Numerical simulation on lean-burn characteristics of a naturally aspirated opposed rotary piston engine fuelled with hydrogen at wide open throttle conditions

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Abstract:

Opposed rotary piston engines are characterized by high power density, which makes them as an ideal power source for hybrid vehicles and range extended electric vehicles. Hydrogen applications can fully exhibit the merits of opposed rotary piston engines, and achieve zero carbon dioxide emissions; however, the applications seriously worsen the nitrogen oxides emissions. In this investigation, lean-burn was adopted to achieve low nitrogen oxides emissions using a three dimensional numerical simulation approach. The results indicated that engine speed of 3000 r/min presented the highest in-cylinder pressure during combustion among the given scenarios, and the pressure over 3000 r/min depended more on the equivalence ratio than that of 1000 r/min and 2000 r/min. Heat release rates were very sensitive to low equivalence ratio. Combustion duration over the equivalence ratio of 0.8 was the shortest among 1000 r/min cases; however, it decreased with equivalence ratio for 2000 r/min and 3000 r/min. Heat loss rates through cylinder walls increased significantly with engine speed, meanwhile they were more dependent on the equivalence ratio over higher engine speed. Maximum nitrogen monoxide formation rates over 3000 r/min occurred slightly earlier than those of 1000 r/min and 2000 r/min. Equivalence ratio of 0.8 showed the highest indicated thermal efficiency over corresponding engine speed, and nitrogen dioxide emission factors were quite low over the equivalence ratio of 0.7 for the given engine speed.

Keywords: opposed rotary piston engines; hydrogen fuel; lean-burn; combustion characteristics; NO_x emissions; engine speed

1. Introduction

Nowadays, global warming caused by carbon dioxide (CO₂) is becoming more and more serious; and on-road vehicles are one of the main sources of CO₂ emission. It was reported by European Commission (EU) (European Commission, 2019a) that passenger cars and light commercial vehicles were responsible for approximately 12.0% and 2.5% of total EU CO₂ emission, respectively. In the new regulation, CO₂ emission factor of new registered cars from 2021 would be lower than 95 g/km which corresponded to a fuel consumption level of approximately 4.1 L/100 km for petrol cars and 3.6 L/100 km for diesel cars (European Commission, 2019b). Hybrid vehicles and range extended electric vehicles, being effective approaches of decreasing CO₂ emission factor (De Haan et al., 2007; Lü et al., 2020; Nanaki and Koroneos, 2013; Tran et al., 2020) as well as hazardous emissions (especially cold start emissions which were the main concerns for the modern vehicles (Gao et al., 2019; Zare et al., 2017)), are gaining large attentions. As the main power

sources of these vehicles, internal combustion (IC) engines need to have characters of high ratio of power/mass, compact designs, high brake thermal efficiency, and low emission factors (Lee et al., 2016; Salanki and Wallace, 1996; Turner et al., 2019). Wankel engines and opposed rotary piston (ORP) engines are alternative power sources of reciprocating engines applied to hybrid vehicles and range extended electric vehicles, because of their high power density, low complexity, and being free of connecting rod mechanism. Since hydrogen was considered to be ultimate fuel due to its high energy density and no CO₂ emission during combustion (Moharamian et al., 2018; Wu et al., 2020), it was widely used in advanced combustion systems, such as micro combustors (Li et al., 2020; Zuo et al., 2020a; Zuo et al., 2020b) and internal combustion engines (Acar and Dincer, 2019; Javed et al., 2016). Hydrogen applications to Wankel engines and ORP engines would promote the developments of hybrid vehicles and range extended electric vehicles, further, achieving environmental friendly travel (Keller and Lutz, 2001; Zohuri, 2019).

Hydrogen as pure fuel and fuel additions of IC engines was widely investigated to improve the overall performance (Amrouche et al., 2016b; Su et al., 2017a; Yontar, 2020). Especially for Wankel engines, hydrogen applications would significantly ease the disadvantages caused by long and narrow combustion chambers which led to high exhaust emissions and low brake thermal efficiency (Ji et al., 2020; Shi et al., 2020). Benefits of hydrogen combustion were mainly attributed to its high flame propagation speed, short combustion durations, excellent lean-burn capability, and short quenching distance (Su et al., 2017a; Vinoth Kanna et al., 2020; Zhu et al., 2020). Hydrogen additions greatly promoted the combustion of other fuels, which contributed to the drop of combustion durations, further, leading to high thermal efficiency (Köse and Ciniviz, 2013; Miyamoto et al., 2011). Meantime, hydrogen additions could decrease the unburned hydrocarbon (HC) and carbon monoxide (CO) emissions, benefited from the fact that hydrogen additions broadened the lean-burn limits, decreased the quenching distance, and increased the in-cylinder combustion temperature (Shivaprasad et al., 2014; Zhou et al., 2014). Additionally, hydrogen additions significantly dropped the coefficient of variations (COV) in maximum pressure and indicated mean effective pressure (Chen, Zhao et al., 2020; Ma et al., 2008; Sun et al., 2013; Wang et al., 2008). It contributed to an enhanced stability of in-cylinder combustion, which would be helpful to decrease idle speed for dropping the idle fuel consumption.

