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Piston Engine Modelling for Hydrogen Fueled Composite Cycle Engines

Nickl, M.*, Winter, F.*, Gümmer, V.**

* Bauhaus Luftfahrt e.V., Taufkirchen, Germany

** TU Munich Chair of Turbomachinery and Flight Propulsion, Garching, Germany

markus.nickl@bauhaus-luftfahrt.net

Abstract.

In order to achieve aviation's ambitious emission reduction targets specified by ACARE [1] radical changes in propulsion system concepts will be necessary. To fulfill the goal of carbon dioxide emission neutrality in 2050 and beyond, plenty propulsion system concepts are currently under investigations, mainly focusing on batteries and hydrogen as energy source. Especially for long range aircraft applications, hydrogen might by favorable due to its outstanding specific gravimetric energy density. Therefore, the Composite Cycle Engine (CCE) concept should be evaluated for hydrogen combustion. In a first step, the applied time resolved 0D piston engine performance simulation model of the CCE is adapted for hydrogen combustion. For example, the heat transfer and combustion characteristics of kerosene and hydrogen combustion differ significantly and require specific modeling approaches. The current publication illustrates the piston engine performance simulation model and the modifications needed to account for hydrogen combustion. Furthermore, results of validation case calculations as well as initial sensitivity studies of the hydrogen fueled piston engines model are presented and discussed in the CCE context. For example, sizing effects and the influence of valve timing on piston engine performance will be evaluated.

Nomenclature

Symbols	Description	Abbreviations	Description		
À	Area	ABDC	After bottom dead center		
b	Piston bore	ATDC	After top dead center		
c	Velocity	BBDC	Before bottom dead center		
С	Constant	BHL	Bauhaus Luftfahrt e.V.		
Т	Temperature	BTDC	Before top dead center		
Q	Heat Loss	CCE	Composite Cycle Engine		
p	Pressure	CEA	Chemical Equilibrium with		
-			Applications		
Р	Power	SAF	Sustainable Aircraft Fuel		
V	Volume	SRIA	Strategic Research and		
			Innovation Agenda		
α	Heat transfer coefficient	PEPSI	Piston Engine Performance		
			SImulation		
λ	Air-fuel equivalence ratio				

Crank angle Φ

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1. Motivation

In order to meet aviation's long term emission reduction targets (i.e. specified by SRIA [1]), radical improvements and step changes in all aircraft associated disciplines are mandatory. As in the past, developments in propulsion system technologies will have to contribute a major part to the required rise of vehicle efficiency. Up to now, the efficiency of turbomachinery has been enhanced continuously making further significant evolutionary improvements much harder in the future.

A novel propulsion system concept, promising 10 - 15 % fuel burn reduction above evolutionary turbomachinery development, is the Composite Cycle Engine (CCE), which has already been discussed by Kaiser et al [2,3,4]. The CCE concept introduces piston engines to the core of modern turbomachinery. Due to their unsteady, pressure gaining combustion, higher pressure and temperature levels can be obtained, leading to higher core efficiency. An illustration of a CCE propulsion system and its thermodynamic cycle design is shown in Figure 1.



Figure 1: Illustration of a CCE aircraft propulsion system (left) and its thermodynamic cycle (right) [5]

Furthermore, with respect to the global CO_2 emission budget to restrict global warming to less than 2 K [6] even CO_2 neutral propulsion system concepts might be necessary. A forecast of aviation's CO_2 emissions and a possible split how the recommended CO_2 budget restriction might be achieved is illustrated in Figure 2.



Figure 2: Emission reduction potential for individual options (modified from [7])

Current research favours battery electric propulsion for small [8,9] and hydrogen based propulsion systems for larger public transportation applications [10]. While the use of hydrogen is already state of the art for both, piston engines and turbomachinery, the CCE concept should be compatible with hydrogen combustion as well, but has not been evaluated in aircraft propulsion system context yet. The current publication focuses on the modelling approach for a hydrogen fueled piston engine during propulsion system predesign and discusses results of piston engine performance characteristics in the CCE context.

2. Methods

For piston engine performance simulation, a BHL internal computation code (Piston Engine Performance SImulation - PEPSI) is adapted, which has been used for thermodynamic cycle calculations of kerosene fueled piston engines [2,3,4]. This chapter illustrates the applied modifications to enable performance simulations of hydrogen fueled piston engines.

