of
 211 this ORP engine can be comparable to the reciprocating engine. Ignition timing of these simulation
 212 cases was the same (17°CA before TDC), and ignition timing should be optimized in future work to
 213 achieve better overall performance.

214

Table 4 Boundary conditions of numerical simulations

Boundary conditions	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5
Intake pressure/ bar	1.30	1.58	1.53	1.60	1.82
Intake temperature/ $^\circ\text{C}$	24.0	28.4	30.0	34.8	42.0
Outlet pressure/ bar	1.31	1.40	1.58	2.00	2.83
Rotation speed/ RPM	1000	2000	3000	4000	5000
Engine load	100%	100%	100%	100%	100%
Fuel type	H_2	H_2	H_2	H_2	H_2
Equivalence ratio	1	1	1	1	1
Time step/ s	6×10^{-5}	3×10^{-5}	2×10^{-5}	1.5×10^{-5}	1.2×10^{-5}

215

216 **3. Results and discussion**

217 In order to preliminarily evaluate the engine performance and make a foundation of the engine
 218 structure optimisation, average in-cylinder pressure evolutions, heat release rates, combustion
 219 durations, and NO_x formations were analysed. In addition, the power density was compared to that

220 of a turbocharged reciprocating gasoline engine.

221 3.1 Combustion characteristics

222 Volumetric efficiency of IC engines dominated the quantity of intake air/fuel mixture (under the
223 same boundary conditions) which significantly affected engine power output and thermal efficiency
224 [48, 49]. Figure 5 presented the volumetric efficiency of this ORP engine over different engine
225 speeds. Volumetric efficiency increased with engine speeds and then decreased rapidly, with the
226 maximum value reaching 93.0% under 4000 RPM. Tendency of volumetric efficiency were
227 attributed to the intake durations in time and velocity of intake air/fuel mixture. Higher engine
228 speeds could cause higher intake fluid velocity, but provided less time of the intake process.
229 Volumetric efficiency of a four-stroke reciprocating gasoline engine was lower than 90.0% when the
230 engine speed was below 4000 RPM [50, 51]. The values of this ORP engine were higher than those
231 of reciprocating engines, which was benefitted from large area of intake ports in ORP engine.
232 Because the intake port size was not limited by the layout of exhaust ports and spark plugs. Such
233 high volumetric efficiency would lead to high engine power output and affect the engine torque
234 characteristics.

235
236 Figure 5 Volumetric efficiency over various engine speeds

237 In-cylinder pressure evolutions significantly affected the engine performance, such as engine power
238 output and brake specific fuel consumption (BSFC). Average in-cylinder pressure of this ORP

239 engine during engine operations is shown in Figure 6. Crank angle (CA) corresponding to the peak
240 in-cylinder pressure changed slightly with engine speeds, being around 10 °CA after TDC. Since the
241 boundary conditions such as intake pressure and temperature were different significantly for these
242 cases, the relations between peak in-cylinder pressure and engine speeds were different from those
243 of naturally aspirated engines [52]. The crank angle corresponding to the peak in-cylinder pressure
244 was slightly earlier than reciprocating engines. As presented by Luo et al. [38] that the peak
245 in-cylinder pressure was approximately 15 °CA after TDC for a 2.3 L turbocharged, port fuel
246 injected, spark ignition engine. High flame propagation speed of hydrogen combustion led to high
247 peak in-cylinder pressure under the same engine operation condition. It was demonstrated by Huang
248 et al. [53] and Navale et al. [54] based on a port fuel injection engine fuelled with the blend of
249 gasoline and hydrogen. Additionally, hydrogen additions effectively dropped the cycle-by-cycle
250 variations of a spark ignition engine [55]. Peak in-cylinder pressure over 4000 RPM was the highest
251 among the five scenarios, resulting from high intake temperature and pressure, and high volumetric
252 efficiency (leading to high combustion rates and much heat release). Expansion stroke in time of
253 5000 RPM engine speed was shorter than other cases, which led to lower peak in-cylinder pressure.
254 Because shorter time caused less hydrogen burned around TDC. In-cylinder pressure of a
255 turbocharged reciprocating engine fuelled with hydrogen was also tested at wide open throttle
256 conditions, with the peak in-cylinder pressure of 35.0~56.0 bar [38]. In-cylinder pressure at the end
257 of power stroke over 1000 RPM was much lower than other cases, which contributed to less
258 pumping losses. Pressure in discharge process of turbocharged engines was higher than naturally
259 aspirated engines. The pressure of a heavy-duty natural gas engine was higher than 10.0 bar at a 1.8
260 bar intake pressure condition [56]. In-cylinder pressure increase rates of this ORP engine showed
261 double-peak except for 1000 RPM, with the maximum value being higher than 2.0 bar (°CA)⁻¹. The

