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Exergy analysis of the lean-burn hydrogen-fuelled engine

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ABSTRACT

Hydrogen is considered an alternative fuel for use in internal combustion engines. The internal combustion engine will likely remain in use for vehicle and stationary applications for the foreseeable future, therefore identifying and quantifying efficiency losses of burning fuels is important. Exergy analysis is a method for investigating the fundamental origins of losses, the limits to efficiency, and the engineering trade-offs required to reduce losses. This comprehensive exergy analysis of a boosted lean-burn hydrogen spark ignition engine investigates the processes involving exergy destruction under real-world conditions. This efficiency of a hydrogen SI engine and the NO emissions are evaluated by quantifying the exergy destruction for various intake manifold air pressures, lean-burn mixtures, compression ratios, and spark timings. Using an improved two-zone engine model to study in-cylinder processes, the results indicate that increasing air dilution enhances exergy transfer to work, due mainly to diverting exhaust exergy into reversible work. However, increasing air dilution also increases combustion-related exergy destruction due to greater entropy generation for leaner mixtures, but reducing heat loss decreases combustion-related irreversibility. Higher manifold air pressures and compression ratios increase the quantity of exergy directed to work and heat, whilst reducing exergy expelled to exhaust. Gaining understanding of the detail of thermodynamic mechanisms of the routes by which the work potential is lost potentially assists in engineering improvements to minimize exergy losses, and to increase efficiency and work output.

1. Introduction

Limitations of fossil fuel reserves, and environmental constraints, are spurring development of alternative internal combustion engine (ICE) technologies [1]. Exergy is a useful concept for evaluating the performance of ICEs by identifying and quantifying the thermodynamic inefficiencies (losses) of the underlying irreversible processes [2,3]. Exergy analysis can be conducted using experimental measurements or modelling engine components and systems [4]. Recent research using exergy analysis has focused on combustion strategies [5–7], alternative fuels [8,9], and waste heat recovery systems [10-12]. Exergy destruction in the combustion process is caused by entropy generation resulting from irreversible processes. Entropy generation (exergy destruction) is caused by four irreversible processes viscous dissipation, mass diffusion, heat conduction, and chemical reactions [13]. Quantification of premixed and diffusion flames showed that the main cause of entropy generation was the chemical reaction in premixed flames, whereas heat conduction was the primary cause in diffusion flames [13]. Previous studies using diesel and gasoline have incorporated detailed numerical chemical analyses into the combustion process to study the effect of operating conditions on exergy destruction or the potential relationship between various engine operating conditions [7,11,14]. Investigations of exergy destruction caused by the combustion process for a range of initial reactant temperatures, pressures, and equivalence ratios concluded that the initial reactants' temperature had the highest impact compared to other parameters [15]. Furthermore, the reactants' temperature and equivalence ratio were the most influential parameters regarding the exergy destruction [14,16].

Hydrogen as an alternative fuel offers several advantages. First, the laminar flame speed is four times greater than that of gasoline. Secondly, the hydrogen diffusion coefficient is almost four times greater than that of gasoline, enhancing the mixing with air, hence better mixture homogeneity. Thirdly, the hydrogen lean-limit is significantly lower than that of gasoline, meaning that hydrogen could operate more stably at lean burn mixtures, providing an effective path towards improving engine efficiency [17]. However, despite the higher Research Octane Number of hydrogen compared to gasoline the performance of hydrogen-fuelled engines is still prone to knock [18]. Furthermore, since the hydrogen/air mixture has lower volumetric energy, automobile

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Nomenclature		EGR	exhaust gas recirculation	
		EVO	exhaust valve opening (Crank Angle)	
Symbols		H_2	hydrogen	
с	specific heat (J/kgK)	H_2O	water vapor	
σ	Stefan-Boltzmann constant (5.67 $ imes$ 10 ⁻⁸ W/m ² K ⁴)	ICE	internal combustion engine	
h	specific enthalpy (J/kg)	IMEP	indicated mean effective pressure (Pa)	
i	species index	ITE	indicated thermal efficiency (%)	
j	environmental species index	IVC	intake valve closing (Crank Angle)	
k	heat transfer coefficient (W/m ² K)	MAP	manifold air pressure (Pa)	
m	mass (kg)	MBT	maximum brake torque	
μ	chemical potential (J/mol)	N_2	nitrogen	
n	number of moles (mol)	NO	nitric oxide	
Р	pressure (Pa)	NOx	oxides of nitrogen	
Ø	equivalence ratio	O_2	oxygen	
Q	heat (J)			
R	universal gas constant (8.314 J/mol K)	Subscrip	ubscripts	
S	specific entropy (J/kgK)	0	dead state	
Т	temperature (K)	chem	chemical	
θ	crank angle (degrees)	Exh	exhaust	
u	specific internal energy (J/kg)	heat	heat	
v	specific volume (m ³ /kg)	ht	heat transfer	
ν	stoichiometric coefficient	Irr	irreversibility	
Х	exergy (J)	mix	mixture	
		TM	thermo-mechanical	
Acronyms		Work	work	
CO_2	carbon dioxide	*	restricted dead state	
CR	compression ratio			

manufacturers are developing boosted and downsized hydrogen SI engines to compete with current gasoline engines. It has been shown that by boosting the intake manifold air pressure, a hydrogen-fuelled SI engine could provide the same load as gasoline at a significantly lower level of fuel consumption [19].

