1 Lean-burn characteristics of a turbocharged opposed rotary piston engine
2 fuelled with hydrogen at low engine speed conditions

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21 **Abstract:**

22 Opposed rotary piston (ORP) engines have high power density and compact designs which meet the
23 requirements of power sources of hybrid vehicles. Hydrogen applications to ORP engines can
24 effectively decrease greenhouse gas emissions; however, hydrogen combustion in ORP engines
25 around stoichiometric ratio generated large quantities of nitrogen oxides (NO_x), especially for low
26 engine speed conditions. Lean-burn as an effective method to decrease NO_x emissions was adopted
27 in this research. A 3D numerical simulation method was used to explore the effect of equivalence
28 ratio (≤ 1) on combustion and NO_x emission characteristics of this ORP engine fuelled with
29 hydrogen. The results indicated that peak in-cylinder pressure increased with equivalence ratio for
30 1000 revolutions per minute (RPM); however, the value over the equivalence ratio of 0.9 was the
31 maximum among 2000 RPM scenarios. The effect of equivalence ratio on heat release rates was
32 greatly dependent on the engine speeds. Start of combustion over 1000 RPM engine speed was
33 advanced with the increase of equivalence ratio; and it was the earliest over the equivalence ratio of
34 0.9 at 2000 RPM conditions. During the exhaust stroke, in-cylinder pressure of free discharge was
35 much higher than atmosphere pressure, which significantly increased the pumping losses of exhaust
36 stroke. Accumulated NO_x emissions over the equivalence ratio of 0.9 reached the maximum value
37 for given engine speeds; and the NO_x emissions were almost zero for severe lean-burn (< 0.7)
38 conditions. Engine power output decreased with the drop of equivalence ratio for 1000 and 2000
39 RPM engine speeds; indicated thermal efficiency over the equivalence ratio of 0.9 was the
40 maximum at 2000 RPM engine speed.

41 **Keywords:** opposed rotary piston engines; hydrogen fuel; lean-burn; combustion characteristics;
42 NO_x emissions

43 **1. Introduction**

44 Nowadays, hybrid vehicles are attracting much attention due to their excellent performances in
45 energy consumption and exhaust emissions [1, 2]. Power sources of hybrid vehicles have the
46 requirements of high power density and compact designs. It promotes the applications of two-stroke
47 engines [3, 4] and Wankel engines [5, 6], and provides an opportunity for the development of
48 opposed rotary piston (ORP) engines [7]. Although two-stroke engines can provide high power
49 density, they have low brake thermal efficiency and high exhaust emissions due to low compression
50 ratio and large overlaps of intake and exhaust valves [8]. Wankel engines have long and narrow
51 combustion chambers and large port overlaps, which contribute to high exhaust emissions because

of incomplete combustion [9-12]. ORP engines, as a new type of internal combustion (IC) engines have high power density and are free of connecting rod mechanisms [13-16]. ORP engines were proved to have a similar level of brake thermal efficiency to reciprocating engines [17]. Other types of engines without connecting rod mechanisms were also investigated when hydrogen fuel was applied, such as a spark-ignited free-piston engine (having the character of high efficient, compact and lightweight [18]) researched by Ngwaka et al. [19] that the maximum power output reached 650 W. The priority of a hydrogen fuelled free-piston engine was highlighted by direct converting thermal energy to electricity in Depcik's research [20] that it would brought much benefits for its practical applications. The effect of variable motions on the combustion of a hydrogen fuelled free-piston engine was also investigated, further the combustion optimization using variable motions was conducted by Xu et al. [21].

Hydrogen fuel applications in IC engines are developing rapidly because of their high thermal efficiency and being free of greenhouse gas emission (CO_2) [22, 23]. High brake thermal efficiency was mainly caused by high flame propagation speed and quenching distances for pure hydrogen fuel [24, 25] and hydrogen fuel addition in different types of fuel such as ethanol [26], natural gas [27], n-butanol [28], gasoline [11], and diesel [29]. As demonstrated by Zhang et al. [30] based on an optical methane spark ignition engine that brake thermal efficiency of IC engines could be improved by direct-injected hydrogen, which was attributed to faster early flame propagation. Edwin et al. [31] presented an increase in brake thermal efficiency under 75% and 100% loads. Brake thermal efficiency increased by approximately 2.0% when the hydrogen energy addition was 10%. Hydrogen addition decreased coefficient of variations (COVs) as well, which was demonstrated by Chen et al. [32] based on a spark ignition engine fuelled with ethanol under lean-burn conditions. 15% hydrogen addition could decrease 75% COVs of peak in-cylinder pressure which was considered to be more suitable for evaluating cyclic variations if less misfire happened [32]. In addition, hydrogen fuel addition effectively extended lean-burn limits of methanol engine from an excess-air ratio 1.6 to 2.2 when the hydrogen addition was 3.0% [33]. Yuan et al. [34] analyzed the performance characteristics of a hydrogen fuelled free-piston engine which had a lower peak pressure and heat release rate compared with conventional reciprocating engines due to its faster piston motion around TDC; meantime, it presented less NO_x formation because of lower combustion temperature and shorter duration of power stroke. Combustion and NO_x emission characteristics of an ORP engine fuelled with hydrogen at wide open throttle and