first peak happened around 10 °CA before TDC, and the second peak was around 5 °CA after TDC. The value of second peak in 4000 RPM scenario was much higher than other cases. Pressure increase rates of this ORP engine were at a similar level to reciprocating engines [38].

(a) Average in-cylinder pressure evolutions

(b) In-cylinder pressure increase rates

Figure 6 Average in-cylinder pressure over various engine speeds

In-cylinder pressure evolutions were mainly dependent on the engine speeds and heat release rates. Peak heat release rates during combustion were around 6 °CA after TDC which changed slightly with engine speeds for this ORP engine, as shown in Figure 7. The heat release profiles presented a second peak after 10 °CA after TDC for high engine speed conditions. Peak heat release rates ranged from 27 to 41 J (°CA)⁻¹ for 1000~5000 RPM engine speeds. The value was approximately 100 J (°CA)⁻¹ for a 2.3 L turbocharged hydrogen reciprocating engine under wide open throttle conditions [38]. Heat release rate profiles of a hydrogen/natural gas engine presented double-peak over various engine loads. The first peak decreased with engine loads; however, the second peak showed the opposite tendency [57]. By contrasting with Figure 6, cylinder pressure at 5000 RPM was higher than 1000 RPM; however, the heat release was lower at the first half of combustion process. It was mainly caused by two reasons: (1) in-cylinder pressure and temperature at the beginning of compression stroke over 5000 RPM were higher than those of 1000 RPM; (2) heat loss of 1000 RPM was much higher than 5000 RPM, which was mainly caused by higher

281 in-cylinder temperature and longer duration in time during combustion over 1000 RPM.
 282 Distributions of heat of reaction could reflect flame propagation to some extent, and the heat of
 283 reaction distributions in cylinders is shown in Figure 8. Heat of reaction was consistent with the
 284 pressure evolutions in Figure 6. At the beginning of combustion process, combustion started from
 285 the bowls of combustion chambers and then propagated into gaps of adjacent pistons. Because of
 286 the short duration in time of power stroke over 5000 RPM, heat release rates at the last half stage of
 287 combustion process were higher than other cases. Crank angle corresponding to the maximum heat
 288 release rates was almost the same for 2000 RPM and 3000 RPM engine speed for a spark ignition
 289 engine fuelled with hydrogen/gasoline over maximum brake torque timing [41].

290
 291 Figure 7 Heat release rates over various engine speeds

Figure 8 Heat of reaction distributions in combustion chambers over various engine speeds

As presented by Li et al. [56], high intake pressure promoted in-cylinder combustion, resulting in higher mass burn fraction (MBF) at the same crank angle over for the given engine speeds. Figure 9 presented the MBF of hydrogen fuel over different engine speeds. High intake pressure and temperature (boundary conditions) promoted hydrogen combustion and enhanced flame propagation speed; however, high engine speed allowed short time for chemical reactions during combustion. MBF profiles were resulted from the combined effects of intake pressure and temperature, and engine speeds. In this section, 10% mass burn fraction (MBF10) of hydrogen was defined as the start of combustion; the position as the series of crank angle for 50% MBF (MBF50) was defined as combustion phase; the duration of crank angle between MBF10 and MBF90 (90% mass burn fraction) was defined as combustion duration. Figure 10 shows the start of combustion, combustion phase, and combustion durations of this ORP engine fuelled with hydrogen. The start of combustion was retarded with engine speeds, except for 4000 RPM case. Combustion duration of this engine was short for medium engine speed conditions, which was consistent with Luo's research [38] where the combustion duration of a hydrogen fuelled turbocharged engine over 2000 RPM was slightly shorter than that of 1500 RPM. The combustion duration in the authors' work was shorter than reciprocating engines and Wankel engines fuelled with gasoline [58, 59], which was mainly caused by hydrogen flame propagation speed. It was supported by the research based on

