ADAPTING AN INTERNAL COMBUSTION ENGINE TO OXY-FUEL COMBUSTION WITH IN-SITU OXYGEN PRODUCTION

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ABSTRACT

In transport applications, reciprocating internal combustion engines still have important advantages in terms of endurance and refueling time and available infrastructure when compared against fuel cell or battery-based powertrains. Although conventional internal combustion engine configurations produce important amounts of greenhouse gases and pollutant emissions, oxy-fuel combustion can be used to mitigate to a great extent such emissions, mainly producing NOx-free, CO2 and H2O exhaust gases. However, the oxygen needed for the combustion, which is mixed with flue gases before entering the cylinder, has to be stored in an additional tank, which hinders the adoption of this technology. Fortunately, the latest developments in gas separation membranes are starting to produce extremely-high selectivity and high permeability oxygen-separation membranes. Using the waste heat of the exhaust gases to heat up a mixed ionic-electronic conducting membrane, and feeding it with pressurized air, it is possible to produce all the oxygen needed by the combustion process while keeping the whole system compact. This works presents a design of an oxy-fuel combustion engine with in-situ oxygen production. The numerical simulations show also that this concept keeps a competitive brake specific fuel consumption, while the high concentration of CO2 in the exhaust gases facilitates the introduction of carbon sequestration technologies, leading to potentially carbon-neutral internal combustion engines.

NOMENCLATURE

BSFC  Brake specific fuel consumption
COTS  Commercial off-the-shelf
EGR  Exhaust gas recirculation
η  Efficiency
φ  Fuel-oxidiser equivalence ratio
HC  Hydrocarbons
HE  Heat exchanger
HP  High pressure
ICE  Internal combustion engine
IMEP  Indicated mean effective pressure
LP  Low pressure
MIEC  Mixed ionic and electronic conducting
\( \dot{m}_{O_2} \)  O2 mass flow permeated through the membrane

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Oxycombustion is a technology that responds to the global interest in reducing greenhouse gases emissions, where combustion processes take place in a O₂/CO₂ atmosphere rather than an O₂/N₂ one, changing combustion characteristics because physicochemical properties of CO₂ are different from those of N₂ [1]. The main advantages that come from the oxy-combustion implementation are the reduction of heat losses, near-zero emissions because of the absence of nitrogen from oxidants and the possibility of CO₂ capture [2]. Different industrial sectors as cement production [3], [4], [5], power plants [6], [7], [8] and oil refineries [9], [10] have studied the application of oxycombustion, where the main results are the reduction of pollutant emissions and the possibility of CO₂ capture, and a decay of the system performance due to the addition of different components to adapt the operation to this type of combustion.

On the other hand, the European Union has reported that 21% of the total emissions of CO₂ are contributed by the road transport [11]. In addition to this, it is shown that 10% of the global emissions are generated by internal combustion engines (ICE), mainly used in the transport sector, being responsible for 25% of the total consumption of fossil fuel oil [12]. For this reason, regulations as the current EURO 6d FULL were released to achieve acceptable levels of emissions in the transport sector. For light and heavy-duty vehicles, Table 1 enlists objective values for the different greenhouse and pollutant gases.

<table>
<thead>
<tr>
<th></th>
<th>Light duty</th>
<th>Heavy duty</th>
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</thead>
<tbody>
<tr>
<td>NOₓ [g km⁻¹]</td>
<td>0.06-0.08</td>
<td>0.40-0.46</td>
</tr>
<tr>
<td>PM</td>
<td>0.005</td>
<td>0.005</td>
</tr>
<tr>
<td>CO [g km⁻¹]</td>
<td>0.5-1.0</td>
<td>1.5-4.0</td>
</tr>
<tr>
<td>HC [g km⁻¹]</td>
<td>0.10</td>
<td>0.13-0.16</td>
</tr>
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**TABLE 1.** Regulation for the different greenhouse gases in EURO 6d FULL normative.
studied an oxy-fuel power plant where a hybrid method for oxygen production using cryogenic and membrane methods and only cryogenic methods were considered where introducing a membrane in the cycle enhanced the economic performance of the whole system by 1.1%. Additionally, Castillo [24] studied a different oxy-fuel plant, comparing its performance where oxygen was produced by cryogenic and membrane means. When using membrane technology, a 4% improvement was achieved compared with the plant operation using a cryogenic method to produce oxygen.

Meanwhile, there are certain conditions required to produce oxygen properly. Vacancy sites in the membrane increase with temperature, with temperatures higher than 700 °C [20], where several authors report temperatures as high as 1000 °C [18]. Also, as it was mentioned, the main driving force to produce oxygen using MIEC membranes is the partial pressure difference, where elevated air pressure in the feed side is demanded [21].