2.1. Thermodynamic Properties

In a piston engine, thermodynamic state conditions vary over a wide range. For example, temperature rises from inlet conditions up to 2500 K, which is accompanied by massive changes in thermodynamic properties of the fluid. Also the fluid composition changes during combustion. The air-fuel equivalence ratio λ can be chosen from no fuel ($\lambda \rightarrow \infty$) up to $\lambda = 1$, which causes significant variations in fluid properties, too. As the dependency of thermodynamic gas properties on pressure is orders of magnitude smaller compared to their sensitivity on temperature, half-ideal gas properties for air and hydrogen combustion products are used.

The National Aeronautics and Space Administration (NASA) provides an open source program [11] which calculates complex chemical equilibrium compositions for different fluids. This 'Computer Program for Calculation of Complex Chemical Equilibrium Compositions and Applications' (CEA) is used to establish a database for the fluid properties of hydrogen-air combustion.

This customized database is validated against further data available in literature [12,13]. The results of the validation show an adequate accordance between the database and the literature data with relative errors up to maximal ± 0.3 % in the relevant area of application. For example, Figure 3 illustrates the relative deviations for the specific enthalpy of air.



Figure 3: Customized data in comparison to literature data for the specific enthalpy of air

2.2. Piston Engine

The piston engine is modeled using a 0D-modeling approach, which provides the advantage to deliver results rapidly. A 0D- or single-zone model resolves the thermodynamic cycle crank angle-/time-wise, however, the spatial flow field is not resolved. Therefore, the 0D-model offers all relevant crank angle resolved thermodynamic information to evaluate the piston engine combustion process $(T(\phi), V(\phi), \dot{m}(\phi))$ as well as integral data like the heat loss Q and the power output P.

The BHL-inhouse piston simulation program PEPSI is based on the reciprocating piston model of van Gerpen [14] and is calibrated and validated against NASA-CR-188232 data [15], but also incorporates several extensions in example for different piston geometries, heat transfer correlations and

emission estimations. As result of the validation, the main performance indicators mass flow rate \dot{m}_1 and \dot{m}_2 as well as the power output vary by less than 0.1 % of the validation data. The time-resolved results for temperature and pressure vary by 0.4 % and 1.0 % respectively which shows a good agreement across the entire cycle [16] (illustration in Figure 4). A more detailed description of the methods of PEPSI can be found in [3].



Figure 4: Validation of crank angle resolved pressure (left) and temperature (right) distribution of the piston engine performance simulation (literature data from [14])

2.3. Heat Transfer

The short duration of the hydrogen combustion process leads to an increased heat emission and hence, to a higher amount of heat losses across the walls of the combustion chamber compared to hydrocarbon fueled piston engines. Furthermore, the increase in thermal wall losses is additionally boosted by the absence of solid soot, which would increase the heat transfer resistance. Since no soot particles are formed by the combustion of hydrogen, on the one hand, water vapor is the radiation generator in this process. However, the radiation forced by water vapor is negligible which leads to a non-existent radiative heat flow [17]. On the other hand, no carbon deposit is formed, which acts as a natural heat insulator on the surfaces of the heat-stressed engine parts [17]. Moreover, the heat transfer inside the combustion chamber is not steady and varies cyclically [18]. As a result, the heat transfer of hydrogen combustion could not be modeled as that of hydrocarbon fuels.

To describe the heat transfer between the hot gas and the piston wall, quasi-steady state conditions are assumed. Then, the heat transfer can be calculated using the Newton law of cooling according to

$$Q = \alpha A (T_{\rm g} - T_{\rm W})$$

where α is the wall heat transfer coefficient, A is the total wall surface area, T_g is the bulk gas temperature and T_W is the wall temperature averaged over the heat transfer surface.

To predict the wall heat transfer coefficient α during hydrogen combustion, new or adapted correlations have to be applied. In literature, various correlations are used to describe the wall heat transfer coefficient α like the Woschni-Vogel correlation [19], the Annand correlation [18] and the Hohenberg correlation [20]. In this study, a newly developed approach to model the hydrogen-fueled piston engine wall heat transfer coefficient by Shudo and Suzuki [21] is used. This approach is based on the Woschni-Vogel correlation, where the gas velocity term (in brackets in equation below) is adapted to hydrogen combustion [21]

$$\alpha = C_1 b^{-0.2} T_{\rm g}^{-0.53} p^{0.8} \left(c_{\rm m} + C_2 \frac{\mathrm{d}Q}{\mathrm{d}t} \frac{T_1}{p_1 V_1} \right)^{0.8}$$

Compared to Woschni-Vogel, the gas velocity term is no more dependent on the pressure but on the apparent rate of heat release dQ/dt. This adaptation leads to a faster increase in heat transfer coefficient and therefore, the heat transfer reaches its maximum earlier [21] corresponding to the faster combustion of hydrogen. Moreover, the parameters C_1 and C_2 are defined as functions of the ignition timing and air excess ratio [21]. According to preliminary studies, the parameters C_1 and C_2 are not adapted to the actual air-fuel equivalence ratio, but they are held constant at the following values defined for stoichiometric combustion: $C_1 = 0.1257$ and $C_2 = 0.8772 \frac{m}{\kappa}$.