stoichiometric conditions were investigated [35] that lower engine speed led to higher NO_x emission factors. In order to compensate the power loss caused by low energy density of gaseous hydrogen by volume, the engine performance over turbocharged conditions was further analyzed [36]. Power density of this engine increased up to 104 kW/L; however, the NO_x emission factors reached up to approximately 14 g (kW h)⁻¹.

As the high in-cylinder combustion temperature of hydrogen fuel or hydrogen fuel blends, nitrogen oxides (NO_x) emission factors were higher than other types of fuels. As indicated by Geo et al. [31] that NO_x emission factors increased from 6.9 to 10.76 g/kW h when hydrogen energy addition in rubber seed oil increased from 0% to 8.39%. However, hydrogen addition effectively decreased the combustion durations, which prevented NO_x formation to some extent. It was presented by Barrios et al. [37] under medium engine speeds and low engine load conditions. Nag et al. [38] studied the joint effects of hydrogen addition and exhaust gas recirculation (EGR) on a dual fuelled single cylinder compression ignition engine. Accumulated NO_x reduction reached 38.4% when 10% EGR rate was applied. Loganathan et al. [39] indicated hydrogen addition in biofuel combined with EGR enhanced engine thermal efficiency and simultaneously reduced NO_x emission. Thermal efficiency of hydrogen-enriched biofuel engine increased from 31.0% to 36.5% when compared to biofuel mode. Lean-burn can effectively drop in-cylinder combustion temperature, resulting in lower NO_x emission factors. Luo et al. [40] investigated the effect of equivalence ratio on the power, combustion stability, and NO_x emission for a turbocharged hydrogen engine at low engine speeds. Engine power and brake thermal efficiency increased with equivalence ratio caused by the speed up of combustion velocity and improved gas exchange process for the lean-burn conditions. NO_x concentration decreased significantly with the drop of equivalence ratio when the equivalence ratio was lower than 0.8 under 2000 RPM engine speed. Retarded ignition timing also decreased the in-cylinder temperature, and was usually used by combining with other technologies. As presented by Lim et al. [41], NO_x emission drop reached 61.7% by retarding 10 °crank angle (CA) with the applications of hydrogen/natural gas blends, compared to a base compressed natural gas engine.

For reciprocating engines, hydrogen fuel or hydrogen addition applications may lead to lower power density, caused by low fuel mass fraction in fuel/air mixtures. Brake mean effective pressure (BMEP) of a spark ignition engine decreased from approximately 4.2 to 3.9 bar when the hydrogen addition was 6% in volume under stoichiometric and partly load conditions [42]. However, hydrogen addition increased BMEP significantly when the excess air ratio was 1.45. An increase of

114 BMEP in a gasoline fuelled Wankel engine was also observed when the hydrogen addition by
115 volume increased from 0% to 5.0%; meantime, the brake thermal efficiency increased from 13.2%
116 to 16.8% under 3000 RPM engine speed, partly load and stoichiometric conditions [43]. Power loss
117 by hydrogen addition was shown as well in the work conducted by Chen et al. [32] that indicated
118 mean effective pressure (IMEP) decreased with hydrogen addition ratio. Power density changes
119 after the hydrogen applications were dependent on the engine operation conditions, baseline fuel,
120 and hydrogen injection methods [44-46]. Power density was still much higher when they were
121 fuelled with hydrogen fuel in theory than gasoline fuelled reciprocating engines, which made the
122 ORP engines to be more promising for hybrid vehicles.