310 a Wankel engine [59] that gasoline/hydrogen blends were burned out in 50 °CA; however, it was
 311 more than 150 °CA for gasoline fuel.

312
 313 Figure 9 Mass burn fraction of hydrogen over various engine speeds

314
 315 Figure 10 Start of combustion, combustion phase, and combustion durations

316 Combustion was mainly happened in bowls of cylinders before TDC, then the flame propagated
 317 into the gaps between the end faces of adjacent pistons in a short time as long as the gaps increased,
 318 as shown in Figure 11. It was mainly caused by quenching and crevices effects [60, 61] due to low
 319 temperature of piston end faces. At the end of combustion process, combustion was mainly
 320 concentrated in the corners and head of combustion chambers, which was clearly presented in Video
 321 1. Similar to Wankel engines that unburned fuel was mainly in the leading and trailing corners of
 322 combustion chambers, which led to low indicated thermal efficiency and high exhaust emissions [4,
 323 61-63]. With the increase of in-cylinder pressure before TDC, much air/hydrogen mixture was

324 squeezed into the gaps between the adjacent cylinders, which prevented the heat release before
 325 TDC. However, it could lead to a rapid combustion after TDC, resulting in a high percentage of
 326 constant volume combustion, which contributed to increasing engine thermal efficiency.

327 Figure 11 Hydrogen mass fraction distributions in combustion chambers over various engine speeds
 328 P-V diagrams were visualised to compare indicated power output of IC engines, as shown in Figure
 329 12. In the compression stroke, differences of P-V lines for various engine speeds were mainly
 330 caused by intake pressure, temperature, and volumetric efficiency; and the differences were quite
 331 small for 2000~4000 RPM cases. Discharge process included free discharge and forced discharge,
 332 and the in-cylinder pressure was much higher than the pressure of outlet ports at the beginning of
 333 the free discharge. Exhaust valves/ports usually opened before BDC to decrease the in-cylinder

334 pressure in short time for reciprocating engines, ensuring low pumping losses in the gas exchange
 335 process [64, 65]. For the ORP engine, early opening of exhaust port did not happened to ensure
 336 complete combustion, which would lead to high in-cylinder pressure in the free discharge process.
 337 The in-cylinder pressure was higher than 6.0 bar at the start of free discharge for the five cases; and
 338 5000 RPM scenario had the highest value which was attributed to the highest percentage of
 339 hydrogen burned at the last half stage of expansion stroke. It took a large crank angle for in-cylinder
 340 pressure reaching a relative low level, especially for high engine speed conditions. In order to
 341 increase the engine thermal efficiency, re-structures of the exhaust port would be conducted to
 342 achieve an early opening.

343
 344 Figure 12 P-V diagrams over various engine speeds

345 3.2 Emission characteristics

346 Due to high combustion temperature of stoichiometric air/hydrogen mixture, much NO_x were
 347 formed during combustion. NO concentration of a hydrogen fuelled reciprocating engine was
 348 approximately 2200 ppm over 2500 RPM [66]. NO_x formations during fossil combustion included
 349 thermal NO, prompt NO, and fuel NO; however, it was only thermal NO for hydrogen combustion
 350 [67]. Thermal NO formation was much slower than prompt NO, such that high engine speeds could
 351 contribute to low NO formation. Pollutants formed in hydrogen combustion process were NO_x