2.4. Calibration and Verification

The piston engine model described in section 2.2 including the modified heat transfer correlation (see section 2.3) is calibrated and verified with data from literature. Therefore, a model of a published piston engine [22] is set up and three operating conditions of the piston engine are calculated. A comparison of the time resolved pressure curves as well as integral data are shown in Figure 5. For all three cases pressure curves fit almost perfectly, whereas integral values of power output and peak pressure deviate within a range of approximately 1 %. More verification calculations for further publications [23] were performed, achieving variations of less than 4 % from published data.

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Figure 5: Comparison of calculated and published [22] data for time resolved (left) and integral (right) data of a hydrogen fueled piston engine

3. Analyses

Based on the presented parametric piston engine performance simulation model, sensitivity analyses were performed. Here, the results of two selected parameter studies are presented. First, the effect of valve timing is analyzed and second, piston cylinder geometry variations and their effect on piston engine key parameter is illustrated. For this purpose, a generic piston engine design is chosen, from which 1D-sensitivities are derived. The settings of the generic piston engine are summarized in Table 1.

Parameter	Unit	Value	Parameter	Unit	Value			
Bore	[m]	0.10	Combustion duration	[deg]	30			
Bore-to stroke ratio	[m]	0.8	Inlet valve opening	[deg]	17 ATDC			
Compression ratio	[-]	10	Inlet valve closing	[deg]	26 ABDC			
Air-fuel equivalence ratio	[-]	3	Exhaust vale opening	[deg]	12 BBDC			
Combustion heat release characteristic parameter	[-]	2	Exhaust valve closing	[deg]	6 ATDC			
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3.1. Valve Timing

Piston engine valves are assumed to be located at the piston head. Two inlet and outlet valves are arranged at the available circular area. The valve cross sectional area is geometrically maximised dependent on piston bore diameter and the number of valves. Additionally, sinusoidal valve opening and closing characteristics are applied. In the first parameter study, the effect of piston engine valve timing is examined. Therefore, the four valve timing parameter are varied independently. The corresponding relative changes in piston engine key parameters are depicted in Figure 6.

Power output, thermal efficiency and peak pressure similarly react on a variation of intake valve opening position (IVO), having a maximum at IVO at piston top dead center (TDC), whereas heat losses behave vice versa. Intake valve closing point (IVC) has no influence on thermal efficiency in the investigated parameter range, but the other parameters have maxima at IVC set at piston bottom dead center (BDC). For exhaust valve opening position (EVO) shifting to later positions, monotonously

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increasing heat losses are detected in the chosen parameter range, whereas piston peak pressure is constant. Therefore, piston thermal efficiency and power output decrease in this direction. Finally, variation of exhaust valve closing position leads also to increasing heat losses and decreasing power output and thermal efficiency in direction of late EVC timings. Piston peak pressure sensitivity is caused by change in scavenging behavior of the piston cylinder and has a maximum 5 deg after TDC position. If beneficial settings of all valve timings (dashed lines in Figure 6) are combined, thermal efficiency of the piston engine can be increased by 0.7 % compared to initial generic piston engine settings (yellow square). Power output, peak pressure and heat losses increase thereby almost homogeneously (approx. +3.6 % each).



Figure 6: Relative changes in piston engine key parameters for valve timing variation

3.2. Geometry Variation

In a second study, piston cylinder's geometric parameters bore, bore-to-stroke ratio and geometric compression ratio (ratio between minimum and maximum cylinder volume, here h_{min}/h_{max}) are varied individually. The parameters are depicted in Figure 7 (top left) together with the sensitivities of piston engine key parameters for the three parameter variations (curve colour indicates the corresponding ordinate scale). In Figure 7 top right, the results of the bore variation are plotted. The swept volume of the piston engine changes with the power of 3 (constant bore to stroke ratio) for linear bore increase. Combined with the constant air-fuel equivalence ratio λ , this leads to a significant increase of power output and heat losses with rising bore (up to 7 times and 15 times, respectively). For large pistons (bore > 0.175m), piston scavenging becomes worse, caused by the limited valve cross flow area for the assumed valve arrangement. Especially, peak pressure reduces for this reason, counteracting and reversing the upstreaming power output trend. Thermal losses further increase for larger pistons due to enlarging surface areas resulting in lower thermal efficiencies.