123 Due to high speed of hydrogen flame propagation, higher mass fraction of fuel was burnt before top
124 dead centre (TDC), especially under low engine speed conditions. It led to higher peak in-cylinder
125 temperature, resulting in more NO_x emission for low engine speed conditions. Low equivalence
126 ratio could effectively decrease in-cylinder combustion temperature to achieve low NO_x emission;
127 additionally, lean-burn was an effective method for improving thermal efficiency under specific
128 conditions [42]. To the authors' knowledge, few investigations are available about the effect of
129 equivalence ratio (≤ 1) on the performance of a turbocharged ORP engine fuelled with hydrogen
130 under low engine speed conditions. Meantime, the investigations of current researches about ORP
131 engine mainly included the two aspects: (1) mathematical equations were used to clarify the engine
132 operation theory; (2) 3D simulations were used to explore the in-cylinder flow without addressing
133 the combustion characteristics and emission formations. In this paper, combustion and emission
134 characteristics of a turbocharged ORP engine were explored under different equivalence ratio for
135 low engine speed conditions. The investigation was conducted by analysing the in-cylinder pressure
136 evolutions, mass burn fractions, heat release rates, and NO_x formation. The main differences of this
137 paper with published ones are that detailed 3D combustion model and emission estimation model
138 were used to estimate the engine performance; however, other published work was based on simple
139 mathematical equations and 1D simulation model, and exhaust emissions were not addressed.

140 **2. Materials and methods**

141 In order to explore the in-cylinder combustion characteristics, 3D numerical simulation was used. In
142 this section, ORP engine model and operation theory were described; then, the effect of mesh
143 number sensitivity and calculation residuals on the simulation results was analysed.

144 **2.1 Configurations of the opposed rotary piston engine**

145 The technical specifications of the ORP engine were presented in Table 1. It is a four-stroke,
 146 four-cylinder, turbocharged spark ignition engine. This engine has three intake ports, one exhaust
 147 port, and two spark plugs, as shown in Figure 1; compression ratio of this engine is the same level
 148 as four-stroke reciprocating engines. In order to compensate the power loss caused by hydrogen
 149 combustion, a turbocharger system is applied to the engine. The turbocharger system is not shown
 150 in Figure 1; however, boundary conditions under turbocharged situations will be used for 3D
 151 numerical simulations.

152 Table 1 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
Bore/ mm	59.5
Crank angle per stroke/ °	90
Intake port number	3
Exhaust port number	1

153

154 Structures of this ORP engine are shown in Figure 1. Combustion chambers are composed of end
 155 faces of adjacent pistons (including bowl surfaces), inner faces of engine blocks, and faces of
 156 engine shafts. Piston1 and piston 3 are connected with shaft 1; piston 2 and piston 4 are connected
 157 with shaft 2. There are two bowls in each end face of pistons. Two spark plugs are opposed
 158 positioned in the two engine blocks; bowls in each piston pass the positions of the two spark plugs.
 159 More details of this engine structures were presented in the authors' previous work [7].

Figure 1 Structures of the opposed piston engine, reproduced from [7]

2.2 Operation descriptions of the opposed rotary piston engine

In order to investigate the engine performance, top dead centres (TDCs) and bottom dead centres (BDCs) were defined in this sub-section. TDCs were defined as the positions, where the combustion chamber volumes were the minimum value; BDCs were corresponding to the maximum combustion chamber volume. So, there were two TDCs and two BDCs for this ORP engine, as shown in Figure S1. “TDC 1” and “BDC 1” were defined as 0° crank angle (CA) and 90° CA, respectively. Figure S1 also shows the fluid domains used for 3D simulations. Operation process of this ORP engine is presented in Video 1. Pistons passed exhaust port and intake ports sequentially. Each stroke lasted 90° CA, and there were not overlaps for exhaust port and intake port opening; there were two intake ports at most could work simultaneously.

2.3 Numerical simulation model

Meshes of the numerical simulation model are shown in Figure S2; hexahedral meshes were applied to all the fluid domains. In this paper, ANSYS software [47] was used to simulate the unsteady flow. Mesh numbers of the ORP engine fluid domain are shown in Table 2. Dynamic meshes were used to simulate the unsteady flow in cylinders. The minimum orthogonal, maximum ortho skew, and

176 maximum aspect ratio were 0.337, 0.663 and 16.726, respectively. In this numerical combustion
177 model, k-epsilon Re-Normalisation Group (RNG) viscous, species transport model, and finite-rate
178 /Eddy-dissipation models were set in FLUENT software. The ignition of hydrogen fuel was
179 achieved by patching high temperature zone. Thermal NO_x formation was activated in the
180 combustion model to investigate the effect of equivalence ratio on emission characteristics. In the
181 simulation, sinusoidal movements of the four pistons were attached as the boundary conditions.
182 Sensitivities of mesh number and calculation residuals on simulation results were discussed in
183 authors' previous work [7], where grid number 779324 and residual 10⁻⁶ were chosen (details
184 shown in Table S2). In order to monitor parameter changes (e.g. average temperature, average
185 pressure, and average hydrogen and NO_x concentration) in cylinders during engine operations, the
186 targeted cell zones (cylinders in this paper) need to be monitored. The average temperature,
187 pressure, and hydrogen and NO_x concentration could be calculated based on parameter distributions
188 in cylinders.