Since the physical and chemical properties of pure hydrogen differ significantly from hydrocarbon fuels, it is beneficial to understand the exergy split to work, heat, irreversibility and exhaust of hydrogen under realistic engine operating conditions. Due to hydrogen's higher burning speed compared to that of hydrocarbon fuels, the exergy transfer to work and heat is greater than that of fuels such as compressed natural gas [20]. However, the exergy destroyed by combustion-related irreversible processes in hydrogen SI engines is lower than that of hydrocarbon fuels, due to lower entropy generation [21]. Lower entropy generation for hydrogen is attributed to its simpler combustion pathway compared to that of hydrocarbon fuels [22]. Exergy and energy analyses of a hydrogen-fuelled HCCI engine with EGR concluded that for hydrogen fuelled engines, the engine speed had a smaller effect on exergy destruction compared to other parameters [23]. Increasing the intake temperature could reduce the combustion losses, due to the reduction in combustion-related entropy generation. Investigating the exergy split of a hydrogen-fuelled SI engine at various equivalence ratios and spark timings showed that as the fuel mixture became leaner, the exergy due to combustion irreversibility increased, mainly due to the decreasing combustion temperature [24]. However, when the spark timing was retarded, the exergy transfer to heat decreased, and the exergy carried by the exhaust gases increased. For a turbocharged hydrogen engine the load was the main influence on the exergy allocation [7]. Hydrogen as a combustion enhancer has also been studied [25-28]. However, a comprehensive exergy analysis of hydrogen-fuelled engines to assess efficiency has not been conducted.

The aim is to evaluate the efficiency of a hydrogen-fuelled engine and the NO emissions by quantifying the exergy destruction for conditions such as intake manifold air pressure, lean burn mixture, compression ratio, and spark timing. From this standpoint, the design of engines becomes a matter of managing the initial exergy resources supplied to the engine by minimizing the exergy losses and maximizing the exergy outflow. Parametrizing the heat loss reveals the compromises required and consequences for the exergy management of a hydrogenfuelled SI engine.

2. Methodology

A modified two-zone combustion model [29] was used to quantify exergy transfers, which were categorized into work, heat transfer, exhaust, and combustion irreversibility. The crank-angle-resolved heat transfer model was refined to accurately predict heat transfer in a hydrogen-fuelled SI engine across various intake manifold air pressures, equivalence ratios, spark timings, and compression ratios. The main assumption of the model is the division of the combustion chamber into two zones: the burned zone, consisting of the combustion products, and the unburned zone, consisting of the reactants. Both zones are treated as ideal gases. The pressure is assumed to be uniform throughout the chamber, and temperatures are characterized as the burned and unburned temperatures. The combustion model was derived based on the equation of state, the first law of thermodynamics, and the continuity equation, as shown in the appendix.

Exergy is the maximum theoretical work that can be extracted from a system with respect to the thermal, mechanical, and chemical equilibrium reference state [3]. The reference state is either equilibrium with the surroundings (the dead state) or a restricted dead state in which the system is only in thermo-mechanical equilibrium (but not chemical). The restricted dead state is defined as the thermo-mechanical exergy at P_0 and T_0 based on the temperature and pressure of the system with respect to the fixed chemical composition of the system. Both dead state and restricted dead state are at P_0 and T_0 ; the transition from the restricted dead state to the dead state requires further interaction with the environment in terms of diffusion of the molecular species and chemical reactions [3].

The exergy balance for an ICE is:

$$X = X_{Chem} + X_{TM} = X_{Work} + X_{Exh} + X_{Irr} + X_{Heat} + X_{others}$$
(1)

where X_{Chem} is the chemical exergy of the fuel, X_{TM} is the physical thermo-mechanical exergy of the in-cylinder mixture, X_{Work} is the exergy transferred to work, X_{Exh} is the exergy expelled by the exhaust, X_{Irr} is the exergy transfers associated with combustion irreversibility, X_{Heat} is the heat, and X_{others} denotes the exergy destruction due to mixing, blow-by gases, losses in valves, etc., caused by the mixing of two or more streams with different thermodynamic properties. Note that X_{others} exergy destructions could not be modelled using the proposed engine combustion model. The exergy analysis divides into thermo-mechanical and chemical exergy. Thermo-mechanical exergy is related to the incylinder properties such as pressure and temperature, and chemical exergy describes the chemical potential of the in-cylinder mixture with respect to a reference condition. The crank-angle-resolved thermo-mechanical and chemical exergy are calculated using Eqs. (2) and (3), respectively,

$$X_{TM} = (U - U_*) + P_0(V - V_*) - T_0(S - S_*)$$
⁽²⁾

$$X_{Chem} = \mu_* - \mu_0 \tag{3}$$

$$\mu_* = h_* - T_0 s_* \tag{4}$$

$$\mu_0 = h_0 - T_0 s_0 \tag{5}$$

where u, v and s are internal energy, volume and entropy, respectively. The subscript 0 corresponds to properties at the dead state (P_0 , T_0). The chemical potential μ was calculated by using Eqs. (4) and (5). The subscript * represents the mixture properties at a restricted dead state. The values for u, v, h and s were calculated as a function of the incylinder mixture composition. Firstly, the chemical potential of each specie was computed, then the total mixture chemical potential using Eq. (6).

