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EGR Strategy for NOx Emission Reduction in a CAI Engine Fuelled with Innovative Biogas

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ABSTRACT

Gaseous fuel utilization reduces pollutant emissions and makes thermal energetic systems less dependent on oil. Their carbon content is low, which means low CO_2 emissions, and a lower cost with respect to conventional fuels.

If gaseous fuels have a non-fossil origin, their adoption would have a beneficial impact on global CO_2 balance and on the dependence of the energy sector from fossil fuels.

Biogas is produced from the anaerobic digestion of organic materials, with the composition depending on the feedstock and on the production processes.

The use of biogas in internal combustion engines (ICE) is very attractive. However, the presence in the biogas of an inert gas like CO_2 has adverse effects on combustion, reducing combustion speed, narrowing flammability limits with harmful effects on combustion stability. A possible way for improving combustion performance of biogas is hydrogen addition. Innovative anaerobic digestion processes, which maximize the H_2 yield, can end up with biogases made of CH_4, CO_2 and H_2.

The biogas, generally adopted as fuel in positive ignition ICEs, is also suitable for Controlled Auto Ignition (CAI) engines.

Aim of this work is to investigate the biogas combustion in CAI ICE by means of numerical simulations. The effect of fuel composition and EGR on engine performance and exhaust emissions was evaluated. Authors compared conventional and innovative biogases composed by CH_4, CO_2 and H_2 of different compositions. CAI systems are controlled with varying intake gas conditions: air-fuel ratio, boost pressure and charge temperature. The temperature depends on recycled exhaust gas content, which has an impact on the combustion process. Authors investigated the effect that EGR has on the in-cylinder gas temperature and reaction mechanism, focusing on NOx emission formations.

1. INTRODUCTION

Energy sources depletion and fossil fuels cost are main concerns for nowadays society. Unconventional oils [1] represent the vast majority of the world oil reserves and their exploitation is technically difficult and expensive [2]. Moreover, the increasing energy demand and the effect on climate induced by carbon dioxide and other greenhouse gases force the development of technologies for the use of renewable energy.

Biofuels represent an important option as their production and usage is spreading thanks to the advantages they offer in terms of immediate energy availability and reduced environmental impact. A correct life cycle assessment can demonstrate that the use of biogases as fuels in energy conversion systems can strongly contribute to CO_2 emission reduction [3]. As a consequence, European Union is nowadays forcing the use of biofuels. In fact the European directive on renewable energy (Directive 2009/28/EC) [4] establishes that all EU countries must ensure that at least 10 % of their fuels for road vehicles come from renewable sources by 2020.

Most common biofuels are bioethanol, biodiesel and biogas.

Bioethanol is a liquid biofuel that can be used in spark ignition engines both blended with gasoline at 10 and 20 % (E10, E20, etc.), or as an almost pure fuel (E85, E100), the number representing the ethanol percentage content in the blend [5]. Moreover, if blended with diesel oils, it can also be used in compression ignition engine [6].

Biodiesel derived from the transesterification of vegetable oils [7] can be straightforwardly used in diesel engine. Both biodiesel and bioethanol, generally, can be used with minor engine modifications or no modifications when present in low percentages [3].

Biogas is produced from the anaerobic digestion of organic matter and its constituents are mainly methane and carbon dioxide. The most important raw materials for biogas production are municipal solid waste [8], farm waste, domestic garbage landfills [9], sewage sludge [10], agricultural products, rice paddies waste, energy crops, palm oil mill effluents [11], animal manure [12, 13] and coal mining waste [14].

Despite its composition depends on the feedstock and the production process, conventional biogas is typically composed of 55-65 % of methane, 30-40 % carbon dioxide, and traces of hydrogen sulphide. The aerobic decomposition of the organic matter produces greenhouse gases, so the use of biogas as a fuel is particularly beneficial for the environment.

The use of biogas in internal combustion engines is therefore very attractive even if the presence of an inert gas like CO_2 has adverse effects on combustion, reducing combustion speed and narrowing flammability limits [15, 16]. In internal combustion engines a slower combustion causes a larger combustion angle with a consequent negative effect on

engine thermal efficiency [17]. The presence of CO_2 also reduces the combustion stability [18]. As the flame speed slows down due to the presence of inert gases, combustion evolution becomes erratic and significant differences appear between consecutive indicated cycles. Such cyclic variations cannot exceed an upper threshold, expressed as the Coefficient of Variation (COV) of either the indicated work or the peak cylinder pressure. If such limits are overcome, engine operation becomes unacceptably irregular [19].