(include NO and NO₂) generally, among which more than 98% of NO_x was NO if air/hydrogen mixture was stoichiometric. Zeldovitch [67] mechanism was used in FLUENT code for estimating NO formation during combustion. Figure 13 shows the accumulated NO formation during combustion. Accumulated NO emission was in the range of 0.65~0.8 mg per cycle per cylinder for engine speeds of 1000~4000 RPM; however, the value over 5000 RPM was approximately 0.35 mg, resulting from short duration in time of high in-cylinder temperature. For low engine speed conditions, accumulated NO decreased slightly after reaching the peak values, and it happened later than 10 °CA after TDC. The simulation results were consistent with the tests [67] that NO mole fraction in hydrogen combustion process increased and then decreased with crank angle. NO concentration drop with residence time during combustion was also demonstrated in the work [68]. NO formation during fuel combustion was a reversible chemical reaction that large amounts of NO formation under low engine speed conditions accelerated the backward reactions, resulting in the drop of accumulated NO emission. Additionally, high in-cylinder temperature was also necessary for the backward reactions. Crank angles corresponding to the maximum NO formation rates were in the range of 5~13 °CA after TDC. NO mass fraction distributions in combustion chambers are shown in Figure 14. Small amounts of NO were generated before 5 °CA before TDC, being mainly distributed in the bowls of the combustion chambers. For low engine speed conditions, measures should be taken to decrease the NO formation, such as EGR [69] and lean-burn [70]. Lean-burn would be explored in the authors' future work, considering the balances between thermal efficiency and NO formation.

Figure 13 Accumulated NO during hydrogen combustion over various engine speeds

Figure 14 NO mass fraction distributions in combustion chambers over various engine speeds

High in-cylinder temperature was one of the main factors promoted NO formation. Average

in-cylinder temperature evolutions during engine operations are presented in Figure 15. Temperature distributions in combustion chambers and the relations between NO formation and average in-cylinder temperature are shown in Figure S1 and Figure S2. NO formation mainly happened in the temperature range of 1600~2400 K, which was concluded by contrasting to Figure 13. In-cylinder temperature over 5000 RPM case was the lowest among the five scenarios, which partly contributed to the least NO formation. Average in-cylinder temperature earlier than 20 °CA before TDC was the highest for 4000 RPM condition; it did not differ much for 1000, 2000 and 3000 RPM scenarios. Although the maximum temperature for 3000 RPM and 4000 RPM engine speed was almost the same, accumulated NO emission of 3000 RPM was higher than that of 4000 RPM, which was mainly caused by the short cyclic period in time for 4000 RPM. Hydrogen additions in fuel would effectively accelerate the combustion and increase the in-cylinder temperature; however, NO_x concentration did not change much with the percentage of hydrogen additions if the spark timing corresponded to individual maximum brake torque for the given scenario (same speed and hydrogen addition) [35]. Additionally, engine load showed a significant effect on NO_x concentration [71] which increased from approximately 600 ppm to 2100 ppm over the brake mean effective pressure (BMEP) of 3.2 bar when hydrogen additions were changed from 0% to 40%; however, it increased from 200 ppm to 700 ppm over the BMEP of 1.6 bar.

Figure 15 In-cylinder temperature during combustion over various engine speeds

3.3 Overall performance evaluations

Because of low hydrogen mass fraction in air/hydrogen mixture, hydrogen applications in IC engines would lead to power loss, as indicated by Luo et al. [66] that the maximum losses of power density reached 50% compared to that of gasoline engines. But the power density of hydrogen fuelled ORP engine was still much higher than that of reciprocating engines fuelled with gasoline, as shown in Figure 16. Brake power of the reciprocating engine in this figure was tested based on a 1.8 L turbocharged engine fuelled with gasoline in the authors' previous experiments (more details of this engine are shown in Table S1). Indicated power density of this ORP engine was approximately 80% higher than the brake power density of the reciprocating engine although the brake power density was slightly lower than indicated power density for a given engine under specific conditions. Such high power density contributed to downsize of IC engines, which promoted the applications of this ORP engine to hybrid vehicles.