189 Table 2 Element 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

190

191 2.4 Boundary conditions of simulation scenarios

192 As the effect of equivalence ratio on engine performance was investigated under low speed
193 conditions, where NO_x emission was high under low engine speed conditions, demonstrated in the
194 authors' previous work. Table 3 lists the boundary conditions of 3D numerical simulation scenarios.
195 Equivalence ratio was in the range of 0.6~0.9, and engine speed was 1000 and 2000 RPM. Inlet

pressure was obtained from a real test of a turbocharged spark ignition fuelled with gasoline. Spark timing of these simulation cases was the same (17 °CA before TDC), and spark timing should be optimized in future work to achieve better performance.

Table 3 Boundary conditions of CFD simulations

Boundary conditions	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8
Intake pressure/ bar	1.30	1.30	1.30	1.30	1.58	1.58	1.58	1.58
Intake temperature/ °C	24.0	24.0	24.0	24.0	28.4	28.4	28.4	28.4
Outlet pressure/ bar	1.31	1.31	1.31	1.31	1.40	1.40	1.40	1.40
Rotation speed/ RPM	1000	1000	1000	1000	2000	2000	2000	2000
Fuel type	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂
Equivalence ratio	0.9	0.8	0.7	0.6	0.9	0.8	0.7	0.6
Time step/ ×10 ⁻⁵ s	6.0	6.0	6.0	6.0	3.0	3.0	3.0	3.0

200

3. Results and discussion

In order to prevent the increase of NO_x emission factors brought by the applications of turbocharger systems to ORP engines, combustion and emission characteristics under lean-burn conditions were explored in this paper by analysing in-cylinder pressure evolutions, heat release rates, combustion duration, NO_x formations, and in-cylinder temperature.

3.1 Combustion characteristics

Applications of turbocharger systems to this ORP engine significantly increased NO_x emission factors at stoichiometric ratio conditions due to enhanced in-cylinder temperature [48] although the power output of this ORP fuelled with hydrogen was compensated greatly (it was proved in the authors' previous work, as indicated in Table S1). Lean-burn, as an effective approach to suppress NO_x formations during combustion [49, 50] was adopted to achieve low NO_x emission in this paper. In-cylinder pressure evolutions of this ORP engine over different equivalence ratio at low engine speed conditions were presented in Figure 2. The effect of equivalence ratio on in-cylinder pressure evolutions was dependent on the engine speeds, as shown in the figure. In-cylinder pressure over stoichiometric ratio condition was higher than that of the equivalence ratio of 0.9 for the engine speed of 1000 RPM; however, it was reverse for 2000 RPM engine speed. When the equivalence ratio was lower than 0.9, the effect of equivalence ratio on in-cylinder pressure was consistent for 1000 and 2000 RPM cases, which was agreed with the results in the work [51]. Peak in-cylinder

219 pressure of a gasoline engine over excess air ratio of 2.5 was lower than that of 3.0 case, and the
 220 corresponding crank angle was around 5°CA after TDC [51]. Peak in-cylinder pressure of a IC
 221 engine decreased from 23.0 bar to 16.0 bar when excess air ratio changed from 1.0 to 1.6, and the
 222 corresponding crank angle was retarded slightly [52], which was consistent with the authors' results.
 223 Lean-burn characteristics of a gasoline fuelled Wankel engine were also explored under part load
 224 conditions by Su et al. [53] that peak in-cylinder pressure decreased from 9.5 bar to 8.9 bar when
 225 excess air ratio increased from 1.0 to 1.3; and peak in-cylinder pressure was more sensitive to
 226 excess air ratio for hydrogen-gasoline fuelled scenarios than that of gasoline [53].

