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A novel internal combustion engine utilizing internal hydrogen production for improved efficiency – A theoretical concept

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ABSTRACT

Starting from the baseline of a Diesel engine, we show that with a suitable in-cylinder catalyst and well controlled injection of fuel and steam mixture during a certain period in the compression stage, a significant increase in the ideal cycle efficiency is achievable (from 67% to 78% for an initial compression ratio of 25). In such an arrangement, the fuel injection session comprises a two-stage process. In the first stage, fuel and water are injected into the hot previously compressed cylinder charge over the catalyst. Residual heat is absorbed due to a steam reforming process to produce hydrogen. The heat absorption cools the compressed mixture and enables a higher compression ratio up to the maximum allowed pressure, while the temperature of the cylinder charge remains constant. In the second stage, only fuel is injected to initiate combustion while the absorbed heat (of the first stage) is released through the hydrogen oxidation. Essentially, the absorbed heat is exploited to produce extra hydrogen fuel, which increases the cycle efficiency.

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Introduction

The cycle starts at point 1 (Fig. 1) where the piston is at BC (Bottom Centre) and the trapped charge (air for DI engines) is at STP conditions. The basic Diesel cycle is shown by points 1–2–3–4–1. In the present new cycle, the charge is compressed by the up-moving piston from state 1 to 2b. During compression, at point 2a, a well prepared mixture of fuel and steam is introduced to the cylinder in the presence of a suitable catalytic surface. In the first stage, when injection takes place, residual heat is absorbed due to a steam reforming

process to produce hydrogen. The heat absorption cools the compressed mixture and enables a higher compression ratio up to the maximum allowed pressure, while the temperature of the cylinder charge is kept constant (2a–2b). In the second stage, after injection has ended (2b), the absorbed heat (of the first stage) is being used during the combustion stage, when the hydrogen undergoes combustion. Essentially, the absorbed heat is exploited to produce extra hydrogen fuel, which increases the cycle efficiency. That contribution is unique to the combined steam and fuel injection in the present study. The fuel injection rate has to be controlled such that the combustion process (of the injected fuel and the previously

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Nomenclature

c_p	heat capacity at constant pressure
c_v	heat capacity at constant volume
m	mass
P	pressure
Q	heat
R	gas constant
T	temperature
t	time
V	volume
K_{p1}	equilibrium constant (eq. (1))
K_{p2}	equilibrium constant (eq. (2))
W	work
x	CO ₂ production (Table 1)
y	methane conversion (Table 1)
η	efficiency
Indices	
0	ambient (STP)

generated hydrogen) is performed from 2b to 3 under constant pressure conditions. Combustion thus takes place between 2b and 3, while injecting the rest of the fuel.

The overall amount of combusting fuel would be the injected fuel of 2a→2b and 2b→3, less the fuel consumed during 2a→2b (by the hydrogen generating reactions), plus the hydrogen fuel generated during 2a→2b. In total, that should have a higher calorific value than just the amount of supplied fuel (during 2a→3 combined), as the hydrogen generating reactions are endothermic in total. If the same amount of supplied fuel is used in a standard Diesel cycle of the same maximum pressure, the fuel injection will take place between 2 and >3. We note however that in the modified-Diesel cycle described here, hydrogen combustion takes place past point 2b, as it actually carries energy of the prior injected fuel (during 2a→2b). Nevertheless, the overall indicatoric work (area of P–V diagram) is larger for the same total amount of injected fuel as in a standard comparable Diesel cycle, hence its superior efficiency to the latter. The point 2a is chosen as the minimal temperature which would still suffice for a significant amount of water steam reformation. On the other hand, the lower that temperature is, the more heat could be absorbed from the compression stroke, hence an optimization of that point could be achieved. Another factor to consider is the rate of catalyzed reaction, which increases with temperature. Using modern catalysts [1,2] can enable a high enough rate, namely, of a time shorter than the time of the compression stroke, at a workable temperature. For this task, a metal-based catalyst with a suitable effective surface area could fit (e.g. Ni/MgAl₂O₄ or Ni/ZrO₂). Larger Diesel engines, however, of slower rpm's could accommodate a wider selection of catalysts, or lower compression temperatures. Process 3–4 is an isentropic expansion, and 4–1 designates the gas exchange process.

In order to evaluate the new cycle efficiency, we use the following approach.

Thermo-chemistry of steam reforming

To model the steam reforming process, we use a simplified system of Methane–Water, and consider chemical equilibrium reactions between them. We assume the dominant simultaneous reactions to be:

1. $\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2$
2. $\text{CH}_4 + \text{H}_2\text{O} \rightleftharpoons \text{CO} + 3\text{H}_2$

With the purpose of reducing times required for equilibriums, the reactions occur in the presence of a catalyst. The first reaction is moderately endothermic, while the second is highly endothermic. The Equilibrium constants [3] for these two reactions are presented in Fig. 2.

The importance of temperature to these reactions could be realized from Fig. 2. An increase in the temperature from 900 K to 1200 K, for example, results in an increase of 3 orders of magnitude in the equilibrium constant in favour of H₂ production.

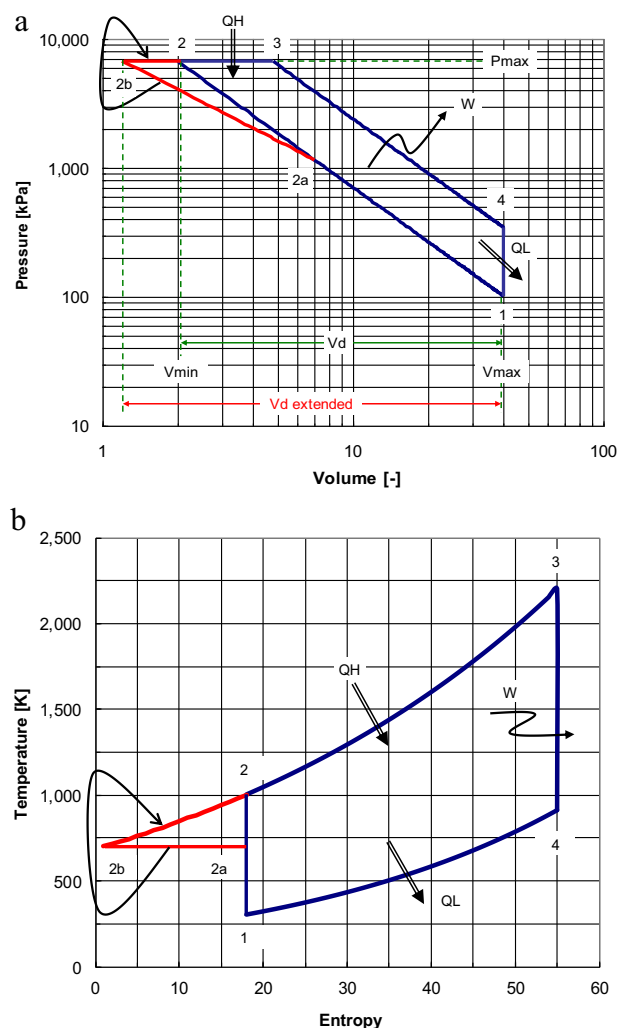


Fig. 1 – The thermodynamic cycles of Diesel and modified-Diesel on a: a) P–V diagram b) T–s diagram.

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