$$G_{mix} = \mu_{mix} = \sum_{i} \mu_{i,0} n_i \tag{6}$$

where G_{mix} is the Gibbs free energy and μ_{mix} is the total chemical potential of the mixture computed as the sum of the chemical potential per mole $\mu_{i,0}$ and the number of moles n_i . The thermodynamic properties for each species are based on curve fitting of the thermodynamic data [30]. The assumptions are that the unburned mixture does not change in composition and that the burned mixture is at equilibrium with respect to dead state. The specific heat, specific enthalpy, specific entropy, and specific internal energy are calculated using Eqs. (7)–(9) to determine unburned and burned mixture properties,

$$\frac{c_p(T)}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$
(7)

$$\frac{h(T)}{R} = a_1 + \frac{a_2T}{2} + \frac{a_3T^2}{3} + \frac{a_4T^3}{4} + \frac{a_5T^4}{5} + \frac{a_6}{T}$$
(8)

$$\frac{s(T)}{R} = a_1 lnT + a_2 T + \frac{a_3 T^2}{2} + \frac{a_4 T^3}{3} + \frac{a_5 T^4}{4} + a_7$$
(9)

The internal energy is given by

$$u = h - RT \tag{10}$$

Two temperature ranges for the values of the coefficients *a* for H_2 , O_2 , N_2 and H_2O are used [30]. The lower range (300–1000 K) is appropriate for the unburned mixture properties, while the higher range (1000–5000 K) is used for the burned mixture properties. The environment is assumed to comprise four primary species, with other components aggregated into a single category [4]. The volume fractions of the environmental species are: 20.35 % O₂, 75.67 % N₂, 0.03 % CO₂, 3.03 % H₂O, and 0.92 % other.

2.1. Exergy transfers

The exergy transfer to indicated work is

$$\frac{dX_{Work}}{d\theta} = (P - P_0)\frac{dV}{d\theta} \tag{11}$$

where *P* is the instantaneous in-cylinder pressure, P_0 is the pressure at the dead state, and *V* is the volume of the cylinder. The in-cylinder pressure was obtained from a previously developed two-zone hydrogen combustion model [29].

The exergy transfer to heat between the in-cylinder mixture and chamber walls is

$$\frac{dX_{Heat}}{d\theta} = -\left(1 - \frac{T_0}{T}\right)\frac{dQ_{ht}}{d\theta}$$
(12)

where T_0 and T are the initial temperature and in-cylinder mixture temperature, respectively. The convective heat loss Q_{ht} is modelled using the Woschni correlation [31], but the heat transfer coefficient in the standard Woschni correlation needs to be multiplied by a factor of 2.2 to match the heat losses of hydrogen [32].

The hydrogen chemical exergy was calculated using

$$X_{Chem} = (U_* + P_0 V_* - T_0 S_*) - \sum_j \sum_i \mu_{i,0} \left(\frac{\nu_{ij}}{\nu_j}\right) n_j$$
(13)

where the chemical exergy X_{Chem} is the chemical potential of the resource at the thermo-mechanical dead state, and the chemical potential of the environmental species *j* is formed from the species originally present in the system *i* at the dead state.

The exergy destruction due to combustion irreversibility is calculated as a function of the reaction rate and the difference between the chemical potential of the reactants and products, based on the Gouy-Stodola theorem [33]. The entropy generation was formulated as

$$\frac{dX_{Comb}}{d\theta} = -T_0 \frac{dS}{d\theta} = -\frac{T_0}{T} \sum_i \mu_{i,0} dm_i$$
(14)

where the chemical potential μ_i is set to be X_{Chem} for the fuel, and Gibbs free energy G_i for other gases.

The exergy transfer to exhaust gases was estimated as the thermomechanical exergy at the EVO,

$$X_{Exh} = X_{\theta = EVO} \tag{15}$$

The in-cylinder exergy was calculated using Eq. (2), when the specific internal energy, volume and entropy of the gas are known.

2.2. NO emissions

Nitric oxides (NOx) exhaust emissions require control in hydrogenfuelled engines. The formation of NOx is dependent on the in-cylinder temperature (>1800 K), oxygen concentration, and reaction duration. Of the possible NOx emissions, nitric oxide (NO) is the main emission [34]. The NO concentration was computed by integrating the chemical rate equations of the extended Zeldovich mechanism [34].

3. Results and discussion

The two-zone hydrogen combustion model was used to investigate the performance and the NO emissions of a boosted lean burn hydrogen fuelled engine. Then the results were used to identify the exergy split to work, heat, irreversibility and exhaust and potential improvements of a boosted lean-burn hydrogen-fuelled SI engine. First, entropy generation due to irreversible combustion-related processes destroys exergy, the entropy generation of hydrogen combustion under various conditions was analysed. Secondly, the efficiency was calculated using a hybrid top-down and bottom-up exergy approach to assess the accuracy of the exergy quantification. The exergy losses of the hydrogen engine operating under various conditions were identified and quantified using the bottom-up approach, whilst and the efficiency, expressed as reversible work, was calculated using the top-down approach by taking the difference in the exergy flow crossing the control volume. Finally, the effect of increasing the energy state through compression ratio increase and heat loss reduction was investigated.