Hydrogen addition to the gaseous fuel represents a way to increase the combustion speed. Ma et al. [20] experimentally investigated a lean burn engine fuelled with hydrogen-enriched natural gas, observing a reduction of the combustion angle as hydrogen content increased. The addition of hydrogen in gaseous fuels also improves combustion stability, reducing cycle-by-cycle variations. Indeed, Mariani et al. observed a reduction of COV in indicated mean effective pressure promoted by hydrogen addition to natural gas in a spark ignition engine [21].

The effect of the addition of hydrogen to a biogas was also investigated in the literature, particularly in spark ignition engines [22]. Chung et al. [23] studied the combustion performance of H_2/biogas in a spark ignition engine by numerical simulation; they showed that the rate of heat release increases while increasing H_2 content. Rakopoulos et al. [24] used a quasi-dimensional multi-zone model to study the biogas/hydrogen combustion in a single cylinder engine; they concluded that the addition of increasing amounts of H_2 in biogas results in a decrease of the flame development period. Park et al. studied the performance and emission characteristics of biogas mixed with hydrogen in SI engine [25, 26]. They found out that the presence of inert gases in the biogas can improve the thermal efficiency and reduce the NOx emissions, though, HC emissions and cycle variation increase. Li et al. investigated the effect of hydrogen enrichment on combustion and heat release of a biogas; they concluded that the overall reaction rate increases with H_2 concentration [27].

Part load operation is a very frequent condition for internal combustion engines, especially for road vehicle applications. At such operating conditions the engine efficiency is negatively affected by the combined effect of the increased relative incidence of rubbing friction and, in spark ignition engines, by intake air throttling losses [19]. An alternative to the conventional spark ignited combustion is the Controlled Auto-Ignition (CAI) combustion, allowing operating the engine at part loads with considerable excess of air, so eliminating the need for throttling. CAI combustion is governed by auto ignition instead of by spark ignition and subsequent flame front propagation [28]. Thanks to its characteristics, CAI engines attracted some attention in the literature [29-32]. The combustion is characterized by the absence of a flame front propagation and by an extremely rapid evolution. This allows an efficiency improvement, limited however by the constraint that cylinder pressure rise rate cannot exceed some limits in order to prevent unacceptable mechanical and thermal loads [29]. Biogases were also used to fuel CAI engines and the influence of the amount of recycled combustion products on combustion timing and angular duration was investigated [30]; Jamsaran et al. [33] investigated the auto-ignition reactivity of natural gas with regard to the effects of intake air temperature and equivalence ratio; Nishi et al. [34] studied the effects of EGR ratio and engine speed on HCCI combustion; Ibrahim et al. [35] improved the performance and extended the load range of

hydrogen fuelled homogeneous charge compression ignition (HCCI) engine through charge temperature control and CO_2 dilution.

Another important aspect related to the use of biogas as fuel in spark ignition internal combustion engines is the reduction of power due to the presence of the inert gases. In biogas fuelled CAI engines it is possible to compensate for the presence of CO_2 in the fuel by changing (increasing) the equivalence ratio. In fact CAI's are operated at lean conditions giving the possibility to control load by varying the ER. In this way the engine would not be affected by any power reduction.

It was already proven that fuelling a CAI engine with hydrogen enriched methane contributes to reduce NOx emissions, essentially because the intake gas temperature, controlled with EGR, is lower than what is required for the auto-ignition of pure methane [36]. Furthermore, a preliminary simplified analysis, where the intake gas temperature is considered as a parameter of the problem, confirmed the NOx emissions reduction also when a CAI engine is fuelled with biogases made of methane, carbon dioxide and hydrogen [37]. Aim of this paper is the investigation of the effects on CAI engine performance and NOx emissions of the use of innovative biogases made of CH_4, H_2 and CO_2, adopting EGR for controlling auto-ignition and combustion phasing. The engine load is here managed by changing the intake charge pressure at constant equivalence ratio. Results show that the innovative biogases allow a very promising reduction of NOx emissions with respect to that of a conventional biogas, mainly due to less boosting and EGR rate requirements, for delivering a reference imep.