However, high in-cylinder combustion temperature of hydrogen and hydrogen enriched fuel led to numerous nitrogen oxides (NO_x) formations. Lean-burn was an effective approach to achieve low

NO_x combustion by dropping in-cylinder temperature; additionally, it could theoretically improve the brake thermal efficiency for some operation conditions. As indicated in the work (Ma et al., 2007), NO_x emission factors decreased from 20 g/(kW h) to lower than 5 g/(kW h) when the excess air ratio increased from 1.0 to 1.6, accompanied by a slight increase of brake thermal efficiency. It was consistent with Gong's (Gong et al., 2019a; Gong et al., 2019b) and Luo's research (Luo et al., 2019) where a turbocharged hydrogen engine was used. Amrouche et al. (Amrouche et al., 2016a) investigated the Wankel engine performance under lean-burn conditions when hydrogen enriched gasoline was used. The results indicated that hydrogen enrichment effectively increased the engine thermal efficiency under the same equivalence ratio as pure gasoline cases; moreover, NO_x emission factors dropped more than 90% when equivalence ratio decreased from 0.9 to 0.6. However, brake thermal efficiency was almost kept the same for the equivalence ratio of 0.8~0.9, then decreased with the drop of equivalence ratio. Su et al. (Su et al., 2018) also researched the lean-burn characteristics of a Wankel engine fuelled with hydrogen enriched n-butanol under low engine load conditions. NO_x emissions decreased more 90% when the equivalence ratio decreased from 1.0 to 0.75; however, brake thermal efficiency dropped as well, resulting from a significant increase of combustion durations. The effect of lean-burn on brake thermal efficiency varied with scenarios, although it was consistent for NO_x emissions (Amrouche et al., 2016a; Su et al., 2018; Su et al., 2017b; Yu et al., 2019). Spark timing should be adjusted for lean-burn situations to balance the effects from prolonged combustion durations which prevented the improvement of brake thermal efficiency. Artificial neural network (ANN) and response surface methodology (RSM) (Banerjee et al., 2017) could be effective technologies to explore the optimal equivalence ratio of low NO_x emissions and high thermal efficiency.

ORP engines (or twin-rotor piston engines), as a new type of vehicle power source, operated smoothly with low carbon footprint, multi fuel capacities, and were considered to be suitable for the applications of hybrid vehicles and range extended electric vehicles. Excellent performance of ORP engines was benefited from the short cyclic period (360° crank angle (CA)) and the layouts of intake ports, exhaust ports, and spark plugs. Volumetric efficiency of a four-cylinder ORP engine was higher than reciprocating engines based on an overall estimation (Gao et al., 2020b); and the power output was demonstrated to be approximately twice of a naturally aspirated reciprocating engine, under the conditions of the same engine displacement (Gao et al., 2020b). Although ORP engines presented many advantages for hybrid vehicles and range extended electric vehicle

applications, the investigations were at an initial stage. Deng et al. (Deng et al., 2013) designed a twin-rotor piston engine and a differential velocity drive mechanism; also, the piston movements and valve timing were analysed using mathematical equations. In addition, thermodynamic processes of the twin-rotor piston engine were analysed using Matlab/Simulink (Zou et al., 2014). The twin-rotor piston engine was restructured as a twin-rotor embedded piston engine to resolve the sealing problem, because the sealing method of reciprocating engines could be directly applied to the twin-rotor embedded piston engine (Chen et al., 2014). Advantages of ORP engines over reciprocating engines were detailed analysed using a 3D numerical simulation method. The engine power density estimated using a 1D simulation approach was approximately 80 kW/L when it was fuelled with gasoline (Gao et al., 2020b). Additionally, pumping loss during the intake process was calculated based on 3D simulation results, with the conclusions that pumping loss was higher than reciprocating engines under the same engine speed conditions (Gao et al., 2020a). Gao et al. (Gao et al., 2020c) demonstrated that NO_x emission factors of hydrogen fuelled ORP engines were high over low engine speed and wide open throttle conditions. To the authors' knowledge, there were few papers reporting hydrogen applications to ORP engines over lean-burn conditions, although hydrogen was the proper fuel for short cyclic period engines to achieve high thermal efficiency. Also, ORP engines fuelled with hydrogen emitted less NO_x than Wankel and reciprocating engines theoretically due to shorter time for NO_x formations.

In summary, lots of researches had been conducted about the hydrogen applications to reciprocating engines and Wankel engines; and benefits of lean-burn were demonstrated over various conditions. However, the investigation of ORP engines was at an early stage. Due to the excellent performance especially for the power density, ORP engines had potentials for the hybrid vehicle applications. Demonstrated by the authors' previous work (Gao et al., 2020c), NO_x emission factors of this hydrogen fuelled ORP engine at low engine speed conditions were quite high when air/hydrogen mixture was stoichiometric. In order to promote the hydrogen fuelled ORP engines to be put into practice, lean-burn technology should be used; meantime, the optimal equivalence ratio should be explored for low NO_x emission and high thermal efficiency to achieve environmental friendly strategy and production. However, the lean-burn characteristics of hydrogen fuelled ORP engines are limited to date. In this paper, lean-burn technology for a naturally aspirated hydrogen ORP engine was explored at low engine speed conditions. It was focused on the in-cylinder combustion, flame propagations, heat loss, NO_x formations, and indicated thermal efficiency. The equivalence

ratio delivering low NO_x emission factors and high thermal efficiency would also be obtained.