Considering this, to operate an engine under oxy-combustion conditions, an in-situ oxygen production method should be considered to produce the required oxygen for the combustion. This work investigates the adaptation of an oxygen production cycle using a MIEC membrane in the operation of a 1.3 L spark ignition engine, comparing its performance with the conventional operation of this engine and optimizing the layouts proposed by Desantes et al. in [25]. To achieve optimal conditions in the membrane, two compression stages are implemented to drive atmospheric air through the system and increase its pressure and heat exchangers with the exhaust gases are also implemented to reach high temperatures. Additionally, these mentioned compressors are moved by considering turbines whose energy is obtained from the oxygen-depleted flow generated due to the oxygen separation from the air, which has high pressure and temperature conditions. This oxygen-depleted flow is also considered to increase air mass flow temperature for its remaining thermal energy. The study is performed by computational means, properly calibrated against experimental data. To the best of authors knowledge, this is the first time a work detailing how a multi-cylinder spark-ignition engine can be operated in oxy-fuel combustion mode with in-situ (onboard) oxygen generation by recovering waste energy from the exhaust gases.

In this sense, the main objectives of this paper are mentioned as follows:

To describe the design of an optimized system that consists of an engine whose oxygen mass flow is obtained by an oxygen production cycle and uses oxy-fuel combustion.

To assess the oxy-fuel combustion engine’s performance compared to the conventional engine operation in terms of brake specific fuel consumption.

To evaluate the different energy flows during the engine operation.

The work is presented as follows: first, the system is de-
scribed; then, the computational method is summarized; following that, the performance of the engine operating at full load at different speeds is shown and discussed; finally, the main conclusions are presented.

SYSTEM DESCRIPTION

The whole system exhibited in Figure 1 consists in the coupling of two codependent cycles, which jointly compound the oxycombustion engine working with in situ oxygen production conditions. Firstly, an oxygen production cycle with a similar structure to that of a regenerative Brayton Cycle with multiple compression, with intermediate cooling and multiple expansion, with reheating, stages (Ericsson Cycle) is used to recover the engine exhaust gases energy: atmospheric air is pressurized, heated up, passed through a MIEC membrane and, finally, expanded in turbines. Initially, there are two compression stages (1, 3 in Figure 1) that are intercooled (2) which move air at ambient conditions into the system. Then, the air rises its temperature at HE-14, where it receives heat from the oxygen/EGR flow from the power cycle. After this, the air is branched using a three-way valve to control the inlet air temperature at the membrane, where a part is passed through two heat exchangers to recover energy at HE-5 and HE-6 from exhaust gases and oxygen/EGR flow, respectively. Then, the air is rejoined and branched again, passing through HE-8 and HE-18, receiving energy from exhaust gases. Later, the air goes into the membrane, where mass and species exchange is achieved, and the air losses its oxygen composition.

Consequently, an oxygen-depleted flow is produced (mainly nitrogen) with a high temperature and pressure. This flow passes through two expansion stages (10,12), interheated in HE-11 by the oxygen/EGR flow. These expansion stages are implemented to drive the compressors mentioned before. Finally, after the low-pressure turbine, the nitrogen flow delivers heat to the air at HE-14, reducing its temperature again and increasing the air temperature. Finally, the O\textsubscript{2}/EGR temperature gives thermal energy to the nitrogen at HE-13, reducing its temperature, and to the air at HE-14, reducing its temperature again and increasing the air temperature. The O\textsubscript{2}/EGR is cooled to ensure a temperature of 85 °C at the cylinders intake, passing also through a compressor that is driven by the exhaust gases turbine. It is also mentioned that the exhaust gases flow at the turbine outlet is used to increase air temperature at HE-5, taking advantage of its remaining thermal energy.

The chosen engine, as it has been mentioned before, is an 1.3 L, turbocharged and direct-injection four-cylinder spark-ignition engine. The extra components used for the oxygen production cycle are commercial off-the-shelf components, such as turbochargers, valves, and coolers, and other elements such as high-temperature heat exchangers and the high-productivity MIEC membrane. The high pressure and the O\textsubscript{2} + EGR turbochargers are the same model, whereas the low-pressure turbocharger is a scaled-up version.

In the following section, the main aspects of the computational method are presented, including the control variables used in the oxy-fuel combustion simulations.

COMPUTATIONAL METHOD

A software called VEMOD [26] is used to model the whole system studied in this paper. Developed at I.U.I CMT – Motores Térmicos, it originally aimed at 0D/1D modeling of thermo-and fluid dynamic processes in engines, especially of compression ignition engines. However, different elements such as turbochargers, coolers, pipes, heat exchangers, membranes, simple electric systems, and control units can be modeled using this program.