2. METHODS

2.1 CAI engine

Controlled Auto-Ignition combustion combines the advantages of spark ignition and compression ignition engines. The combustion is characterized by an extremely rapid evolution with high thermal efficiency. However, the cylinder pressure rise rate tends to be very sharp and, if not limited, it can lead to unacceptable mechanical and thermal loads and noise. With the absence of flame front propagation, CAI combustion is dominated by chemical kinetics. Implementation of a detailed reaction mechanism is therefore necessary for CAI combustion analysis. The complex gas-phase chemical kinetics is here modelled with the detailed radical chain reaction mechanism GRI-Mech 3.0 [38], designed for methane. It is made of 325 elementary chemical reactions and 53 species, including those to predict NOx formation; all kinetic constants are provided. GRI-Mech 3.0 mechanism includes all the reactions required to accurately describe both biogas and hydrogen combustion, also allowing to consider the effect of EGR on the auto-ignition, reaction rates and emission formation.

The combustion process of a CAI engine is studied using the Package HCCI of Chemkin 17.0 [39]. The engine cycle simulation does not consider the gas exchange process. The CAI model predicts the combustion in an internal combustion engine under auto-ignition conditions. The implemented single-zone CAI combustion model permits detailed description of the chemical kinetics by assuming homogeneous gas properties in the combustion chamber. The single-zone model can adequately predict the ignition.
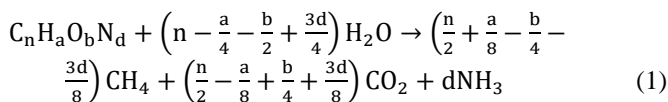
However, because it does not account for low-temperature regions within the thermal boundary layers and crevices, the model underestimates carbon monoxide and unburned hydrocarbon emissions. For this reason here the authors focused on NOx emissions only. The main characteristics of the engine selected for the simulations are reported in Table 1. This type of engine is used for stationary applications, i.e. power generation at constant engine speed (usually 1500 rpm). The investigated engine is supercharged; as a consequence cylinder pressure at start of compression is above ambient pressure. Temperature at start of compression can be controlled by varying the amount of residual gases in the cylinder using an EGR system [30-32]. The presence of residual gases has an impact on the combustion process as the burning mixture composition consequently changes.

Table 1. Engine parameters and operating conditions

Engine type	4-stroke
Compression ratio	16.7:1
Bore [mm]	135
Stroke [mm]	170
Engine speed [rpm]	1500

2.2 Biogas

Biogas is typically obtained from the dark anaerobic digestion of organic matter and mainly composed of methane and carbon dioxide. The molar ratio CH_4/CO_2 in a biogas can be predicted with the Buswell equation for the anaerobic digestion of organic matter [40]:

$$C_nH_aO_bN_d + \left(n - \frac{a}{4} - \frac{b}{2} + \frac{3d}{4}\right)H_2O \rightarrow \left(\frac{n}{2} + \frac{a}{8} - \frac{b}{4} - \frac{3d}{8}\right)CH_4 + \left(\frac{n}{2} - \frac{a}{8} + \frac{b}{4} + \frac{3d}{8}\right)CO_2 + dNH_3 \quad (1)$$

Equation (1) predicts a CH_4/CO_2 ratio ranging from 1, for simple carbohydrates like starch $(C_6H_{10}O_5)n$, or proteins $(C_5H_7NO_2)$ to 2.35, for the conversion of lipids, e.g., $C_{57}H_{104}O_6$. It is experimentally found that for the anaerobic digestion of water buffalo manure the CH_4/CO_2 ratio is about 2 [41, 42]. Being 2 an intermediate value, it was decided to keep the CH_4/CO_2 ratio constant and equal to 2 for all biogases considered in the present study.

Hydrogen is an intermediate product of the anaerobic fermentation and thus, if the digestion process is accurately designed and controlled the H_2 yield can be maximized so to produce an innovative biogas mainly made of CH_4, H_2 and CO_2 [44]. Water buffalo manure naturally contains the eubacteria responsible of the hydrogen production [43] and thus it can be considered as a very promising substrate to produce the innovative biogas [45]. The authors then assumed water buffalo manure as a reference organic matter from which, as experimentally demonstrated, an innovative biogas with an H_2/CO_2 molar ratio of about 1 and a maximum H_2/CH_4 molar ratio of 0.25 can be produced [46]. The authors thus decided to keep H_2/CO_2 molar ratio value constant and equal to 1 in the innovative biogases studied and to investigate two different H_2/CH_4 ratios equal to 1/9 and 2/8, respectively. As a matter of comparison also a traditional biogas without H_2 is investigated.