2. Materials and methods

In order to explore the effect of lean-burn on hydrogen ORP engine performance at low engine speed conditions, a 3D simulation approach was applied to various scenarios. Firstly, the engine structures, operation process, and potential advantages to reciprocating engines were described; then, the 3D simulation model and theory were introduced.

2.1 Configurations and operation process of the opposed rotary piston engine

The ORP engine was designed for the applications of hybrid vehicles and range extender electric vehicles, such that it was a small scale engine with a displacement of 0.5468 L. Its rated power output was approximately 40 kW at 5000 RPM when fuelled with gasoline, being estimated using a 1D simulation approach (Gao et al., 2020b). It was a four-stroke, four-cylinder engine, having a compression ratio of 9.73. As this engine was fuelled with hydrogen, which was ignited using spark plugs. This engine had two spark plugs, two shafts, two engine blocks, one exhaust port, and three intake ports. More details of this ORP engine were presented in the authors' previous work (Gao et al., 2020a). Figure 1 shows the configurations of this ORP engine. Combustion chambers of this engine were covered by end faces of pistons, surfaces of shafts, and inner faces of engine blocks. Pistons 1 and 3 were connected with shaft 1; pistons 2 and 4 were connected with shaft 2. Positions of pistons should be adjusted to ensure the correct valve timing. There were two bowls at the end faces of each piston. Judged from the engine structures, the potential merits of this ORP engine compared to reciprocating engines were as the follows:

- (1) This engine had a compact design, was free of connecting rod mechanism, and operated smoothly. These advantages would be helpful for the applications to hybrid vehicles and range extended electric vehicles. It also contributed to less noise in theory.
- (2) Volumetric efficiency of this ORP engine was supposed to be higher than reciprocating engines. It was benefited from the fact that intake and exhaust ports were not limited by spark plugs and cylinder head area.
- (3) It had a higher power density than reciprocating engines due to its short cyclic period of 360° CA. Short cyclic period also contributed to decreasing NO_x emissions because of less time for thermal NO_x formations.
- (4) It had a low possibility of engine knock, which was resulted from the separations of combustion chambers and exhaust ports in the combustion process. Exhaust ports were one of the main reasons

causing hot points leading to engine knock.

(5) It had a high percentage of constant volume combustion, because two spark plugs contributed to a short flame propagation distance, further more hydrogen combustion around top dead centre. It promoted to the increase of brake thermal efficiency.

(6) It had low a possibility of backfire due to the existing of two spark plugs.

(7) It did not have any early opening of intake ports, which decreased the probability of backfire if hydrogen fuel was applied to this engine.

(8) It could significantly decrease the possibility of backfire achieved by the fact that intake port 1 (the one close to the exhaust port) provided the fresh air, and intake ports 2 and 3 delivery rich fuel/air mixture. The residual gas from last cycle would be cooled down by fresh air from intake port 1.

(9) Heat loss through cylinder walls was less than that of reciprocating engines and Wankel engines in theory due to its short duration in time of high temperature process.

Figure 1 Configurations of the opposed rotary piston engine, reproduced from the work (Gao et al., 2020b)

As this ORP engine was a new type engine, its investigations were at an initial stage. Issues of this ORP engine should be addressed before practical applications, such as lubrication, seal, and thermal load. Operation process of this ORP engine included intake stroke, compression stroke, expansion

stroke, and exhaust stroke, with each stroke lasting 90° CA. Its operation process was shown in Video 1. Top dead centres (TDCs) and bottom dead centres (BDCs) of this engine are shown in Figure 2, and their corresponding crank angle was also presented. Sinusoidal rotations were attached to the two shafts during simulations (Gao et al., 2020b).

Figure 2 Engine model, fluid domains, and meshes of this ORP engine

Meshes of this ORP engine model are also presented in Figure 2(c), and the mesh number of individual parts is shown in Table 1. Minimum orthogonal, maximum ortho skew, and maximum aspect ratio of overall mesh quality were 0.337, 0.663, and 16.726, respectively. Sensitivity analysis of mesh number (mesh size) and calculation residuals was discussed in the authors' previous work (Gao et al., 2020a) (see Table 2), where grid number of 779324 and calculation residual of 10^{-6} were chosen. Dynamic meshes were applied to simulate the unsteady flow in the engine. FLUENT (ANSYS, 2013) code and Renormalization group (RNG) k-epsilon model were used in the simulation. The meshes shown in Table 1 were corresponding to the engine status in Figure 2(c). NO_x emission model was activated during simulation, and NO_x formation was based on Zeldovich mechanism in FLUENT software. Hydrogen/air mixture ignition was achieved by patching high temperature zones in the regions of spark plugs. The patched temperature was 2073 K. Ignition timing for the given scenarios in this investigation was the same (17°CA before TDC).

Table 1 Element numbers of fluid domains

Sub-domain	Elements
Intake pipe 1	12210
Intake pipe 2	12210
Intake pipe 3	16632
Exhaust pipe	40664

Spark plug	18202
Bowl	37718
Cylinder	53376

Table 2 Sensitivity analysis of mesh number and residual setting, reproduced from (Gao et al., 2020a)

Mesh number	Residuals	Time step/ s	Average in-cylinder pressure at the end of intake process/ Pa
593246	10^{-6}	10^{-5}	99599
	5×10^{-6}	10^{-5}	99595
	10^{-6}	2×10^{-5}	99598
779324	10^{-6}	10^{-5}	99593
	10^{-6}	0.5×10^{-5}	99589
	0.3×10^{-6}	10^{-5}	99591
102672	10^{-6}	10^{-5}	99597

2.2 Three dimensional numerical simulation theory

Part of work in this section was introduced in the authors' previous work (Gao et al., 2021).