227 Figure 2 In-cylinder pressure evolutions over different equivalence ratio at low engine speeds

228

229 The crank angle corresponding to peak in-cylinder pressure was advanced with the increase of
 230 equivalence ratio for 1000 RPM conditions. Because flame propagation speed decreased
 231 significantly with the drop of equivalence ratio [54, 55]. Spark timing should be advanced to

232 achieve high indicated thermal efficiency under severe lean-burn cases. The profiles of in-cylinder
 233 pressure increase rates presented single-peak for small equivalence ratio scenarios; however, they
 234 were double-peak for medium and high equivalence ratio cases. The first peak was almost
 235 overlapped over different equivalence ratio for the same engine speeds. As can be seen, in-cylinder
 236 pressure almost reached the peak value around TDC if corresponding in-cylinder pressure increase
 237 rates showed single-peak; however, the in-cylinder pressure would increase to a much higher value
 238 after TDC if the corresponding pressure increase rates were double-peak. The value of the first-peak
 239 was approximately $2.0 \text{ bar } (^{\circ}\text{CA})^{-1}$ for 1000 RPM, and it was $2.5 \text{ bar } (^{\circ}\text{CA})^{-1}$ for 2000 RPM.
 240 Heat release as the series of crank angle was the dominated factor affecting in-cylinder pressure for
 241 given engine speed conditions. Heat release rates of hydrogen combustion in this turbocharged ORP
 242 engine are shown in Figure 3. Heat release rates showed double-peak, with the first peak being
 243 around 5°CA after TDC and the second one being around 12°CA after TDC. For 1000 RPM speed
 244 conditions, the first peak over equivalence ratio of 1.0 reached $30 \text{ J } (^{\circ}\text{CA})^{-1}$ which was much higher
 245 than other cases; however, the values were almost the same over equivalence ratio of 0.9 and 1.0 for
 246 2000 RPM. Peak heat release rates of a direct injection gasoline engine were similar for the
 247 equivalence ratio of 0.3 and 0.4 at part load conditions, being approximately $12 \text{ J } (^{\circ}\text{CA})^{-1}$ [51].
 248 Peak heat release rates of a hydrogen-enriched gasoline engine decreased significantly with the
 249 increase of excess air ratio [52], and the value over stoichiometric ratio was approximately twice of
 250 the excess air ratio of 1.0; additionally, the corresponding crank angle was retarded from 10°CA
 251 after TDC to 25°CA after TDC. The test data had a similar tendency with the authors' simulation
 252 results. Peak heat release rates were significantly dependent on the engine type, fuel type, engine
 253 speed, engine load, engine displacement, and so on.

254 Figure 3 Heat release rates over different equivalence ratio at low engine speeds

255 For low equivalence ratio conditions in this ORP engine, more heat was released later than 30 °CA
 256 after TDC than high equivalence ratio cases, which was mainly caused by weakened hydrogen
 257 flame propagation due to severe lean-burn. It significantly decreased the power capacity of burned
 258 gas. Flame propagation could be reflected by heat of reactions to some extent, although they were
 259 different things. Figure 4 shows the distributions of heat of reactions in combustion chambers over
 260 different cases (only parts of figures are shown in the main document, others are presented in
 261 support information). It was agreed with the in-cylinder pressure evolutions that high equivalence
 262 ratio promoted in-cylinder combustion. As shown in Figure 4, higher engine speed contributed to
 263 more heat release and faster combustion due to high intake temperature and pressure in this paper.

264 (a) 1000 RPM (other cases shown in Figure S3)

265 (b) 2000 RPM (other cases shown in Figure S4)

266 Figure 4 Distributions of heat of reactions in combustion chambers over various engine speeds

267
 268 Mass burn fraction profiles were consistent with in-cylinder pressure evolutions that higher mass

burn fraction at the same crank angle would lead to higher in-cylinder pressure, as presented in Figure S5. In theory, slight lean-burn could effectively accelerate the combustion due to more oxygen available; however, lean-burn meant lower fuel mass fraction in hydrogen/air mixture.

Figure 5 presented the start of combustion, combustion phase, and combustion duration for different scenarios. Start of combustion referred to the crank angle being corresponding to 10% mass burn fraction (MBF, CA_{10}); and combustion phase was corresponding to 50% MBF (CA_{50}); combustion duration was the crank angle between 10% MBF and 90% MBF (CA_{10-90}). CA_{10} and CA_{50} decreased with the increase of equivalence ratio for 1000 RPM engine speed conditions, resulting from high hydrogen flame propagation speed over high equivalence ratio scenarios; however, the values of CA_{10} , CA_{50} , and CA_{10-90} over the equivalence ratio of 0.9 were the smallest for 2000 RPM conditions. The influence of equivalence ratio was also partly dependent on the engine operation conditions, as demonstrated in the study [56] using experiments. The effect of equivalence ratio on start of combustion, combustion phase, and combustion duration also varied with fuel types [52, 57-59]. Start of combustion and combustion duration of a reciprocating engine were retarded with the increase of excess air ratio when the engine was fuelled with ethanol and hydrogen-enriched ethanol [58]. For a hydrogen-enriched gasoline engine, slight lean-burn advanced the start of combustion; and combustion duration increased then decreased with the increase of excess air ratio [59]. Flame developing period decreased significantly with the increase of equivalence ratio for natural gas fuelled conditions [56]; however, the equivalence ratio corresponding to the shortest fame developing period for 10% hydrogen-enriched natural gas was around 0.7.