Changing the ratio of bore and stroke, affects monotonously rising characteristics for peak pressure and thermal efficiency and decreasing trends for power output and heat losses (Figure 7, bottom left). Again, the latter mainly results from the change in swept volume of the piston cylinder. Last, piston compression ratio variation obviously leads to peak pressure shift in the same direction (Figure 7, bottom

bore Variation of piston bore 1.2 Piston (TDC) 0.8 0.6 04 Piston (BDC) 0,2 0.3 0.05 0.075 0,1 0,125 0,15 0,175 0.25 Variation of piston compression ratio Variation of bore-to-stroke ratio 1,5 2.4 1.04 1,6 1.9 1 01 12 1,4 0,98 0.9 0.95 0.9 0.8 04 0.92 0.7 0.4 1.4 al Effic

right). Additionally, piston power output and thermal efficiency improve with rising compression ratio, even though heat losses increase, too.

Figure 7: Illustration of piston cylinder geometric parameters (top left) and relative changes of piston engine key parameters for piston geometry variation (top right: bore, bottom left: bore-to-stroke ratio and bottom right: compression ratio)

4. Discussion

In the following, the results of the parametric studies are discussed together with further aspects in the CCE context. Especially the expected impact on hydrogen fueled CCE design are highlighted. First, the valve timing study indicates, that valve timing has to be chosen beneficially, but partial dependencies of piston engine key performance parameters are very flat when valve timing is modified. Consequently, only second order effects on H_2 -CCE design are expected. In contrast, significant influences on (for example) piston peak pressure were shown for different piston engine geometries. On the one hand, the piston system dimensions need to be accommodated within the core engine cowling. On the other hand, geometric relations have to be set properly for best CCE performance. Most likely, a compromise between piston peak pressure and power output has to be found.

Furthermore, piston peak pressure level was identified as a technological limitation for CCE design. This limitation will be even harder for H_2 -CCEs due to hydrogen's combustion characteristic. The high combustion velocity results in a short combustion duration and the peak in combustion heat release shifts towards early phases during the combustion phase. Both effects lead to higher peak pressures compared to kerosene fueled CCEs. Additionally, increased piston wall heat transfer is detected for hydrogen combustion. This might motivate a recovering system for piston engine heat losses on CCE level.

Another finding from CCE investigations in the past was the beneficial combination of CCE with intercooling technology. By cooling the piston inlet mass flow, volume flow reduces, allowing smaller and therefore lighter piston systems. Moreover, lower peak temperatures occur within the piston thermodynamic cycle, cutting down the criticality of piston cooling system. It is expected, that intercooling will be a synergistic technology for H_2 -CCEs, too.

5. Conclusion and Further Work

In order to find technologies for realizing the pathway to a CO_2 neutral aviation sector until 2050, as requested by the Paris Agreement, the piston system of the revolutionary aircraft propulsion system concept of a Composite Cycle Engine (CCE) is analyzed with regard to its compatibility with hydrogen combustion. Therefore, required modifications of the used 0D - piston engine performance simulation program are presented, which cover adaptions of the thermodynamic property database, correlation of the piston wall heat transfer coefficient and the combustion characteristic. The applied methodologies are verified by recalculation of published data for hydrogen fueled piston engines. Time resolved as well as integral parameters are reproduced for different operating conditions with small relative deviations (<1 %). Then, sensitivities of valve timing settings as well as the influence of piston geometry parameter variations on hydrogen fueled piston engine performance are illustrated. The results are discussed with regards to the expected impact on hydrogen fueled CCE design. It is found, that valve timing settings have a second order effect on piston engine performance, whereas piston geometry has to be optimized for CCE integration to find the best compromise between piston peak pressure and thermal efficiency and shaft power output.

Future work will focus on the integration of the hydrogen fueled piston performance modelling to the turbomachinery performance simulation environment to enable design studies on H_2 -CCE level. For evaluation of these studies on aircraft level, weight estimation methods for both, hydrogen fueled piston engine and turbomachinery have to be conveniently adopted, too.

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