Continuity equation is shown in Equation 1,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m \quad (1)$$

t is time; ρ is the working fluid density; $\vec{v}$ is fluid velocity; S_m is the mass added to the continuous phase or the user-defined source.

Conservation of momentum is shown in Equation 2,

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\bar{\tau}) + \rho \vec{g} + \vec{F} \quad (2)$$

t is time; ρ is the working fluid density; $\vec{v}$ is fluid velocity; p is the static pressure; $\bar{\tau}$ is the stress tensor; $\rho \vec{g}$ is the gravitational body force; $\vec{F}$ is external body force.

Energy governing equation is shown in Equation 3,

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho \vec{v} h) = -\frac{dp}{dt} + \nabla \cdot (k \nabla T) + \Phi \quad (3)$$

Where, t is time; h is the specific enthalpy; ρ is density; $\vec{v}$ is fluid velocity; p is the static pressure; k is thermal conductivity; T is temperature; Φ is the dissipation function representing the work done against force.

In FLUENT code, the combustion model is described in a similar form to energy balance equation (Kozubkov áet al., 2012), as shown in Equation 4,

$$\frac{\partial}{\partial t}(\rho Y_{i'}) + \frac{\partial}{\partial x_i} \cdot (\rho \bar{u}_i Y_{i'}) = - \frac{\partial}{\partial x_i} \cdot \bar{J}_{i',i} + R_{i'} + S_{i'} \quad (4)$$

Where, t is time; ρ is density; $Y_{i'}$ is local mass fraction of the species i ; $\bar{u}_i$ is average velocity; $\bar{J}_{i',i}$ is the diffusion flux of species i ; $R_{i'}$ is production rates of species i ; $S_{i'}$ is production increase of distributed phase.

The turbulent flame speed closure is computed using a model for wrinkled and thickened flame fronts (Zimont et al., 1998), as indicated in Equation 5.

$$U_t = A(u')^{3/4} U_l^{1/2} \alpha^{-1/4} l_t^{1/4} = A u' \left(\frac{T_t}{T_c} \right)^{1/4} \quad (5)$$

A is model constant; u' is root-mean-square velocity; U_l is laminar flame speed; α is molecular heat transfer coefficient of unburnt mixture; l_t is turbulence length scale; T_t is turbulence time scale; T_c is chemical time scale.

The laminar flame speed (Metghalchi and Keck, 1982) is calculated using Equation 6,

$$U_l = U_{l,ref} \left(\frac{T_u}{T_{u,ref}} \right)^\gamma \left(\frac{p_u}{p_{u,ref}} \right)^\beta \quad (6)$$

$U_{l,ref}$ is reference laminar flame speed; T_u is the unburnt reactant temperature; p_u is pressure ahead of the flame; $T_{u,ref}$ is 298 K; $p_{u,ref}$ is 1.0 bar. γ and β are the functions of equivalence ratio ahead of the flame front.

Ignition delay model in FLUENT code is shown in Equation 7,

$$T_{id} = \frac{C_1 + 0.22 \bar{S}_p}{6N} \exp \left[E_a \left(\frac{1}{RT} - \frac{1}{17190} \right) + \left(\frac{21.2}{P - 12.4} \right)^{e_p} \right] \quad (7)$$

T_{id} is ignition delay; C_1 is 0.36; $\bar{S}_p$ is average value of the source term of the pressure; N is engine revolution speed per minute; E_a is the effective activation energy; e_p is the pressure exponent; T is temperature; p is pressure.

In the FLUENT code, the NO formation mechanism was based on Zeldovitch (Knop et al., 2008), and NO formation process was shown in Equations 8~10.

2.3 Boundary conditions of simulation scenarios

Based on the authors' previous research (Gao et al., 2020c), NO_x emission factors of this ORP engine over low engine speed conditions were much higher than those of high speed scenarios. In this paper, lean-burn was used to decrease NO_x emissions at low engine speed conditions. The boundary conditions of the simulations are presented in Table 3. As the cyclic period in time changed with engine speed, time step setting was different for various engine speed. However, the setting ensured that same time step was corresponding to the same crank angle for different scenarios. Intake mixture of the intake pipes were set as H₂, O₂, and N₂, which were uniformly mixed. The temperature of cylinder walls was set as a constant value of 573 K, which could generate errors (such as heat loss rates). In reality, the temperature changed greatly with the engine operations rather than a constant value.

Table 3 Boundary conditions of simulation scenarios

Boundary conditions	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8	Case 9
Intake pressure/ bar	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Intake temperature/ K	293	293	293	293	293	293	293	293	293
Outlet pressure/ bar	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Rotation speed/ RPM	1000	1000	1000	2000	2000	2000	3000	3000	3000
Fuel type	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂
Equivalence ratio	0.7	0.8	0.9	0.7	0.8	0.9	0.7	0.8	0.9
Time step/ $\times 10^{-5}$ s	6.0	6.0	6.0	3.0	3.0	3.0	2.0	2.0	2.0
Wall temperature/ K	573	573	573	573	573	573	573	573	573

3. Results and discussion

In order to decrease NO_x emissions, lean-burn was applied over low and medium engine speed conditions. Lower equivalence ratio would lead to higher cycle-by-cycle variation (CCV) (Ma et al., 2008), and excessive lean-burn would drop the indicated thermal efficiency, so equivalence ratio of hydrogen/air mixture should be proper.