The results for in-cylinder pressure were validated using published data [35]. Fig. 1 compares the simulated and experimental in-cylinder pressure at equivalence ratios (\emptyset) of 0.77 and 0.50. The combustion model was predicting accurately the in-cylinder pressure for both equivalence ratios at different spark timings. Understanding the exergy transfer mechanisms enables the engine model to identify potential improvements in hydrogen engine performance.

3.1. Hydrogen engine performance

The optimal spark timing in an ICE is determined by the characteristics of flame propagation within the combustion chamber and parameters such as engine load, fuel composition, intake pressure, intake temperature, and engine speed. To ensure maximum thermal efficiency under all simulated conditions the spark timing was set at the minimum spark advance for the maximum brake torque (MBT). Fig. 2a shows the variation of indicated mean effective pressure (IMEP) with spark timing at different equivalence ratios for naturally aspirated conditions. It can be seen that the MBT shifts away from the TDC when the mixture became leaner. The MBT timing was found to be at 11, 10, 8, 6 and 4 °CA bTDC for Ø of 0.45, 0.5, 0.65, 0.77 and 0.9, respectively. The shift of the MBT timing away from TDC for leaner hydrogen mixtures is explained by the increased combustion duration due to the slower burning speeds for greater air-diluted hydrogen mixtures. Fig. 2a also shows that the IMEP was reduced by 46 % when the \emptyset was reduced from \emptyset of 0.9 to \emptyset of 0.45 at their respective MBT timing under the naturally aspirated condition. Whereas in Fig. 2b, the IMEP under Ø of 0.77 at various MAP values shows that as the MAP increased, the MBT timing shifted closer to TDC. This was because of the increase of the charge density at the higher MAP values. For Ø of 0.77 as the MAP was increased from 80 kPa to 100 and 120 kPa, the IMEP at MBT timing increased by 7 % and 16 %, respectively. The power increase is explained by the increase of the incylinder charge density for higher MAP [36].

The indicated thermal efficiency (ITE) demonstrates how effectively chemical energy is converted into mechanical work. Fig. 3 displays the effect of equivalence ratio (\emptyset) and manifold air pressure (MAP) on ITE, under MBT timing at a fixed engine speed of 2000 rpm. It is evident that ITE increases proportionally with increasing MAP. For \emptyset of 0.9, the ITE increased by 4 % and 7 % when the MAP was raised to 100 kPa and 120



Fig. 1. Comparison of the simulated and experimental in-cylinder pressure of [35] at Ø of 0.77 and 0.50 (CR = 11.5, $ST_{\emptyset=0.77}$ = 3 °CA bTDC, $ST_{\emptyset=0.5}$ = 12 °CA bTDC).

kPa, respectively, from the naturally aspirated condition of 80 kPa. The ITE also increased when the hydrogen/air mixture became leaner; for the naturally aspirated condition of 80 kPa, the ITE increased by 10 % when the \emptyset was shifted from 0.9 to 0.45. This increase was caused by the greater expansion of leaner mixtures due to the increase of the specific heat ratio. The peak ITE, observed at an \emptyset of 0.45 with a boost of 40 kPa, was 43 %. This finding aligns with previous studies [37,38]. Concurrently, the benefit of boosting MAP was counteracted by an increase in NO emissions, mainly due to the rise in in-cylinder temperature, which strongly influences NO formation. For \emptyset of 0.9, the NO emissions increased by 5 % and 23 % when the MAP was increased from 80 kPa to 100 kPa and 120 kPa, respectively. However, a reduction in NO emissions was achieved by operating the mixture at a leaner hydrogen mixture; the NO emissions were reduced by 87 % when the \emptyset was shifted from 0.9 to 0.45 under naturally aspirated conditions (MAP = 80 kPa).

3.2. Hydrogen entropy generation

Hydrogen allows for high dilution rates with air or exhaust-gas recirculation (EGR), thus reducing NOx emissions [39]. However, this reduces engine power output and potentially limiting hydrogen-use in high-density powered applications. Moreover, the lower power of lean-burn hydrogen operation reduces the in-cylinder temperature, increasing the combustion irreversibility ratio. This increase in irreversibility or the destruction of available energy is directly proportional to the rate of entropy generation. Entropy can be generated by processes such as unrestrained chemical reactions, friction, heat transfer across different temperature zones, and mixing of different gases [13], but exergy transfer does not necessarily mean exergy destruction. Entropy generation (exergy destruction) must be reduced to improve the fuel conversion efficiency. The entropy generation ($S_{gen} = S_{products} - S_{reactants}$) at various operating conditions was calculated by assuming adiabatic, constant volume, and closed combustion chamber conditions. As mixtures became leaner (Ø of 0.90 to 0.45), entropy generation increased (Fig. 4) because the lean combustion with excess air provides a greater quantity of the product species, meaning an increase in the product chemical component of entropy. The entropy generation increased significantly when the \emptyset was reduced from 0.90 to 0.45.

