Article

A Diesel Engine with a Catalytic Piston Surface to Propel Small Aircraft at High Altitudes—A Theoretical Study

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Abstract: Due to the oxygen shortage at high altitudes, the use of diesel engines in small aircraft is limited to a low ceiling level. Here, we propose to significantly extend the ceiling level by introducing an in-cylinder steam reforming system. In this arrangement, the fuel direct-injection assembly comprises of a two-stage process. In the first stage, a blend of methanol and water is injected into the hot previously compressed cylinder charge onto an in-cylinder catalyst. Residual heat is absorbed due to the blend evaporation and the steam-reforming process to produce hydrogen. In the second stage, diesel fuel with a lower ignition temperature than the hydrogen fuel is injected to initiate combustion, while the absorbed heat (from 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. In this arrangement, the in-cylinder oxygen content is significantly increased due to the additional oxygen atoms that are included in the methanol and in particular in the water molecules. These are released when the methanol and water are decomposed during the steam-reforming process. We show that owing to the addition of the oxygen content in the cylinder, the flight ceiling level can be extended from 5000 to 9000 ft, and that the indicated efficiency can be increase up to 6%.

Keywords: diesel engine; small aircraft; in-cylinder steam reforming; flight ceiling

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1. Introduction

While considering a basic naturally aspirated diesel engine, the employment of a suitable in-cylinder catalyst may significantly increase the ideal cycle efficiency by more than 10% [1]. In this arrangement, a blend of fuel and steam is pre-injected during the compression stroke onto the piston head surface that is coated by a specially designed catalyst. Then, the blend is transformed by a steam-reforming process (SRM) into a hydrogen-rich mixture. This is a promising type of internal heat recovery approach that can be used (among other widely used applications) in diesel-operated miniature air vehicles (MAVs) [2,3] at high altitudes. Due to its high hydrogen-to-carbon ratio, sulfur-free composition, high energy density, and availability [4], we consider here a blend of methanol and water.

During the last two decades, steam reformers (SRM) have been considered to recover a part of the exhaust gas thermal energy. Suitable catalysts were installed downstream the exhaust pipe to harvest a part of the exhaust gas energy while generating hydrogen, which is fed directly back into the cylinder [5–7]. An interesting simple miniature methanol reformer for miniature air vehicles (MAVs) was developed by Telotte [8]. This SRM system was designed to produce a small amount of hydrogen for generating a net power of a few dozen Watts.

In a previous work [1], an in-cylinder steam reforming has been designed and employed. The fuel direct-injection system comprises of a two-stage process. In the first stage, a blend of methanol and water is injected into the hot previously compressed cylinder

charge onto the catalyst. Residual heat is absorbed due to the blend evaporation and the steam-reforming process to produce hydrogen. In the second stage, diesel fuel (or alike) with a lower ignition temperature than the hydrogen fuel is injected to initiate combustion, while the absorbed heat (of the first stage) is released through the hydrogen oxidation (exothermic reaction). Essentially, the absorbed heat is exploited to produce extra hydrogen fuel, which increases the cycle efficiency [1]. In this arrangement, the temperature and the pressure of the in-cylinder charge at the end of the compression stroke are lowered (from point 5 to point 3 in Figure 1), and a higher compression ratio (which results in an extended displacement volume) is therefore allowed (point 4); thus, further improvement of the thermodynamic efficiency is achieved at the same engine load. Therefore, cylinder compression occurs simultaneously with the heat absorption by the SRM process. In order to maximize the SRM advantage, the blend injection should be carefully designed such as the temperature of the cylinder charge remains constant toward the end stages of the compression stroke (the red line from point 2 to point 4 in Figure 1). The corresponding T-s diagram may be found in Sher and Sher [1].

Figure 1. A modified diesel cycle in which residual heat is absorbed during the compression stroke due to a steam-reforming process of methanol/water blend to produce hydrogen fuel (modified from [1]). The displacement volume is the volume swept by the piston in a single stroke.

In addition, by utilizing a portion of the in-cylinder thermal energy to generate hydrogen, we are using thermal energy that otherwise would have been partially rejected from the cylinder.

The unique thermo-physical properties of hydrogen, its low fuel-lean flammability limit, high burning velocity, high heat of combustion value, high diffusivity to the air, and zero carbon content make it an ideal efficient and clean fuel. However, the present concept calls for an additional fuel tank for the liquid methanol/water blend.

Due to the oxygen shortage at high altitudes, the use of naturally aspirated diesel engines in small aircraft is limited to a low ceiling level. In the present article, we propose to significantly extend the flight ceiling level of a small diesel-propelled aircraft by introducing an in-cylinder steam-reforming system.