3.1 Combustion characteristics

Volumetric efficiency dominated the quantity of hydrogen/air mixture, further affecting the performance of IC engines (Gumus, 2011). Volumetric efficiency of this hydrogen fuelled ORP engine is shown in Table S1 that it significantly depended on the engine speed. The volumetric efficiency increased from approximately 86% to 90% when the engine speed changed from 1000

RPM to 3000 RPM; however, it was almost free of the influence of equivalence ratio. Volumetric efficiency of this ORP engine was at a similar level to reciprocating engines, concluded by comparing with the reported results (Masi and Gobbato, 2012; Song et al., 2017). Average in-cylinder pressure during combustion is also relied on the volumetric efficiency to some extent, and the in-cylinder pressure evolutions of the given scenarios are shown in Figure 3. Peak in-cylinder pressure over 3000 RPM was higher than that of the other two engine speed, which agreed well with the volumetric efficiency (Table S1). The amount of hydrogen over the equivalence ratio of 0.8 was less than the cases of 0.9; however, the in-cylinder pressure changed slightly when the equivalence ratio dropped from 0.9 to 0.8, which was mainly caused by short combustion duration for the equivalence ratio of 0.8. Lean fuel/air mixture was demonstrated to be helpful to accelerate the in-cylinder combustion, which conducted to increasing engine thermal efficiency. However, the optimal equivalence ratio in terms of thermal efficiency varied with fuel types, engine types, and engine conditions (Cho and He, 2008; Gong et al., 2019b; Ma et al., 2007). Crank angle corresponding to peak in-cylinder pressure over 3000 RPM was retarded compared with that of 1000 RPM and 2000 RPM over the equivalence ratio of 0.8 and 0.9. Peak in-cylinder pressure under the equivalence ratio of 0.7 dropped slightly compared with that of 0.8 and 0.9 for 1000 RPM and 2000 RPM; however, it decreased significantly for 3000 RPM, which was mainly caused by short cyclic period in time and slow combustion (in terms of crank angle) caused by lean-burn. Peak in-cylinder pressure over the equivalence ratio of 0.7 was greatly advanced compared with that of 0.8 and 0.9. It was mainly caused by slower combustion and less hydrogen mass over the equivalence ratio of 0.7, which led to less heat release rates after TDC compared with the other two equivalence ratios.

Figure 3 Average in-cylinder pressure over various engine speed

Hydrogen applications would fully present the merits of ORP engines in theory due to fast combustion of hydrogen/air mixture. It was supported by the fact that peak in-cylinder pressure was increased by hydrogen additions for a natural gas engine (Ma et al., 2007) and a gasoline engine (Ceviz et al., 2012) over given scenarios; meantime, the corresponding crank angle was advanced. Peak in-cylinder pressure of a natural gas/methanol dual-fuel engine decreased significantly with the drop of equivalence ratio, (Chen, Zhanming et al., 2020), which was slightly different from the authors' results. The difference was partly caused by the fact that the ignition timing was the same for all the scenarios in this investigation. Peak in-cylinder pressure decreased from approximately 24.0 bar to 17.0 bar when the equivalence ratio dropped from 1.0 to 0.62 for a hydrogen enriched natural gas engine, and the corresponding crank angle was retarded (Zhao et al., 2013). Similar conclusions were obtained by Niu et al. (Niu et al., 2016) based on a hydrogen/gasoline engine; additionally, the crank angle corresponding to peak in-cylinder pressure was significantly dependent on the amount of hydrogen additions in gasoline. Peak in-cylinder pressure drop by decreasing equivalence ratio was also observed in a hydrogen fuelled engine over water direct injection situations (Xu et al., 2020).

Heat release rates of this hydrogen fuelled ORP engine presented double peaks over the three

engine speed, as shown in Figure 4. The position and intensity of the peak were determined by the engine speed and equivalence ratio. Heat release rates around TDC decreased with the drop of equivalence ratio. For a hydrogen enriched natural gas engine, the heat release rates dropped from 90 J/(°CA) to 40 J/(°CA) when the equivalence ratio decreased from 1.0 to 0.62, and the corresponding crank angle was greatly retarded (Zhao et al., 2013), resulted from less hydrogen and slow combustion. It was different from the authors' results where the heat release rates were less dependent on the equivalence ratio. The distributions of heat of reactions in combustion chambers are presented in Figure S1. For the same crank angle being earlier than 15 °CA after TDC, equivalence ratio of 0.8 showed the highest value for local heat of reactions. The intensity of heat of reactions around 25 °CA after TDC over the equivalence ratio of 0.8 dropped to be lower than that of 0.7 and 0.9. Combustion over the equivalence ratio of 0.7 was much slower than that of 0.8 and 0.9; additionally, hydrogen mass was the least among the three equivalence ratios. Both aspects might lead to the large difference in peak pressure and heat release rates between the equivalence ratio of 0.7 and the other two equivalence ratios. However, the difference over the equivalence ratio of 0.8 and 0.9 was minor. It was mainly caused by the mixture temperature before ignition, because the combustion was very sensitive to mixture temperature. The temperature before ignition was the highest over the equivalence ratio of 0.8 (as shown in following section, Figure 10).