In addition, the oxy-fuel combustion system with in-situ oxygen production was benchmarked against the base configuration. An IMEP corresponding to the maximum achievable in the base configuration was used in both cases. Experimental data were used to calibrate the base engine model. In oxy-fuel combustion operation, an O\textsubscript{2} mass concentration of 30 % was used in all cases.

Modelling

The different elements implemented in this paper are solved by 0D/1D calculation means. For ducts, Euler’s fluid dynamics equations in 1D are solved by a finite-volume approach. Additionally, Colebrook-White’s and Colburn’s correlations are used to determine friction and heat transfer coefficients, respectively. Other elements such as heat exchangers and the MIEC membrane are solved by 0D means, using continuity and energy conservation equations. In the case of the MIEC membrane, the model described in [27] is used to determine the oxygen transfer from the feed side to permeate air by considered 1D simplifications.
Turbocharger efficiency calculation:

\[ \eta_{\text{total}} = \eta_{\text{LP turbine}} \cdot \eta_{\text{LP compressor}} \cdot \eta_{\text{HP turbine}} \cdot \eta_{\text{HP compressor}} \] (1)

Oxy-fuel combustion engine control:

In the control of the oxygen production cycle, the global turbocharger efficiencies \( \eta_{\text{total}} \) of the air turbomachines are maximized (i.e., the efficiency of the low-pressure turbocharger times the efficiency of the high-pressure turbocharger), as in Equation 1. This is achieved by changing the position of the turbine stator vanes.

Additionally, the power cycle performance is optimized by minimizing its brake specific fuel consumption while maintaining the IMEP of the conventional combustion mode for the same rotational speed. This is achieved by changing the spark timing, keeping a restriction of 15 MPa for the maximum in-cylinder pressure, which was the mechanical limit of the experimental facility used for obtaining the heat release rates.

The EGR rate and, thus, the concentration of oxygen going into the cylinders is controlled by changing the position of the stator vanes of the \( \text{O}_2 + \text{EGR} \) turbine. A bypass valve is also
kept for cases where it is not enough to open the turbine vanes fully.

The temperature at the inlet of the $O_2 +$ EGR turbine is controlled through the bypass valve marked as 7 in Figure 1, so it never surpasses 950 °C.

The temperature of the MIEC feed air is controlled using the bypass valve marked as 4, diverting more flow through HE-5 and HE-6 when the temperature is too low and bypassing them entirely when the temperature is bigger than 950 °C.

Finally, the engine power output is controlled with the amount of $O_2$ permeated through the MIEC membrane, injecting enough fuel to keep the equivalence ratio equal to 1. The flow of $O_2$ is regulated by using a throttle valve just downstream of the intake filter, upstream of the low-pressure air compressor. This valve is not affecting the pumping losses of the engine cylinders since they are not directly throttled.

Assumptions, simplifications and restrictions

The following considerations are taken to perform the calculations of the system:

Energy consumption of auxiliary components is not considered.
Combustion parameters of the Wiebe law have been changed according to an empirical model obtained from computational fluid dynamics simulations fitted to an experimental database, as described in [36].
For air composition, only $N_2$ (79 %) and $O_2$ (21 %) are considered.
Heat exchanger efficiencies remain constant.

The simulations were run taking into account all these. The main results are presented in the following section, including a comparison of the efficiency of the cycle against that of the original engine.

PERFORMANCE EVALUATION

Conventional and oxy-fuel combustion mode comparison

Oxy-fuel combustion affects the duration of the combustion and the shape of the heat release law inside the cylinder. Figure 2 shows the shape of the rate of heat release obtained in normal operation and in oxy-fuel combustion mode in a point of maximum $IMEP$ at 3000 rpm. In this figure, both laws present the same start of combustion to ease their comparison. The high concentration of $CO_2$ inside the combustion chamber clearly reduces the flame speed in oxy-fuel combustion mode, which is consistent with the results obtained by other authors such as in [13].

In Figure 3 it is shown the brake specific fuel consumption ($BSFC$) comparison between conventional and oxy-fuel combustion scenarios for engine speeds between 1250 and 5000 rpm. There is a minimum fuel consumption at 2500 rpm for the oxy-fuel combustion scenario of 294.5 $gkW\cdot h^{-1}$, while a maximum consumption of 323.6 $gkW\cdot h^{-1}$ is reported at 5000 rpm. Meanwhile, for the same engine speed range, it can be found a minimum ($BSFC$) at 2000 rpm, where 252.6 $gkW\cdot h^{-1}$ are found for this speed, and a maximum consumption at 5000 rpm of 321.4 $gkW\cdot h^{-1}$.