Figure 5 Start of combustion, combustion phase, and combustion duration

292 In this paper, spark timing for all the scenarios was the same. Lean-burn was usually accompanied
 293 by advanced spark timing in practice to compensate the drop of indicated thermal efficiency caused
 294 by slow combustion (lean-burn). It would inevitably increase NO_x formations in combustion
 295 chambers for advanced spark timing, so balances between NO_x emissions and indicated thermal
 296 efficiency should be made in future work. Figure 6 presented the hydrogen mass fraction
 297 distributions in combustion chambers, which was consistent with the distributions of heat of
 298 reactions. Hydrogen was mainly in the top and corners of cylinders at the end of combustion
 299 process, where heat of reactions was still high.

Note: EQ, equivalence ratio; CA, crank angle

(a) 1000 RPM (other cases shown in Figure S6)

Note: EQ, equivalence ratio; CA, crank angle

(b) 2000 RPM (other cases shown in Figure S7)

Figure 6 Distributions of hydrogen mass fraction in combustion chambers over various engine speeds

304 P-V diagrams of this ORP engine fuelled with hydrogen at different conditions are shown in Figure
 305 7. At the beginning of expansion stroke at 1000 RPM conditions, in-cylinder pressure over the

306 stoichiometric ratio situations continued to increase after TDC; it was almost kept at a constant
 307 value for equivalence ratio of 0.7~0.9; and it decreased significantly as long as the combustion
 308 chamber passed TDC for the equivalence ratio of 0.6. For 2000 RPM engine speed conditions, the
 309 in-cylinder pressure increased to a quite high value after TDC for the equivalence ratio of 0.9; and
 310 they had similar tendency with those of 1000 RPM cases for equivalence ratio of 0.6~0.8.
 311 In-cylinder pressure at the end of expansion stroke changed slightly for different equivalence ratio.
 312 Discharge process included free discharge and forced discharged, and the combustion chamber
 313 volume change during free discharge was more dependent on the engine speeds than equivalence
 314 ratio. As for the reciprocating engines, exhaust valves were opened before TDC generally, which
 315 significantly promoted the drop of in-cylinder pressure during free discharge [60, 61]. So, the
 316 pumping losses during discharge process of this ORP engine were higher than that of reciprocating
 317 engines in theory if they had same engine displacement.

318 Figure 7 P-V diagrams over various engine speeds

319 3.2 Emission characteristics

320 During hydrogen combustion, NO_x were the main pollutants; and only thermal NO_x were formed
 321 due to no carbon and nitrogen elements in hydrogen fuel. The main purpose of the lean-burn
 322 technology was to drop NO_x emissions in this paper. Accumulated NO_x per cylinder per cycle
 323 during hydrogen combustion are presented in Figure 8. The tendency of accumulated NO_x
 324 formations with equivalence ratio was the same for 1000 and 2000 RPM conditions. Accumulated
 325 NO_x emissions over the equivalence ratio of 0.9 were higher than that of equivalence ratio of 1.0,
 326 which was consistent with many published results [56, 62]. Slight lean-burn would promote NO_x
 327 formations during combustion; then, the accumulated NO_x decreased significantly with the drop of
 328 equivalence ratio. It almost achieved zero-NO_x emissions when the equivalence ratio was 0.6; and it

329 was believed to be kept at a low level when the equivalence ratio continued to decrease. It should be
 330 noted that accumulated NO_x over stoichiometric ratio was higher than that of equivalence ratio of
 331 0.9 for 1000 RPM before the peak value; however, it was inverse for 2000 RPM engine speed. It
 332 was mainly caused by fast combustion of corresponding high emission cases.