Figure 4 Heat release rates over various engine speed

Start of combustion, combustion phasing, and combustion durations over the given scenarios are presented in Figure 5. In this paper, start of combustion was defined as the crank angle corresponding to 10% mass burn fraction (MBF) of hydrogen; combustion phasing corresponded to the position where MBF was 50%; combustion duration was the crank angle duration between 10% MBF and 90% MBF. The residual hydrogen fraction in combustion chambers is also shown in Figure S2. The three key parameters presented the smallest values under the equivalence ratio of 0.8 over 1000 RPM engine speed; however, the trend was different for 2000 RPM and 3000 RPM. Start of combustion was advanced and the combustion duration was shortened by high equivalence ratio (< 1) for a natural gas/methanol fuelled engine (Chen, Zhanming et al., 2020) and a hydrogen fuelled engine (Xu et al., 2020). Combustion duration of a hydrogen fuelled reciprocating engine varied from 6.5 °CA to 10.5 °CA for the given ignition timing over 1400 RPM engine speed (Xu et al., 2020), and the duration was much shorter than that of this hydrogen fuelled ORP engine. The effect of equivalence ratio on combustion duration was still in debated. Combustion duration of a natural gas engine (Ma et al., 2007) was significantly dependent on the equivalence ratio that the duration was almost twice when the equivalence ratio dropped from 1.0 to 0.56; additionally, the combustion duration was dropped by hydrogen additions, and the duration was less sensitive to the equivalence ratio for higher hydrogen additions (Ma et al., 2007). However, the combustion duration increased to 42 °CA from approximately 15 °CA when the equivalence ratio dropped from 1.0 to 0.4 for a spark ignition engine fuelled with the blends of hydrogen and natural gas (Zhao et al., 2013).

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

Distributions of hydrogen mass fraction in combustion chambers are shown in Figure 6. At the end of combustion, hydrogen was concentrated in the top regions of the combustion chambers. Residual hydrogen in combustion chambers was quite few later than 25 °CA after TDC for the equivalence ratio of 0.9 over 3000 RPM, which was consistent with Figure S2.

Figure 6 Hydrogen mass fraction distributions in combustion chambers under different equivalence ratio over 3000 RPM (more figures shown in Figure S3)

Hydrogen fuelled engines usually have faster combustion and higher combustion efficiency compared with other types of fuel, such as gasoline (Acikgoz and Celik, 2012; Nieminen and Dincer, 2010), natural gas (Hairuddin et al., 2014; Park et al., 2011), methane (Kamil and Rahman, 2015), and n-butanol (Su et al., 2018). It was one of the main reasons that hydrogen additions contributed to increasing engine thermal efficiency. It was demonstrated by the fact that the

combustion rates increased significantly when hydrogen additions increased by 6% for a gasoline engine over specific conditions (Ji and Wang, 2009). Faster combustion would also lead to more complete combustion of fuel. The combustion efficiency of this hydrogen fuelled ORP engine is shown in Figure 7. As presented in the figure, combustion efficiency increased with the equivalence ratio over individual engine speed scenarios. Combustion efficiency of this ORP engine over 3000 RPM engine speed was much higher than that of 1000 RPM and 2000 RPM. It agreed well with the phenomenon in Figure 5. The combustion efficiency of this hydrogen fuelled ORP engine was high, which was partly caused by the neglect of the crevices between the pistons and cylinders. In reality, the crevices between pistons and cylinders significantly decreased the combustion efficiency due to the crevice effect. The effect of equivalence ratio on combustion efficiency would be obvious when crevices were considered.

Figure 7 Combustion efficiency over the given scenarios

P-V diagrams during the ORP engine operations were shown in Figure 8. P-V diagrams over the equivalence ratio of 0.8 and 0.9 changed slightly over individual engine speed. The area covered by P-V lines indicated the power capacity to some extent. The decrease of the area over the equivalence ratio of 0.7 by comparing with the equivalence ratio of 0.8 and 0.9 over 3000 RPM was higher than that of 1000 RPM and 2000 RPM. In addition, the pumping loss was much higher for 3000 RPM than 1000 RPM and 2000 RPM, which was also demonstrated in the authors' previous work (Gao et al., 2020a).

Figure 8 P-V diagrams over various engine speed

3.2 Heat loss during combustion by cylinder walls

As mentioned in Section 2.1, heat loss of this hydrogen fuelled ORP engine was less than that of reciprocating engines over the same engine speed theoretically. Less heat loss contributed to increasing engine thermal efficiency. Its effect was similar to adiabatic engines (Beg et al., 2002; Mitianiec, 2016) which were widely investigated to decrease the heat loss for improving engine thermal efficiency. However, the benefits brought by the heat isolation approach in adiabatic engines were not significant, because much more heat was lost though exhaust. It would be slight helpful for energy recycle technology such as organic Rankine cycle (Chen et al., 2019; Zhao et al., 2018) which would be applied to vehicles to improve the overall energy efficiency. The heat loss during the compression stroke and power stroke are shown in Figure 9. Heat loss per cycle difference was minor for the equivalence ratio of 0.8 and 0.9 under individual engine speed. Heat loss rates through cylinder walls increased significantly with engine speed. Temperature fluctuations in the layer near the walls led to the fluctuations of heat loss rates; however, the fluctuations would be seriously weakened over higher engine speed due to much shorter period. It led to lower fluctuations (smoother lines) of the heat release rates over higher engine speed.