Higher differences between conventional and oxy-fuel combustion operations in fuel consumption are seen at low engine speeds while at higher speeds, consumption tends to converge.

It has to be remarked that the operation of the conventional engine is conducted with a variable equivalence ratio to perform correctly while this parameter remains constant for the oxy-fuel combustion operation, as it is also seen in Figure 3.

Discussion

Petrol engines operating by oxy-combustion means and the same compression ratio are expected to perform with higher values of $BSFC$ for a given indicated mean effective pressure, as the specific heat capacities ratio inside the combustion chamber is smaller due to the greater concentration of triatomic molecules such as $CO_2$ and water vapor. On the other hand, there is a non-negligible efficiency penalty in conventional combustion in this engine at high speeds, as the fuel-air mixture has to be enriched to reduce the turbine inlet temperature at the maximum $IMEP$. This enrichment is seen in Figure 3, where even values in the equivalence ratio of 1.2 can be reached to avoid inlet temperatures at the turbine higher than 950 °C. In contrast, in oxy-fuel combustion, the equivalence ratio is kept equal to 1 during the whole operation. The efficiency of the cycle is also affected
by the differences in heat release rate observed between conventional and oxy-fuel combustion: the high concentration of CO₂ and H₂O in the combustion chamber increases the duration of the combustion, which also increases the fuel consumption for a given power output.

As oxy-fuel combustion conditions reduce the detonation tendency inside the cylinder, the ignition timing does not need to be retarded and the combustion can be centered. Also, the mixture can be burnt in stoichiometric conditions since the turbine inlet temperature is naturally limited as the exhaust gas passes through a heat exchanger, leading to lower BSFC values than in conventional combustion for high engine speeds where in-cylinder and exhaust temperatures increase.

Generating pure O₂, even by using high productivity MIEC membranes, requires important amounts of power. The waste heat in the engine exhaust line is recovered to directly produce high temperatures and pressures to promote the transport of O₂ across the membrane: first, for heating the feed air and, then, for driving the turbocompressors. Figure 4 shows the fraction of fuel power available on the brake, recovered for compressing the MIEC feed air and recovered for heating the MIEC feed air. The amount of heat used to heat the MIEC feed air is around 40% of the lower heat capacity of the fuel, whereas 10% is used for compressing the air. The oxygen-depleted gas leaving the MIEC membrane still has an important amount of energy, which is partially recovered in the turbines that power the turbocompressors.

The O₂ + EGR turbine is used as a valve to control the EGR concentration and may be, indeed, swapped by an actual valve. As it recovers part of the exhaust energy, however, it is also used to increase the volumetric efficiency and reduce the pumping losses.

Figure 5 shows the O₂ production (\(n_{O_2}\)) over the MIEC map, which is a function of the membrane size, the ratio between the average O₂ partial pressure at the feed side (\(p_{feed}\)) and the permeate side (\(p_{perm}\)), and the flow temperature (\(T_{MIEC}\)). The permeability is highly affected by low flow temperatures: at the lowest speeds, the temperature achievable at the MIEC inlet port is more than 100 °C and 200 °C smaller than at higher speeds, for 1500 rpm and 1250 rpm respectively. For this reason, the O₂ partial pressure ratio has to be increased substantially for these low engine regimes in order to keep the desired production levels.

At any operating point, an important amount of this energy is recycled from the gases downstream of the turbines, from both the oxygen-depleted air and from the oxygen-enriched stream, from HE-11 and HE-14. The EGR stream is also used in both HE-8 and HE-18, and the MIEC membrane itself exchanges heat between all its input and output flow branches. The relative amount of available energy to be recovered for producing the O₂ flow from these sources varies widely between low and high rotational speeds, however, and extra heat has to be recovered in HE-5 and HE-6 from the exhaust gases and the oxygen-depleted flow, respectively. That is the case of low rotational speeds, as can be seen in Figure 6. While the rotational speed increases, the bypass (item 4 in Figure 1) has to decrease the amount of air flow passing through HE-5 and HE-6 so the MIEC inlet temperatures are kept below a maximum safe value. This can be seen in Figure 7, where the heat entering the modified Brayton cycle through HE-5 and HE-6 is much smaller than through all the other heat exchangers. At 5000 rpm, the bypass valve completely diverts the flow and no heat is recovered through HE-5 and HE-6, as it is shown in Figure 8. An extra bypass valve is used (item 7 in Figure 1) to control the temperature at the EGR+O₂ turbine, so it never surpasses 950 °C. This increase in complexity, which in-
creases the cost of the system as well as its size, weight and technological risks, may limit its application to stationary engines or hybrid-electric applications. Changing the EGR concentration may be also used to control the gas temperature and the available energy at different operating points, possibly reducing the complexity of the whole system. Attention must be paid to the coefficient of variation in combustion at EGR rates over 70 %, as discussed in [36].