In agreement with pervious work using hydrocarbon fuels [16], increasing the reactant temperature monotonically reduced entropy generation. For Ø of 0.90 under the pressure of 30 bar, the entropy generation was reduced by 61 % and 86 % at the temperature of 1800 K when the reactant temperature was increased from 300 to 500 and 900 K, respectively. This could be explained by the reduction of the difference between the reactant and product temperatures, directly reducing the combustion entropy generation. This entropy reduction could reduce combustion irreversibility if it were possible to keep the reactant temperature as close as possible to product temperatures just before the combustion starts. This could be achieved by high compression of the fresh charge [26], but raising the reactant temperature increases the likelihood of combustion abnormalities and NOx emissions. In Fig. 4 the reactant pressure has a slight effect on the entropy generation for constant internal energy-volume combustion, mainly due to the suppression of product dissociation [16]. However, the pressure influence on entropy generation was more noticeable when the pressure rose from 10 to 30 bar, but less significant for engine-relevant combustion pressures (>30 bar).

3.3. Hydrogen engine exergy

The exergy split to work, heat, irreversibility and exhaust of a hydrogen-fuelled SI engine as a function of crank angle are shown in Fig. 5. At the intake valve closure (IVC) at 240 °CA, the total input exergy equals the chemical exergy with a small increment from the thermo-mechanical exergy. During the compression process, work was supplied from the piston to the mixture, as it can be seen by the negative



Fig. 2. a) IMEP at different spark timing for various Ø at naturally aspirated conditions (MAP = 80 kPa), and b) IMEP at different spark timing for various MAP under Ø of 0.77.



Fig. 3. a) Indicated thermal efficiency at various \emptyset and MAP at MBT timing and b) NO emissions at various \emptyset and MAP under MBT timing (CR = 11.5, N = 2000 rpm).

work exergy values. During compression:

- the in-cylinder pressure and temperature increased, thus the incylinder thermo-mechanical exergy increased,
- the exergy transfer to heat is negligible during this phase, and
- the pressure and temperature of the premixed hydrogen/air mixture are not sufficient to start the oxidation; therefore, the chemical exergy is constant.

With the start of combustion at 4°CA bTDC, the chemical exergy dropped rapidly as the fuel burned, while the thermo-mechanical exergy increased due to the significant rise in in-cylinder pressure and temperature. As combustion occurred and the expansion process progressed, the exergy transfer to work and heat increased, eventually contributing to the decrease of the total in-cylinder exergy. After the end of the combustion process, as the piston approached bottom dead centre (BDC), the total in-cylinder exergy continued to decrease because of the exergy transfer to heat, work, and combustion-related exergy



Fig. 4. Entropy generated by combustion at various pressures, temperatures, and equivalence ratios in a hydrogen-fuelled SI engine.



Fig. 5. In-cylinder exergy balance from intake valve closing to exhaust valve opening for \emptyset of 0.90 at spark timing of 4 °CA bTDC under naturally aspirated condition (MAP = 80 kPa, CR = 11.5, N = 2000 rpm).

destruction. The remaining exergy of the in-cylinder mixture at the end of the expansion process was defined as the exergy expelled by the exhaust gases, because the pressure and temperature at the instant of exhaust valve opening (EVO) were greater than those of the dead state.

The main destinations of exergy — work, heat, combustion, and exhaust —for a boosted lean-burn hydrogen SI engine at MBT timing are shown in Fig. 6. The largest proportion of exergy was associated with reversible work, under all operating conditions. Moreover, the proportion of reversible work increases with increasing dilution ratios. When the \emptyset reduces from 0.90 to 0.45, the useful work ratio increases by 4 %. This increase was mainly due to the exhaust enthalpy being diverted into reversible work, which eventually increases the efficiency due to a better expansion ratio. The exergy transfer to work correlates with the ITE (Fig. 3a). Conversely, the exergy to heat transfer and exhaust reduces by 35 % and 64 % when \emptyset reduces from 0.90 to 0.45, respectively.



Fig. 6. Exergy split to work, heat, irreversibility and exhaust NO emissions at MBT timing for various equivalence ratios (MAP = 80 kPa, CR = 11.5).

The reduction in exergy transfer to heat results from reducing the difference between the mixture and chamber wall temperatures for leaner hydrogen mixtures. This study does not account for any unburned hydrogen residuals which might reduce thermal efficiency [40]. Furthermore, for \emptyset of 0.90 the exergy transfer to heat accounted for 36 % of the exergy input. This was because of the greater difference between the in-cylinder temperature and the combustion chamber wall. In cases where exergy transfer to heat was dominant, heat reduction technologies such as the low heat rejection method [41] might improve hydrogen-fuelled engine performance. However, this approach might be less beneficial for leaner mixtures ($\emptyset < 0.50$), where the exergy to heat transfer was not as significant. For Ø of 0.45, the exergy transfer to heat accounted for 23 %. The exhaust exergy available represents the in-cylinder available exergy at EVO. Once the exhaust exergy is transferred to the environment, it is completely destroyed as it irreversibly equilibrates with the environment. Increasing the air dilution rates reduces exhaust exergy.

The exergy destruction of combustion increases for leaner hydrogen/

air mixtures, since the difference between the reactant and product entropy increases due to the reduced amount of hydrogen in higher airdiluted mixtures. Additionally, the combustion reaction generates more entropy because of the lower burned temperatures for leaner hydrogen mixtures (see Section 3.2). The efficiency of ultra-lean hydrogen mixtures ($\emptyset < 0.50$) may be limited due to the increase of the combustionrelated irreversibility. The increased air ratio reduces the exhaust exergy by increasing combustion exergy destruction rather than using the exhaust to benefit work output. However, the fact that lean burn hydrogen results in lower NO emissions cannot be overlooked. Lower temperatures lead to less NO formation, and if the temperature remains below 1800 K, NO emissions would be significantly reduced. From Fig. 6, it is evident that for the naturally aspirated hydrogen engine, NO emissions were reduced by 30 % and 87 % when Ø shifted from 0.90 to 0.77 and from 0.77 to 0.45, respectively. This reduction is attributed to the significant decrease in in-cylinder temperature at higher air dilution rates.