Figure 8 Accumulated NO_x during hydrogen combustion over various engine speeds

333
 334
 335 Accumulated NO_x decreased slightly after reaching the peak value, which was agreed with the test
 336 results by Knop et al. [63] and Konnov et al. [64]. This phenomenon was caused by reverse
 337 reactions of NO_x formations which were reversible chemical reactions, as indicated in Zeldovich
 338 mechanism [63]. Seen from Figure 8(a), NO_x formations were retarded with the drop of equivalence
 339 ratio at 1000 RPM engine speed conditions; however, it was much earlier for equivalence ratio of
 340 0.9 than other cases at 2000 RPM. Most of NO_x were formed earlier than 20 °CA before TDC for all
 341 the given cases; and only small amounts of NO_x were formed before TDC, which could be seen
 342 from Figure 9 which presented NO_x distributions in combustion chambers. NO_x concentration

343 increased slightly when excess air ratio increased from 1.0 to 1.1 for a hydrogen-enriched ethanol
 344 reciprocating engine [58]; in addition, NO_x concentration was almost zero when excess air ratio was
 345 approximately 1.5, which was consistent with the authors' simulation results. NO_x concentration in
 346 Luo's research [40] where a turbocharged hydrogen engine was used, was also quite low for the
 347 equivalence ratio of 0.6. NO_x concentration drop with the increase of equivalence ratio was more
 348 significant for a hydrogen-gasoline fuelled Wankel engine than that of gasoline [53]. This hydrogen
 349 fuelled ORP engine would be a promising power for future hybrid vehicles by adopting low
 350 equivalence ratio (<0.7) such that after-treatment would be unnecessary; meantime, hydrogen
 351 fuelled IC engine could still keep high thermal efficiency and operate steadily; additionally, power
 352 density of this hydrogen fuelled ORP engine under lean-burn would still be higher than
 353 reciprocating engines (see the following section). Lower in-cylinder temperature contributed to less
 354 heat losses, and further decreasing the size and energy consumption of coolant pumps.

355 (a) 1000 RPM (other cases shown in Figure S8)

(b) 2000 RPM (other cases shown in Figure S9)

Figure 9 Distributions of NO_x mass fraction in combustion chambers over various engine speeds

Temperature was one of the main factors contributing to NO_x formations [62]. In-cylinder temperature evolutions of this ORP engine fuelled with hydrogen were shown in Figure 10. Peak in-cylinder temperature increased with equivalence ratio, which showed a similar result with Su et al. [53], where peak in-cylinder pressure and temperature decreased continuously with the increase of excess air ratio for a Wankel engine fuelled with gasoline and hydrogen-enriched gasoline at part load conditions [53]. Peak in-cylinder temperature of this ORP engine reached 2500 K for stoichiometric hydrogen/air mixture; crank angle corresponding to the peak in-cylinder temperature was similar to that of peak accumulated NO_x .

Figure 10 In-cylinder temperature during combustion over various engine speeds

Peak in-cylinder temperature over the equivalence ratio of 0.6 was higher than 1800 K, and NO_x formations were quite low; however, large quantities of NO_x were generated when in-cylinder temperature was lower than 1800 K for high equivalence ratio scenarios, as presented in Figure S10. Equations 1~3 show the Zeldovitch mechanism of NO formation. As indicated in FLUENT tutorial [65], reaction rate constants of forward reactions in Equations 1~3 were the function of in-cylinder temperature; Equation 3 was considered to happen at near-stoichiometric and fuel-rich conditions; and NO could be formed under relative low temperature through Equation 3 for near-stoichiometric conditions. NO formation mainly came from Equations 1 and 2 for low equivalence ratio cases (<0.7), whereas in-cylinder temperature was low due to serious lean-burn. Accumulated NO was the joint effects of the forward and reverse reactions of Equations 1~3. Temperature distributions in

combustion chambers were similar to that of NO_x formations, as shown in Figure 11. High temperature zones were mainly formed in the bowls at the beginning of combustion, and then they were spread into the gaps between the end faces of adjacent pistons.

(a) 1000 RPM (other cases shown in Figure S11)

(b) 2000 RPM (other cases shown in Figure S12)

Figure 11 Temperature distributions in combustion chambers over various engine speeds