Figure 9 Heat loss rates through cylinder walls

Heat loss rates of this ORP engine were partly dependent on the in-cylinder temperature. Figure 10 shows the average in-cylinder temperature evolutions during engine operations. The equivalence ratio of 0.9 and 0.8 over 3000 RPM presented higher in-cylinder temperature than other cases, which could lead to higher heat loss rates. Figure 11 shows the temperature distributions in combustion chambers over various scenarios. High temperature regions propagated from the bowls to other regions of the combustion chambers. At the start of combustion, the heat loss was dominated by the bowls in cylinders. Such high temperature would generate high thermal load for this engine, which was also an issue that need to be addressed in practical applications.

Figure 10 In-cylinder temperature evolutions during combustion over various engine speed

Figure 11 Temperature distributions in combustion chambers under different equivalence ratio over 3000 RPM (more figures shown in Figure S4)

3.3 Nitrogen monoxide emission characteristics

High flame propagation speed of hydrogen fuel would significantly promote the increase of brake thermal efficiency; however, it led to high NO_x emission factors (Al-Baghdadi, 2004; Subramanian et al., 2007) because of high temperature. In FLUENT code (FLUENT, 2001), Zeldovich mechanism was used to predict the NO formations. Accumulated NO formation per combustion chamber during hydrogen combustion is presented in Figure 12. For the equivalence ratio of 0.8 and 0.9, 3000 RPM showed the highest accumulated NO, followed by 1000 RPM and 2000 RPM. It was mainly caused by the highest combustion temperature over 3000 RPM, which was indicated in Figure 10. The crank angle corresponding to peak NO formation rate was around 7°CA after TDC

for 3000 RPM; however, it was 12 °CA and 15 °CA after TDC for 1000 RPM and 2000 RPM, respectively. NO formations over the equivalence ratio of 0.7 were much lower than other cases that the value was almost zero. NO concentration by volume in the combustion chamber during combustion was also shown in Figure S6, and it showed a similar tendency with accumulated NO. In the reported work (Xu et al., 2020), maximum average in-cylinder temperature dropped from approximately 1640 K to 1500 K when the equivalence ratio changed from 1.05 to 0.7, which was inconsistent with NO_x concentration that reached maximum value over the equivalence ratio of 0.85. In this investigation, ignition timing of the nine scenarios was always the same (17 °CA before TDC) which didn't correspond to the maximum torque over the given scenarios (given equivalence ratio and engine speed). NO emission would increase if ignition timing was optimized to achieve higher thermal efficiency and power output. Distributions of NO mass fraction in combustion chambers are presented in Figure 13. NO mass fraction was the highest in the bottom and top regions of the cylinders and in the centre of the bowls around 12 °CA after TDC, which was consistent with temperature distributions in combustion chambers.

Figure 12 NO formations during hydrogen combustion over various engine speed

Figure 13 NO mass fraction distributions in combustion chambers under different equivalence ratio over 3000 RPM (more figures shown in Figure S7)

3.4 Performance evaluations

Overall performance of this hydrogen fuelled ORP engine, including indicated power output, indicated NO emission factors, indicated thermal efficiency, and energy loss through cylinder walls and exhaust are shown in Figure 14. Indicated power output and indicated NO emission factors increased with equivalence ratio for the given engine speed. Indicated power output of 3000 RPM engine speed depended more on the equivalence ratio than that of 1000 RPM and 2000 RPM. NO emission factors over 3000 RPM were higher than those of 1000 RPM and 2000 RPM under the equivalence ratio of 0.8 and 0.9, which was mainly caused by high combustion temperature; however, it was inverse for the equivalence ratio of 0.7, resulting from short duration of high temperature for 3000 RPM. In the published reports (Ceviz et al., 2012; Ma et al., 2007), the equivalence ratio corresponding to maximum NO_x emission factors was in the range of 0.8~0.9 when the engines fuelled with hydrogen or hydrogen blended fuel. NO_x emission factors of the natural gas fuelled engine reached the maximum value around the equivalence ratio of 0.8, and NO_x emission factors increased with hydrogen additions in natural gas (Ma et al., 2007); however, the equivalence ratio was 0.9 in the work (Zhao et al., 2013) where the maximum NO_x emission factors were approximately 32 g/kWh. Also, the equivalence ratio corresponding to the maximum NO_x emission rates decreased with hydrogen additions (Ma et al., 2007). It was also demonstrated that

NO_x emission factors changed slightly over different hydrogen additions if ignition timing corresponded to the optimal value of brake thermal efficiency (Ma et al., 2007). Additionally, NO_x emission factors were less than 3 g/(kW h) when the equivalence ratio was smaller than 0.6 (Zhao et al., 2013). However, slight increase was observed for NO_x concentration when the equivalence ratio was lower than 0.5 for a hydrogen enriched gasoline engine (Niu et al., 2016). Minimum NO_x emission factors were also reported by Smallbone et. al (Ngwaka et al., 2020) over the equivalence ratio of lower than 0.5 when hydrogen fuel was applied to a free-piston engine.