3.3.1. Effect of spark timing on exergetic processes

For \emptyset of 0.77 and 0.9, Fig. 7a and Fig. b show that the exergy associated with heat transfer decreases, but that the exhaust exergy increases as the spark timing shifts away from MBT timing. However, the magnitudes of exergy transfer associated with heat and exhaust are greater for Ø of 0.90 compared to the leaner case Ø of 0.77. The difference between energy and exergy analyses of exhaust is the inability of energy analysis to distinguish useful exhaust energy which could be extracted by recovery systems, from irreversibility which cannot (only minimized). As the spark timing shifts away from MBT timing, the exergy associated with heat transfer and work transfer is reduced due to reductions in the hydrogen engine IMEP (Fig. 2a and Fig. 2b). Reducing exergy transfer to work and heat causes increases the exergy expelled by the exhaust gases and is commensurate with the second law of thermodynamics which states that the system rejects the unused exergy and generated entropy. Therefore, reducing the exergy transfer to work and heat necessitates that the remaining exergy be expelled at the exhaust. When \emptyset was 0.77, the exergy expelled by the exhaust doubled when the spark timing was advanced by 10° CA from the corresponding MBT timing. However, the exergy associated with combustion irreversibility did not vary significantly (<2 %) with spark timing, as combustion related irreversibility is influenced most by mixture composition. Fig. 7a and Fig. 7b show that NO emissions were reduced when the spark timing was advanced or retarded from the corresponding MBT timing, which is

due to the reduction of the in-cylinder temperature.

3.3.2. MAP effect on exergy split

The hydrogen SI engines require an increase in MAP to compete with the load capabilities of gasoline engines [19]. Fig. 8 shows that at MBT timing the exergy transfer to reversible work increases with increasing MAP. For \emptyset of 0.90, the exergy to work transfer increased by 7 % when the MAP was increased from 80 kPa to 120 kPa. This increase was caused by the increased charge density associated with boosting resulting in a greater difference between the in-cylinder temperature and combustion chamber walls, as indicated by the increase in exergy associated with heat transfer. For Ø of 0.90 (Fig. 8c), the exergy associated with heat transfer increased by 8 % when the MAP was raised from 80 to 120 kPa. In contrast, the exergy expelled by the exhaust decreases as the MAP increases because the increase in exergy transferred to work and heat. Specifically, the exhaust exergy was reduced by 70 % and 22 % when the MAP increased from 80 to 120 kPa for \emptyset of 0.45 (Fig. 8a) and \emptyset of 0.90 (Fig. 8c), respectively. Meanwhile, the exergy associated with combustion irreversibility slightly reduced with increasing MAP but was not significantly affected, suggesting that the exergy transfer to combustion irreversibility mainly depends on the equivalence ratio. When the Ø shifted from 0.45 to 0.90 for the naturally aspirated condition (MAP of 80 kPa) the exergy due to irreversibility was reduced by 72 % due to the combustion product entropy reducing as Ø became richer, and coupled with an increase in the in-cylinder temperature. The exergy transfer to work increased with increasing MAP mainly because of the significant exhaust exergy losses and some contribution from reductions in combustion irreversibility. Consequently, the increase in efficiency and the reduction of the exhaust exergy with increasing MAP are promising; however, these benefits are counteracted by an increase in NO emissions (Fig. 8(a-c)). For all modelled Ø, NO emissions increased when the MAP shifted from 80 to 120 kPa, highlighting a trade-off between improving engine performance and managing emissions.

3.3.3. Compression ratio effect on the exergy split

Increasing the compression ratio also raises the reactant temperature, influencing entropy generation, hence potentially reducing the irreversibility losses associated with combustion. Whether this rise in reactant temperature is sufficient to influence the exergy due to combustion irreversibility of a hydrogen-fuelled engine is not understood. Increasing the compression ratio also increases the likelihood of com-



Fig. 7. Exergy split to work, heat, irreversibility and exhaust and NO emissions for various spark timings for Ø of 0.77 and 0.90 (MAP = 80 kPa, CR = 11.5, N = 2000 rpm).



Fig. 8. Exergy split to work, heat, irreversibility and exhaust for various MAP and Ø at and NO emissions at MBT timing (MAP = 80 kPa, CR = 11.5, N = 2000 rpm).

bustion abnormalities occurring [42], but these are not modelled in this study. In Fig. 9, the effect of increasing the compression ratio from 11.5 to 13.0 shows that exergy transfer to work increases by 9, 7, 6, 4, and 3 % for \emptyset of 0.45, 0.50, 0.65, 0.77, and 0.90, respectively. The peak exergy transfer to work, at 44 %, occurred at \emptyset of 0.45. The load increase with compression ratio could be explained by the increase in pressure and temperature during compression, which increases the flame speed and decreases the combustion duration. The exergy associated with combustion irreversibility did not vary significantly with the increase of the energy state by increasing the compression ratio. For \emptyset of 0.90 under naturally aspirated conditions, the exergy associated with combustion irreversibility reached a plateau around 7 %, even though the energy state increased with increasing compression ratio or by reducing heat loss (see Section 3.3.4). Whereas, for \emptyset of 0.45, the exergy transfer to combustion-related irreversibility could not be reduced by more than 25



Fig. 9. Compression ratio effect on the exergy split to work, heat, irreversibility and exhaust for MAP = 80 kPa NO emissions at MBT timing for various equivalence ratios.