2. Steam-Reforming Kinetics

During the years, the model has been extensively validated for quite a wide range of engine types against experimental observations. For the present purposes, we employed the GT-POWER engine simulation software where the chemical reactions scheme has

been modified to include the in-cylinder steam-reforming (SRM) process. We used the Langmuir–Hinshelwood mechanism as validated by Poran and Tartakovsky [7] in the entire range of the present in-cylinder relevant temperatures and pressures. In this scheme, the SRM is considered to occur when the methanol/water blend hits the catalyst surface through two possible parallel paths [9]. The 1st possible path includes two-stage reactions: the methanol decomposition (MD) reaction and the water gas shift (WG) reaction (Figure 2). The 2nd possible path is a single step reaction, the steam reforming (SR), which transforms methanol and steam directly to hydrogen and carbon dioxide.

Figure 2. The chemical reactions mechanism.

The endothermic methanol decomposition (MD) reaction:

The exothermic water gas shift (WG) reaction:

The endothermic direct steam-reforming (SR) reaction:

Following Peppley [9], there are two distinct types of active sites on the surface of the $\text{CuO}/\text{ZnO}/\text{Al}_2\text{O}_3$ catalyst: one small-size active site for the smaller species and one big-size active site for the bigger species [10]. The rates of reactions that occur on the surface of the catalyst per unit mass of the catalyst in $\left[\frac{\text{kmol}}{\text{kg}\cdot\text{s}}\right]$ are [11]:

$$\frac{d[\text{H}_2]}{dt} = (3r_{\text{SR}} + 2r_{\text{MD}} + r_{\text{WG}}) \cdot S_A \quad (4)$$

$$\frac{d[\text{CO}]}{dt} = (r_{\text{MD}} - r_{\text{WG}}) \cdot S_A \quad (5)$$

$$\frac{d[\text{CO}_2]}{dt} = (r_{\text{SR}} + r_{\text{WG}}) \cdot S_A \quad (6)$$

$$\frac{d[\text{CH}_3\text{OH}]}{dt} = -(r_{\text{SR}} + r_{\text{MD}}) \cdot S_A \quad (7)$$

$$\frac{d[H_2O]}{dt} = -(r_{SR} + r_{WG}) \cdot S_A \quad (8)$$

where S_A is the specific surface area per unit mass of fresh catalyst (here $S_A = 101.72 \left[\frac{m^2}{g} \right]$), and r_{MD} , r_{WG} , and r_{SR} , are the reaction rates of the methanol decomposition (MD), the water gas shift (WG), and steam reforming (SR), respectively. The reaction rates are complex functions [9,12] of the partial pressures of each species, equilibrium constants of each elementary chemical equation, and the total surface concentration of the active site related to each individual species.

In the present proposed configuration, following the hydrogen formation, fossil fuel (n-heptane in this simulation) is injected into the cylinder, and owing to the higher ignition temperature of the hydrogen, 800 K as compared to 490 K of the n-heptane fuel, the latter is ignited first. The combustion process is simulated here by a reduced mechanism of n-heptane/air mixture (1738 simultaneous elementary reactions and 106 species) that includes the hydrogen combustion mechanism [13–15].

3. Model Validation

The GT-POWER engine simulation software [16] is a well-established engine performance simulation software that is widely used today by a number of major engine manufacturers and vehicle original equipment manufacturers (OEMs) worldwide. We note that the GT-Power model considers premix combustion rather than mixing controlled combustion. This approach is appropriate when high injection pressures are applied to generate small enough droplets to facilitate fast evaporation and mixing, and thus, it fits well our present case. The GT-POWER software has been used to predict the time evolution of the pressure, temperature, and relevant species quantities inside the cylinder, from which the engine performance map is calculated under various ambient conditions including operation (flight) altitude level. During the years, the model has been extensively validated for quite a wide range of engines types against experimental observations. For the present purposes, we employed the GT-POWER engine simulation software where the chemical reactions scheme has been modified to include the in-cylinder steam-reforming (SRM) process. We used the Langmuir–Hinshelwood mechanism as suggested by Peppley [11] and validated by Poran and Tartakovsky [7]. Based on the vast experience of the GT-POWER engine simulation program in which its results were validated satisfactorily against experimental observations in the entire range as relevant to the present work, its predictions are highly confident.