Figure 14 ORP engine performance calculated using 3D simulation

Energy loss through cylinder walls and exhaust were also presented in Figure 14 (c) and Figure 14

(d), respectively. Heat loss through cylinder walls over 1000 RPM were the highest among the three engine speed, which was resulted from long cyclic period in time although the in-cylinder temperature was lower than that of 3000 RPM. Exhaust energy of the nine scenarios were more than 52% of the fuel energy, and it was higher than other types of engines fuelled with hydrogen under wide open throttle conditions (Wang et al., 2019); and it presented the highest value over 2000 RPM. Less heat loss through cylinder walls led to more exhaust energy which contributed to increasing the efficiency of waste energy recycling. Heat loss rates through cylinder walls were consistent with the evolutions of average in-cylinder temperature. Heat loss through cylinder walls was mainly caused by the temperature layer closing to walls rather than the average value. At the start of combustion, the increase of average temperature was mainly caused by the combustion in the bowls which had large surfaces and small volumes. See from Figure 10, the average temperature at the start of combustion over equivalence ratio of 0.8 was higher than that of 0.7 and 0.9, which leading to high heat loss rates.

Equivalence ratio of 0.8 presented the highest indicated thermal efficiency for individual engine speed, which was caused by enhanced in-cylinder combustion over lean-burn conditions. Indicated thermal efficiency of 3000 RPM engine speed was dependent more on the equivalence ratio than 1000 RPM and 2000 RPM. Indicated thermal efficiency could reach a higher value if spark timing was optimized for the scenarios (it was same for all the cases in this investigation). It was consistent with the reported results (Chen, Zhanming et al., 2020) where the efficiency increased and then dropped with equivalence ratio, and the optimal equivalence ratio was approximately 0.75 in terms of brake thermal efficiency. In addition, it was around 0.7 for a hydrogen enriched natural gas engine (Zhao et al., 2013). However, the indicated thermal efficiency of a hydrogen fuelled reciprocating engine over 1400 RPM engine speed increased continuously with the drop of equivalence ratio for the given range (Xu et al., 2020). The optimal equivalence ratio in terms of brake thermal efficiency was also affected by the percentage of hydrogen additions. It was demonstrated by the work that (Niu et al., 2016) the optimal equivalence ratio was 1.0 for low hydrogen additions (4%~5%), 0.85 for medium hydrogen additions (5%~8.5%), and 0.65 for high hydrogen additions (8.5%~10%). Be superior to exhaust gas recirculation (EGR) approach of decreasing NO_x emissions (Banerjee et al., 2015), lean-burn technology could ensure low NO_x emission factors and high thermal efficiency simultaneously.

As indicated thermal efficiency and NO_x emission factors were the two most important key

performance indicators, the choice of equivalence ratio of the hydrogen/air mixture should ensure relative low NO_x emission factors and few penalty of indicated thermal efficiency. The optimal equivalence ratio for practical applications of this hydrogen fuelled ORP engine should be in the range of 0.7~0.8; meanwhile, the higher of the engine speed, the suggested equivalence ratio should be closer to 0.8.

4. Conclusion

Hydrogen fuelled opposed rotary piston engines as a potential power source for hybrid vehicles and range extended electric vehicles, have high power density and can achieve zero CO_2 emission. However, the applications of hydrogen fuelled engines are still struggling with high NO_x emissions. The effect of equivalence ratio on combustion characteristics and NO_x formations of a hydrogen fuelled ORP engine was investigated. The main conclusions are as the follows:

- (1) The difference of peak in-cylinder pressure over 0.8 and 0.9 was minor for individual engine speed; however, the pressure decreased significantly for the equivalence ratio of 0.7, and the corresponding crank angle was advanced greatly.
- (2) More heat was released between 0 °CA and 20 °CA after TDC over the equivalence ratio of 0.8 and 0.9 than that of 0.7 during combustion. Equivalence ratio of 0.8 presented the earliest combustion over individual engine speed; the effect of equivalence ratio on combustion duration depended on the engine speed. Combustion efficiency increased with equivalence ratio, and 3000 RPM had a higher value than that of 1000 RPM and 2000 RPM.
- (3) Heat loss rates of this hydrogen fuelled ORP engine through cylinder walls increased with equivalence ratio and engine speed; however, the difference was minor between the equivalence ratios of 0.8 and 0.9. 3000 RPM engine speed presented the highest average in-cylinder combustion temperature, which was mainly caused by high volumetric efficiency.
- (4) Indicated power output and NO emission factors of this hydrogen fuelled ORP engine increased with equivalence ratio; Equivalence ratio of 0.8 showed the highest indicated thermal efficiency being higher than 38% over 3000 RPM, and equivalence ratio of 0.7 presented the lowest NO emission factors being lower than 1.5 g/kWh.

This research made a foundation for the performance evaluations of hydrogen fuelled ORP engines, and explored lean-burn characteristics to achieve low NO_x emissions and high thermal efficiency. The applications of the hydrogen fuelled ORP engines to hybrid vehicles would significantly

decrease CO₂ emission and hazardous pollutants to achieve cleaner production and environmental friendly travel.

CRedit authorship contribution statement

Jianbing Gao: Formal analysis, Investigation, Methodology, Resources, Validation, Visualization, Writing - original draft, Writing - review & editing. Guohong Tian: Conceptualization, Funding acquisition, Methodology, Project administration, Resources, Software, Supervision, Visualization, Writing - review & editing. Chaochen Ma: Investigation, Writing review & editing; Shikai Xing: Visualization, Writing - review & editing. Liyong Huang: Conceptualization, Data collections.

Declaration of competing interest

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

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