%. However, increasing the compression ratio has been shown to be more effective at reducing the exergy at exhaust compared to combustion-related losses. The exhaust exergy was reduced by 88 %, 41 %, and 37 % when the compression ratio was increased (from 11.5 to 13.0) for \emptyset of 0.45, 0.77, and 0.9, respectively. Concurrently, the increase of the in-cylinder energy state increases the NO emissions by 229 % and 36 % for \emptyset of 0.45 and 0.90, respectively. This illustrates the trade-off where enhancements in performance may increase emissions.

3.3.4. Low heat rejection effect on the exergy split

To better understand the coupling of the main exergy contributors, reductions in heat transfer were studied to fundamentally understand which exergy contributor needs to be minimized to achieve higherperformance hydrogen fuelled engines. It is important to distinguish between an adiabatic and a no-heat-transfer engine. An adiabatic engine does not have heat transfer (which is impossible based on the definition), whereas a no-heat-transfer engine allows balanced heat transfer in and out of the gas [30]. While there will be no net heat transfer, exergy destruction will still occur due to the temperature difference between the burned and unburned mixture [43]. Reductions in heat transfer could be feasible by improving the insulation of the combustion chamber walls, and is known as a low heat rejection (LHR) engine [41].

The heat from the burned mixture could be used to increase the expansion work, thus increasing engine power output. For \emptyset of 0.45 (Fig. 10a) the heat loss reduction increased work efficiency by 37 %, 24 % and 9 % for 50 %, 60 % and 80 % heat loss reductions, respectively. However, it also increased the exergy transfer to the exhaust, where the expelled exergy increased by 60 %, 42 % and 28 %, for 50 %, 60 % and 80 % heat loss reductions respectively. The same trend was observed for all \emptyset (Fig. 10(a–c)). This is consistent with the second law of thermodynamics, which states that a steady-state system must reject the input and generated entropy. Therefore, the reduction of the entropy generated by heat transfer, by reducing heat loss, requires the entropy to be rejected at the exhaust. Without mechanical modifications the reduction of heat loss increases exergy transfer to the exhaust, increasing the exhaust temperature and therefore the temperature difference with the



Fig. 10. Exergy split to work, heat, irreversibility and exhaust for various Ø and heat loss percentages (MAP = 80 kPa, ST = MBT, CR = 11.5, N = 2000 rpm).

environment. However, the work and efficiency increases [41]. From Fig. 10 it can be seen that the combustion-related irreversibility reduced with decreasing the heat loss. This was mainly due to the increasing in-cylinder temperature caused by raising the energy state by reducing the heat loss.

3.4. Combined top-down and bottom-up approach

The efficiency of a hydrogen-fuelled engine at an \emptyset of 0.90 is calculated using two approaches: 1) the bottom-up approach, and 2) the top-down approach (Table 1). In the bottom-up approach, the irreversibility due to heat transfer, combustion, and exhaust are summed. Whereas, the top-down approach calculates the total engine irreversibility by taking the difference between the exergy input and the output. The top-down approach is a global method that does not identify or quantify losses, but depending solely on the exergy flows crossing the control volume boundary. The bottom-up and top-down exergy methods differ by approximately 11 J in the total irreversibility, which is defined

Table 1

Exergy balance for the case of \emptyset of 0.90 under the naturally aspirated condition)n
MAP = 80 kPa (CR = 11.5, N = 2000 rpm, ST = 4 °CA bTDC).	

	Process	Bottom- Up	Top- Down
Exergy input (J)	Fuel Chemical Exergy	465	465
Irreversibility (J)	Heat Transfer	170	
	Combustion	33	
	Exhaust	79	
Exergy output (J)	Reversible Work		172
Exergy input- Exergy output			292
(J)			
Total Irreversibility (J)		282	293
$1 - \frac{\text{Irreversibility}}{\text{Exergy input}}$ (%)		39 %	37 %

as unaccounted exergy. This unaccounted exergy could be due to mechanical friction [43].