3.3 Performance evaluations

Overall performance of this ORP engine fuelled with hydrogen over different equivalence ratio at low engine speed conditions are presented in Figure 12. High equivalence ratio significantly

promoted the power output of this engine at 1000 RPM conditions, with the power output increasing from 7.1 kW to 11.8 kW, which was mainly caused by high mass fraction of hydrogen in hydrogen/air mixture for high equivalence ratio cases. Indicated NO_x emission factors increased and then decreased with the drop of equivalence ratio, with the maximum value being approximately 20 g (kW h)^{-1} at 1000 RPM conditions, which was consistent with the published data in terms of the tendency [66-68]. The drop of indicated thermal efficiency with the increase of equivalence ratio was observed in a reciprocating engine [40]. The effect of equivalence ratio on indicated thermal efficiency was significantly dependent on the engine speeds. As demonstrated in Figure 12(b), slight lean-burn significantly promoted in-cylinder combustion for 2000 RPM scenarios; however, it was inversed for 1000 RPM. Effect of lean-burn on engine power output and NO_x emissions was also conducted by Luo et al. [40] based on a turbocharged reciprocating engine. Equivalence ratio of 0.8 contributed to the maximum power output for 1500 RPM; and it was 0.9 at 2000 RPM, which was inconsistent with the results of authors' ORP engine whose power decreased continuously with the drop of equivalence ratio. In addition, the maximum brake thermal efficiency was corresponding to the equivalence ratio of 0.65~0.80 for both 1500 and 2000 RPM engine speeds [40]. Indicated thermal efficiency of this ORP engine fuelled with hydrogen was higher than that of reciprocating engines generally, concluded by comparisons with the work [40]. Indicated thermal efficiency at excess air ratio of 1.5 was proved to be the highest for the excess air ratio range of 1.0~3.0 [51]; and it was also indicated that the changes of indicated specific fuel consumption with excess air ratio were different for various fuel injection pressure. Ma et al. [69] indicated that lean-burn (<0.85) contributed to an improvement of engine power, and a reduction of combustion duration and cycle-to-cycle variations; however, little difference was observed for near-stoichiometric conditions (>0.85) [69]. In summary, the effect of equivalence ratio on engine performance differed greatly for different situations including engine type, fuel, engine speed and torque, fuel injection methods and so on. For this ORP engine, advanced spark timing was recommended for future explorations of better engine performance under lean-burn (<0.7) conditions.

Figure 12 Performance comparisons of ORP engine over different equivalence ratio and low engine speed conditions

4. Conclusion

In this paper, a 3D numerical simulation method was used to explore the effect of equivalence ratio (≤ 1) on combustion and emission characteristics of this ORP engine fuelled with hydrogen under low engine speed (1000 and 2000 RPM) conditions. The main conclusions are as the follows:

- (1) Peak in-cylinder pressure over 1000 RPM engine speed decreased continuously from approximately 54 bar to 39 bar when the equivalence ratio decreased from 1.0 to 0.6; however, peak in-cylinder pressure over the equivalence ratio of 0.9 was much higher than that of stoichiometric ratio cases for 2000 RPM, which was caused by the enhanced combustion for slight lean-burn conditions. Maximum pressure increase rates were almost overlapped for different equivalence ratio

430 over given engine speeds, and it happened around 10 °CA before TDC for 1000 and 2000 RPM
431 engine speeds.

432 (2) Peak heat release rate was approximately 30 J (°CA)⁻¹ for stoichiometric ratio cases, and it was
433 much higher than lean-burn scenarios for 1000 RPM engine speed; however, the value was almost
434 the same for the equivalence ratio of 0.9 and 1.0 over 2000 RPM engine speed. Combustion
435 duration was in the range of 22.5~31.9 °CA for 1000 RPM engine speed, and it was in the range of
436 21.5~31.7 °CA for 2000 RPM. Start of combustion and combustion duration for the equivalence
437 ratio of 0.9 over 2000 RPM were lower than those of stoichiometric ratio cases.

438 (3) The changes of combustion chamber volume in the free discharge process depended on the
439 engine speed rather than the equivalence ratio. High in-cylinder pressure in the free discharge
440 process significantly increased the pumping losses, which was mainly caused by the late opening of
441 exhaust port.

442 (4) Accumulated NO_x formations under the equivalence ratio of 0.9 were the highest among the
443 given engine speed conditions; NO_x formations over the equivalence ratio of 0.6 was almost zero,
444 which significantly promoted the applications of hydrogen fuelled ORP engines to hybrid vehicles
445 and range extender electric vehicles. The crank angle corresponding to the peak in-cylinder
446 temperature and peak accumulated NO_x was similar for individual scenario.

447 (5) Engine power output decreased continuously with the drop of equivalence ratio for 1000 and
448 2000 RPM engine speeds. Indicated thermal efficiency and indicated NO_x emission factors reached
449 the maximum value over the equivalence ratio of 0.9 for 2000 RPM engine speed. The level of
450 indicated thermal efficiency of this hydrogen fuelled ORP engine was higher than that of
451 reciprocating engines under lean-burn situations.

452

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