4. Results and Discussion

4.1. In-Cylinder Parameters

Figure 3 shows the time evolution of the major species inside the cylinder from -40 to $+40$ crank-angle degree, where 0 designates the top center piston position. In the presented case, a liquid blend of methanol and water with a mass ratio of 1:1, is injected to the cylinder volume during 10 crank-angle degrees starting (SOI) at -40 CA. Soon after, the methanol and water vaporize and their mole fractions are built-up. The methanol decomposes (MD) to carbon monoxide and hydrogen through an endothermic reaction of $90,100 \frac{kJ}{kmol}$ (Equation (1)), while the carbon monoxide reacts exothermally ($-41,000 \frac{kJ}{kmol}$) with the water (WG—water gas shift) to produce carbon dioxide and additional hydrogen (Equation (2)). The rate of the MD reaction at this crank angle (at this moment $p \approx 4.5$ Mpa and $T \approx 600$ K that correspond to a compression ratio of 1 : 15) is rather slow— $0.02 \frac{kmole}{m^3s}$, and the rate of the WG reaction is $0.07 \frac{kmole}{m^3s}$. In parallel, the steam is reformed (SR) through an endothermic reaction of $49,000 \frac{kJ}{kmol}$ (Equation (3)) with a relatively high rate of $1.2 \frac{kmole}{m^3s}$. The strong effect of the SR reaction on the in-cylinder temperature and pressure traces is clearly demonstrated in Figure 4a,b respectively. Here, the mass of the fuel injected per cycle was matched, as the total energy released during the combustion in the modified cycle (methanol and fuel) and the conventional cycle (fuel

only) is equal. It shows that under these conditions, the temperature is kept nearly constant from -35 to -10 CA, and consequently, the pressure during the compression stroke is lower than that in the conventional (with no blend injection) engine. When the main fuel is injected, the pressure and the temperature are recovered as a result of the hydrogen combustion ($H_2 + O_2 \rightarrow 2H_2O$), which is a highly exothermic reaction of $-475,000 \frac{\text{kJ}}{\text{kmol}}$. It is clearly seen visually that as compared to the conventional cycle, the present cycle needs less work to compress the cylinder charge, and it produces higher work in the expansion stroke. Therefore, higher cycle efficiency is expected.

Figure 3. Mole fraction of some major constituents inside the cylinder during the blend injection and fuel injection periods. Sea level conditions, engine compression ratio (CR) = 16.5, engine power = 9 kW, engine speed = 3000 rev/min, blend ratio (BR) = 0.75, start of injection (SOI) of the main fuel = -18 CA degrees, combustion duration = 30 CA degrees. Here, the blend ratio is defined as the ratio between the mass of the injected blend and the mass of the injected main fuel, during a single cycle.

4.2. Engine Performance

In this section, we evaluate the effects of the blend injection timing, the fuel injection timing, and the blend-to-fuel ratio on the engine indicated efficiency and flight ceiling altitude. The effects are examined for both the conventional and the modified (with SRM) engines.

In all cases, the blend timing, which includes the start of injection angle and the injection duration, are determined while the in-cylinder temperature is kept constant during the injection (the later part of the compression stroke—from point 2 to point 4 in Figure 1). It was found that the sensitivity of the engine performance to these two parameters within the practical range of their values is pretty small as long as the blend is injected at the time when the temperature of the cylinder content is above the light-off temperature of the catalyst, and the injection duration is short enough to allow injection completion before the main fuel injection starts. The effects of the main fuel injection timing (start of injection and injection duration) on the engine-indicated efficiency are shown in Figures 5 and 6.

(a)

(b)

Figure 4. In-cylinder temperature (a) and pressure (b) traces. The black curve is for the conventional engine (with no blend injection), and the red curve is for the engine with the steam-reforming process. Sea level conditions, engine compression ratio (CR) = 16.5, engine power = 9 kW, engine speed = 3000 rev/min, blend ratio (BR) = 0.75, start of injection (SOI) of the main fuel = -18 CA degrees, injection duration = 30 CA degrees.

It seems that for any flight level of up to 5000 ft, the indicated efficiency of the conventional engine maximizes as the main fuel injection starts at around -18 crank angle degree. The efficiency mildly deteriorates as the SOI retards for a few crank degrees. For the SRM engine, the indicated efficiency shows quite a similar behavior while the efficiency is slightly higher (around 2.5% above). The sensitivity to this specific angle is rather low. It is important to note that the Lambda parameter (λ), which represents the ratio between the required and the stoichiometric air–fuel ratios, decreases with the flight altitude. Noting that in this range of flight altitude levels, the engine power does not change noticeably; while the air density deteriorates, oxygen shortage conditions are inevitably attained. Thus, for the present system, the flight ceiling is limited to 5000 ft.