4. Conclusions

A two-zone hydrogen combustion model was used to identify exergy transfers of a boosted lean-burn hydrogen-fuelled SI engine. The amount of exergy transferred to work increased with decreasing equivalence ratio, as the exhaust enthalpy was diverted into reversible work. However, the combustion-related irreversibility rate increased due to the reactant and product entropy difference, arising from the reduced amount of hydrogen fuel. For Ø of 0.90 at a pressure of 30 bar and temperature of 1800 K the combustion related entropy generation reduced by 86 % when the reactant temperature was increased from 300 K to 900 K. When the spark timing was shifted away from the corresponding MBT timing, the exergy associated with work and heat decreased because of reductions in IMEP. The reductions in exergy transfer to work and heat caused the exergy expelled by the exhaust gases to increase. Additionally, increasing the MAP or compression ratio reduced the exergy expelled by the exhaust, as the exergy used for work and heat transfer left less exergy to be expelled. For Ø of 0.90 the exergy expelled by exhaust reduced by 22 %, whereas exergy transfer to work and heat increased by 7 % and 8 %, respectively, when the MAP was increased from 80 kPa to 120 kPa. In contrast, the exergy associated with combustion irreversibility was not significantly affected by spark timing, MAP, or compression ratio. However, it was strongly influenced by the equivalence ratio because of the difference between the reactant and product entropy. For a ϕ of 0.45, approximately 26 % of the incoming exergy was lost due to the irreversibility of the combustion reaction, limiting the maximum possible efficiency of the hydrogenfuelled SI engine to 74 %. Reducing equivalence ratio below 0.45 could lead to combustion instability due to increased flame instability [44]. Whereas, reducing heat loss increased the exergy transfer to work, but also increased the exergy expelled by the exhaust. With reduced heat

loss, the combustion-related irreversibility decreased due to the increased temperature. While this theoretical approach showed potential benefits for hydrogen engine efficiency, the improvements in exhaust enthalpy must be further addressed to maximise the benefit from entropy reductions by reducing heat loss. Improvements to using or converting exhaust heat into useful energy may enhance the overall engine performance and efficiency.

CRediT authorship contribution statement

D.N. Rrustemi: Writing - original draft, Visualization, Validation,

Appendix

Combustion model

Software, Methodology, Investigation, Formal analysis. **L.C. Ganippa:** Writing – review & editing, Methodology. **C.J. Axon:** Writing – review & editing, Supervision, Conceptualization.

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.

The combustion chamber is modelled assuming two-zones: 1) the unburned zone comprising the reactants, and 2) the burned zone comprising the products. The main input of the two-zone combustion model is the mass fraction burned profile calculated using the Blizard and Keck [4] approach. The laminar flame speed of the hydrogen/air mixture was calculated using an empirical correlation [5]. Whereas, the thermodynamic properties were calculated using the empirical correlations of state properties for each in-cylinder species [6]. After rearranging the equation of state, the first law and continuity equation, following first order differential equations were derived to model combustion process. The subscript u and b refer to unburned and burned zone respectively,

$$\begin{aligned} \frac{dT_u}{d\theta} &= \frac{1}{m_u c_{pu}} \left(V_u \frac{dP}{d\theta} - \frac{dQ_u}{d\theta} \right) \\ \frac{dT_b}{d\theta} &= \frac{1}{m_u c_{pu}} \left[P \frac{dV}{d\theta} - \left(R_b T_b - R_u T_u \right) \frac{dm_b}{d\theta} - \frac{R_u}{c_{pu}} \left(V_u \frac{dP}{d\theta} + \frac{dQ_u}{d\theta} \right) + V \frac{dP}{d\theta} \right] \\ \frac{dP}{d\theta} &= \frac{1}{\frac{c_{yu}}{c_{pu}} V_u} - \frac{c_{yb}R_u}{R_b c_{pu}} V_u + \frac{c_{yb}}{R_b} V \left\{ \left(1 + \frac{c_{yb}}{R_b} \right) P \frac{dV}{d\theta} - \frac{dQ}{d\theta} + \left[\left(u_b - u_u \right) - c_{yb} \left(T_b - \frac{R_u}{R_b} T_u \right) \right] \frac{dm_b}{d\theta} + \left(\frac{c_{yu}}{c_{yu}} - \frac{c_{yb}R_u}{R_b c_{pu}} \right) \frac{dQ_u}{d\theta} \end{aligned}$$

The following equations are used to account for convective heat transfer,

$$\begin{split} \frac{dQ}{d\theta} &= \frac{dQ_u}{d\theta} + \frac{dQ_b}{d\theta} \\ \frac{dQ_u}{d\theta} &= \frac{30A_u}{N} \left[h_{cu} (T_{gu} - T_w) + \beta \sigma \left(T_{gu}^4 - T_w^4 \right) \right] \\ \frac{dQ_b}{d\theta} &= \frac{30A_b}{N} \left[h_{cb} (T_{gb} - T_w) + \beta \sigma \left(T_{gb}^4 - T_w^4 \right) \right] \end{split}$$

where A is the surface area, h is convective heat transfer coefficient, β is a constant value of 0.6 and σ is Stefan-Boltzmann constant 5.67 \times 10⁻⁸ W/m²K⁴.

Although the results support development of hydrogen-fuelled ICEs, experimental work is required to substantiate the proposed boosted lean-burn strategies because the trade-offs and limitations are complex. Boosting intake air pressure enhances thermal efficiency but increases the likelihood of combustion abnormalities as hot spots or emissions from unburned hydrogen from the previous cycle can cause pre-ignition in hydrogen ICE. Pre-ignition was not considered since the hot spots could not be identified using a zero-dimensional combustion model. Similarly, the model does not account for mixing of the fuel and air. The zero-dimensional exergy analysis considered work, heat, combustion irreversibility, and exhaust, but does not provide complex details of the physics and chemistry processes. By using fluid dynamics simulations, it may be possible to gain deeper insights into the loss mechanisms within engine processes and components, and offer a clearer path to minimize exergy losses and enhance overall engine performance.

Data availability

Data will be made available on request.

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