At 1250 rpm, it is seen in Figure 6 that 9.8 % of the recovered heat in the heat exchangers is valorized as an oxygen enthalpy flow that returns to the power cycle, while the remaining energy is wasted by friction in turbochargers and heat to the ambient. Additionally, 36.3 % of the energy obtained by the fuel combustion is wasted by means of friction, heat losses and intercooling in the power cycle of the engine. A different scenario is calculated for a medium speed of 3000 rpm, whose energy flow are exhibited in Figure 7. In this case, 16.2 % of the recovered heat can be used again in the engine cycle as oxygen enthalpy flow while 30.6 % of the fuel energy dissipated by friction and heat. Finally, for higher speeds (as in 5000 rpm as shown in Figure 8), the fraction of energy recovered as oxygen enthalpy flow decreases slightly to 15.6 % of the available heat.

Given this, it is seen that the available thermal energy in the exhaust has its better utilization at middle speeds, which incidentally coincides with the points of better fuel consumption. At medium rotational speeds, an increase in volumetric efficiency is also achieved, which also explains part of the increase in efficiency of the cycle.

The different operating points are plotted over the compressor maps in Figure 9 for the O_2 - EGR compressor, Figure 10 for the high pressure compressor and Figure 11 for the low pressure compressor. The rotational speed of the low-pressure air compressor varies widely between the minimum and the maximum engine speeds, whereas the change is reduced in the high-pressure compressor. In both cases, the compressor operates in a relatively-centered part of the map where its efficiency is close to its maximum. The O_2 + EGR compressor, in the other hand, operates at low rotational speeds, covering a range from almost-zero corrected speed (N∗) to 60 % of its maximum operating corrected speed. Its pressure ratio p_{comp} is quite reduced when compared with that of the air compressors, reaching values lower
than 1.5, with a maximum at medium engine speeds. It operates at corrected mass flows $\dot{m}^*$ close to choke at the maximum engine speed, with a reduced efficiency: it achieves its best usage of the energy recovered in the $O_2$ + EGR turbine at medium engine speeds, leading to lower pumping losses, better volumetric efficiencies and lower values of BSFC.

In all cases, there are still important amounts of medium-grade heat in the exhaust gases (both in the engine exhaust and in the oxygen-depleted air stream), which may be further recovered for powering other elements. The engine exhaust stream, being composed by $CO_2$, $H_2O$ and possible traces of other species such as unburnt hydrocarbons, should be cooled down to separate the $CO_2$ and capture it.

The main conclusions are presented in the following section.

**CONCLUSION AND FUTURE WORKS**

By looking at the simulation results presented in this work, recovering the exhaust waste heat in a spark-ignition engine can be used to generate the pure $O_2$ for oxy-fuel combustion employing a modified Brayton cycle feeding a high productivity MIEC membrane at high loads. COTS components can be used to build the Brayton cycle, except for some components such as the MIEC membrane, thus reducing the risk of developing such a system.

The efficiency of the system, although lower than that of the conventional spark combustion engine due to inherent thermodynamic limitations of oxy-fuel combustion with high EGR rates, is somewhat better at high speeds and high indicated mean effective pressures as the risk of knocking is limited and the maximum in-cylinder pressure can be increased. Strategies to limit inlet temperature at turbines as increasing the equivalence ratio as it is seen in the conventional engine are not necessary in the oxycombustion scenario, which counts with heat exchangers that assure acceptable temperatures at these turbomachines without affect-
ing its proper operation. That said, better efficiencies may be achieved by increasing the compression ratio before detonation, which is an interesting method for making these cycles more attractive and should be studied in future works.

A complex heat exchanger network has to be implemented, as there are important differences in the amount of energy available in the exhaust line between low engine speeds and high engine speeds, which generates differences between their energy flows. HE-5 and HE-6 are necessary when the available energy directly from the exhaust and O₂/EGR lines is not enough to increase the air temperature, which explains the difference between low speeds, where temperatures are lower, and high speeds. However, this heat exchanger network and the turbochargers are able to recover an average value of 50% of the lower heating values from the burnt fuel to produce oxygen.

The high concentration of CO₂ in the exhaust line, with easily separable H₂O, should enable an easy path for sequestering it. However, further studies are needed to design an optimum cycle for carbon capture.

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