Figure 5. Indicated efficiency vs. main fuel start of injection at different altitudes for a conventional and for SRM engines. Engine compression ratio (CR) = 16.5, engine power = 9 kW, engine speed = 3000 rev/min, blend ratio (BR) = 0.75, combustion duration = 30 CA degrees.

Figure 6. Indicated efficiency vs. main fuel injection duration at different altitudes for a conventional and for SRM engines. Engine compression ratio (CR) = 16.5, engine power = 9 kW, engine speed = 3000 rev/min, blend ratio (BR) = 0.75, start of injection (SOI) of the main fuel = −18 CA degrees.

When the SRM is applied at 5000 ft, λ is still well above 1 (1.32), which indicates that an excess air is still available and therefore, a higher flight ceiling is possible. We find that when methanol is introduced (SRM), less main fuel is needed for the same combustion energy. This is attributed to the additional oxygen atoms that are included in the methanol and in particular in the water molecules. We note that the anaerobic dissociation process of the methanol (Equation (1)) generates CO molecules. In a later stage, CO is oxidized by the water through a highly exothermic reaction to produce CO₂. In this exothermic reaction, the water is used to oxidize the CO, while leaving free some oxygen from the air. Consequently, more fuel (and thus energy) can be added to the cylinder while using the extra free oxygen.

The effect of the fuel injection duration is depicted in Figure 6. For each case, the fuel injection rate was adjusted to keep the engine power constant. In practice, it may correspond to a different orifice size. It seems that for any flight level of up to 5000 ft, the indicated efficiency of both the conventional and the SRM engines exhibits the maximum

level as the main fuel injection duration is smaller than 30 crank angle degrees. The efficiency slowly deteriorates as the injection duration stretches beyond 30 crank angle degrees. It is interesting to note that the efficiency deterioration rate with increasing the injection duration for the SRM engine is much smaller and practically is insignificant. This is attributed to the hydrogen combustion process, which occurs very fast after ignition and therefore is independent of the injection duration of the main fuel.

Figure 7 summarizes the effect of the blend-to-fuel ratio on the air excess ratio (λ) at several flight levels. It shows that for the SRM engine, a higher blend-to-fuel ratio results in an increase in the air excess ratio. This is due to the additional oxygen atoms that are included in the blend (in particular in the water molecules) that are released when the methanol and water are decomposed during the steam-reforming process. As discussed earlier, the flight ceiling is limited by the oxygen shortage that constrains the amount of fuel that can be oxidized to generate the required power. When the SRM is applied, the resulting air excess compensates the low ambient air density and thus can be used to climb higher than the flight ceiling level of the conventional engine. Figure 7 suggests that the ceiling level can be significantly improved to some 9000 ft with the SRM.

Figure 7. Air excess ratio (λ) versus blend-to-fuel mass ratio at different flight levels. The blend-to-fuel mass ratio is defined as the ratio between the mass of the blend and the mass of the main fuel, i.e., $m_{blend} / m_{main\ fuel}$. Engine power = 9 kW, Engine speed = 3000 rev/min. Start of injection and fuel injection duration are optimal for best indicated efficiency.

5. Summary

Due to the oxygen shortage at high altitudes, the use of naturally aspirated diesel engines in small aircraft is limited to a low ceiling level. Here, we propose to significantly extend the flight ceiling level of a small diesel-propelled aircraft by introducing an in-cylinder steam-reforming system. This system facilitates heat absorption during the compression stroke, with its subsequent release during the expansion stroke. In addition, in this arrangement, the in-cylinder oxygen content is significantly increased due to the additional oxygen atoms that are included in the methanol and in particular in the water molecules. These are released when the methanol and water are decomposed during the steam-reforming process. We show that owing to the addition of the oxygen content in the cylinder, the flight ceiling level can be extended significantly from 5000 to 9000 ft. Moreover, we show that the indicated efficiency can be increased up to 6%.

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Abbreviations

AF	Air fuel mass ratio
BR	Blend ratio $m_{blend}/m_{main\ fuel}$
CA	Crank angle
CR	Compression ratio
MAV	Miniature aerial vehicle
MD	Methanol decomposition reaction (Equation (1))
SOI	Start of injection
SR	Steam reforming reaction (Equation (3))
SRM	Steam reforming
TC	Top center piston position (0 CA degree)
WG	Water gas shift reaction (Equation (2))

Nomenclature

m	Mass
p	Pressure
r	Reaction rate
S_A	Specific surface area per unit mass of fresh catalyst
T	Temperature
t	Time
λ	Excess air ratio = $AF/AF_{Stoichiometric}$

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