Figure 16 Power density comparisons of this ORP engine and a reciprocating engine

The overall performance of this ORP engine is shown in Figure 17, including engine power output, engine torque, NO emission factors, and indicated thermal efficiency. The maximum indicated power reached 52.0 kW, and indicated torque was higher than 195.0 N m for wide open throttle conditions. This ORP engine had good torque characteristics that high engine torque could be delivered in the engine speed range of 2000~4000 RPM. It would benefit for vehicle accelerations over high vehicle velocity after the applications of ORP engines to hybrid vehicles. In addition, engine torque at 5000 RPM case could be enhanced by re-structuring exhaust and intake ports, and advancing sparking timing. Brake thermal efficiency of a hydrogen fuelled reciprocating engine was higher than 33.0% when the engine speed was higher than 1500 RPM; the efficiency was almost 7% higher than a gasoline reciprocating engine [66]. Indicated thermal efficiency of this ORP engine was higher than 34.0% when the engine speed was lower than 4000 RPM; the efficiency was at a similar level to reciprocating engines. It was demonstrated by comparisons to Ma's [42] test that the indicated thermal efficiency of a hydrogen reciprocating engine was approximately 37.0% over 1200 RPM engine speed. Indicated thermal efficiency over 5000 RPM was approximately 27.0%, which was mainly caused by late spark timing. Emission factors of this turbocharged ORP engine were high, especially for medium engine speed conditions; and they were much higher than gasoline engines and natural gas engines [72]. Lean-burn would be explored in

the authors' future work to achieve low NO emission and high thermal efficiency; in addition, it could decrease the thermal load of the engine.

Figure 17 Summary of engine performance calculated using 3D simulation

4. Conclusions

This paper investigated the combustion and NO_x emission characteristics of a turbocharged ORP engine fuelled with hydrogen. This ORP engine is a promising power source of hybrid vehicles and range extender electric vehicles. The main conclusions of this paper are as the follows:

1. Volumetric efficiency of this ORP engine was higher than 89.0% for the given scenarios, with the maximum value being approximately 93.0% over 4000 RPM engine speed, resulting from the joint effects of intake air/hydrogen mixture velocity and intake duration in time. Peak in-cylinder pressure was in the range of 51.0~69.0 bar; and the maximum value happened at 4000 RPM condition, benefiting from high intake pressure and temperature, and high volumetric efficiency. At the end of combustion process, unburned fuel was mainly in the corners and top of the combustion chambers, due to being far from the bowls.
2. Combustion duration of this ORP engine was more dependent on the engine speed than combustion phase and the start of combustion. 4000 RPM case presented the highest burn rate of the air/hydrogen mixture, contributing to high indicated thermal efficiency. Discharge pressure of

445 this ORP engine was much higher than the pressure of exhaust port at the beginning exhaust stroke,
446 which went against high thermal efficiency. The engine thermal efficiency could benefit from
447 exhaust port layout by providing early opening.

448 3. Accumulated NO formation per cycle during low and medium engine speed conditions was
449 high; it decreased slightly after reaching to the peak value. However, NO formation over 5000 RPM
450 engine speed was approximately 50% lower than other engine speed conditions, due to low
451 in-cylinder combustion temperature and short duration in time of expansion stroke.

452 4. Maximum power density of this ORP engine was approximately 104.0 kW L⁻¹ over 5000 RPM
453 speed, and it showed excellent torque characteristics at medium and high engine speed conditions.
454 Indicated thermal efficiency of this engine was higher than 34% for the engine speed of 1000~4000
455 RPM. These advantages would promote its applications to hybrid vehicles.

456

457 **CRedit authorship contribution statement**

458 Jianbing Gao: Formal analysis, Investigation, Methodology, Resources, Validation, Visualization,
459 Writing - original draft, Writing - review & editing. Guohong Tian: Conceptualization, Funding
460 acquisition, Methodology, Project administration, Resources, Software, Supervision, Visualization,
461 Writing - review & editing. Chaochen Ma: Investigation, Writing review & editing; Shikai Xing:
462 Visualization, Writing - review & editing. Phil Jenner: Conceptualization, Data collections.

463 **Declaration of competing interest**

464 The authors declare that they have no known competing financial interests or personal relationships
465 that could have appeared to influence the work reported in this paper.

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