Fuel compositions are summarized in Table 2.

Table 2. Fuels composition

Fuel	CH_4 mol. fraction	H_2 mol. fraction	CO_2 mol. fraction
Biogas 1	0.67	0	0.33
Biogas 2	0.580	0.065	0.355
Biogas 3	0.500	0.125	0.375

2.3 Hydrogen

Hydrogen is a gas of very low density with a critical temperature of -239.91°C. On volume basis, it requires less air than methane for a stoichiometric combustion whereas it is the opposite on mass basis. The effect of the low hydrogen density is important also on the heating value. When the mass based lower heating value is considered, hydrogen shows a very high energy content per kg of gas, much higher than methane, conversely on volumetric base the opposite holds. Hydrogen has a higher auto-ignition temperature, thermal conductivity and Octane Number than methane. In spark ignition engines, important properties are also its fast flame speed and wide flammability limits. It is important to consider hydrogen properties in the model in order to understand the effect on the combustion process.

2.4 Engine operating parameters

The equivalence ratio (ER) is defined as the ratio between the actual and the stoichiometric fuel-to-air mass ratio:

$$ER = \frac{\left(\frac{m_f}{m_a}\right)_{actual}}{\left(\frac{m_f}{m_a}\right)_{stoic.}} \quad (2)$$

CAI's operate with lean air-fuel mixtures (ER<1) in order to have a better control of pressure gradient in the cylinder. For this reason the analysis is carried out considering a reference ER of 0.4 [30].

Indicated Mean Effective Pressure (imep) is an engine performance index independent from engine size, obtained dividing the indicated work per cycle by the displacement, V_d:

$$imep = \frac{\oint p dV}{V_d} \quad (3)$$

Engine indicated efficiency is defined as:

$$\eta_i = \frac{P_i}{\dot{m}_f \cdot LHV} \quad (4)$$

where P_i is the indicated power, $\dot{m}_f$ is the fuel mass flow, LHV the lower heating value of the fuel.

3. RESULTS AND DISCUSSION

3.1 Biogas: Effect of EGR

The intake temperature is an important control parameter for the combustion in CAI's. The combustion takes place only if the in-cylinder gases reach the conditions for the auto-ignition. Engine performance strongly depends on the initial gas temperature as it directly affects the combustion phasing relative to the top dead center. In CAI's the temperature can be controlled with varying the EGR rate. Hot exhaust gases are

recirculated and mixed with the fresh charge, an air-fuel mixture whose composition is defined by the ER. The air is usually mixed with the fuel downstream the compressor. Normally, in boosted i.c. engines, the air is cooled down before entering the cylinders to improve volumetric efficiency and reduce knock. In this analysis the air cooler was not considered because the air temperature increase due to the compression is beneficial for auto-ignition. Intake temperature consequently depends on the compressor pressure ratio and EGR rate.

Figure 1 shows the effect of EGR on Biogas 1 combustion at intake pressure equal to 230.5 kPa and intake temperature, equal to 435 K. The temperature and pressure traces are plotted versus the crank angle in Figure 1a and 1b, respectively. With no EGR the combustion does not take place and for this reason the corresponding temperature and pressure traces were not included in the plots. As the EGR rate increases from 10 % to 20 %, the combustion start angle moves towards top dead center because in-cylinder gases reach earlier the thermodynamic conditions for the auto-ignition. Engine indicated efficiency is consequently affected. In fact, if the auto-ignition occurs too late, the peak cylinder pressure is positioned later in the expansion stroke and is reduced in magnitude with negative effects on imep; if it is too advanced, peak cylinder pressure occurs too early so increasing the compression work [19]. The solid line (10 % EGR) shows the best combustion phasing.
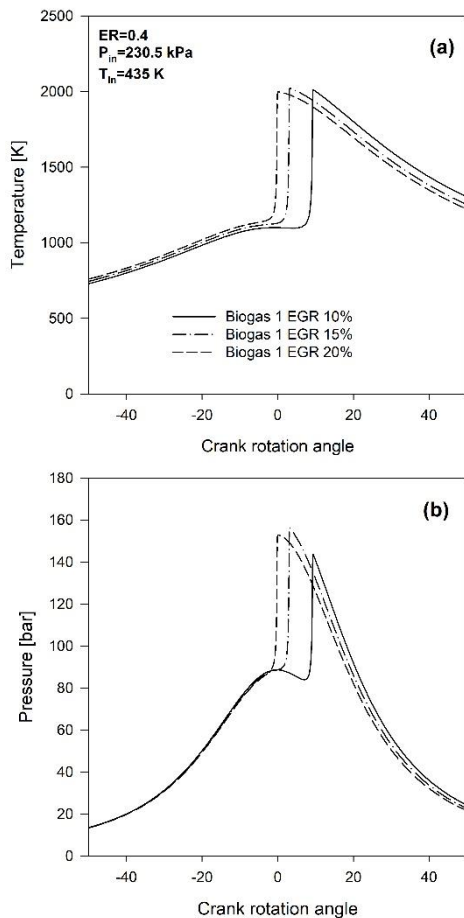
Figure 1. Temperature (a) and Pressure (b) traces vs. crank angle at different EGR rates (Biogas 1)

Figure 2 shows the effect of EGR on engine performance and emissions when Biogas 1 is adopted. Imep (a) and efficiency (b) are higher with 10 % EGR because of better combustion phasing. Conversely, the peak Temperature (c) is essentially unaffected by the EGR. Concerning the NOx emissions (d) the minimum is found with EGR = 10 %. Indeed, higher EGR rates reduce the engine power output and cause higher NOx emissions due to higher peak cylinder temperature and/or due to longer exposition of the combustion products to high in-cylinder temperature (see Figure 1a).
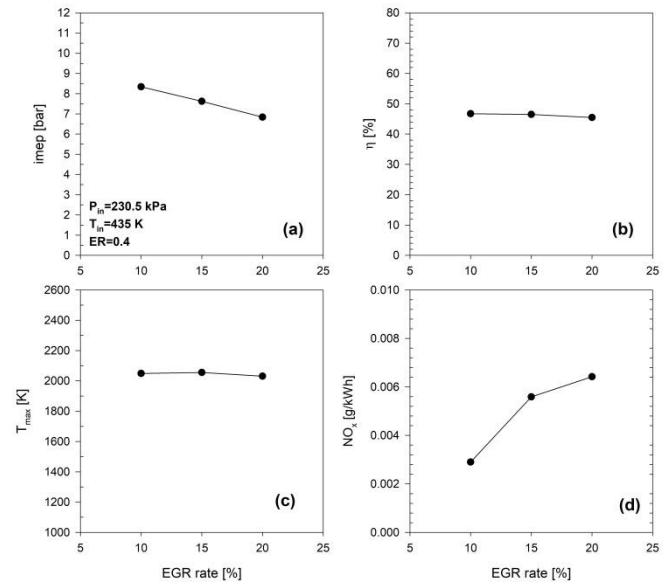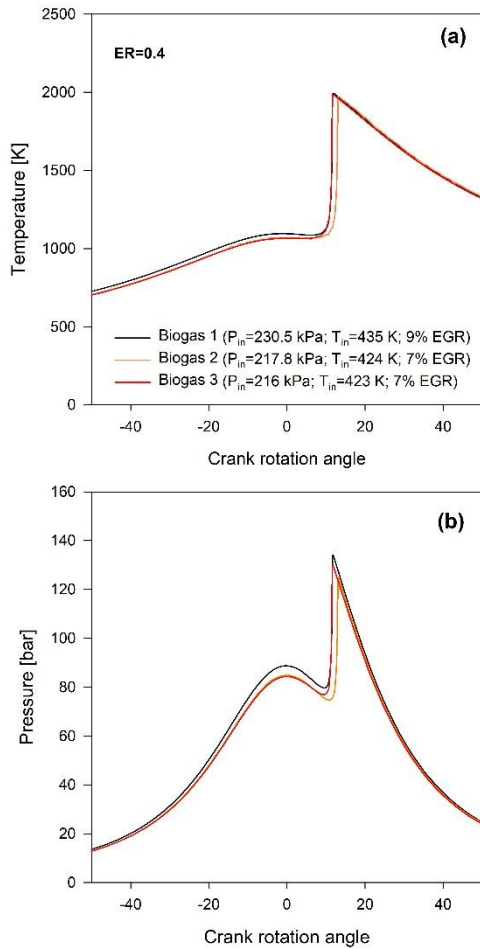

Figure 2. Effect of EGR rate on imep (a), efficiency (b), maximum temperature (c) and NOx emissions (d). Biogas 1

### 3.2 Comparison between conventional and innovative biogases

Innovative biogases (Biogas 2 and 3) contain hydrogen which reduces the auto-ignition temperature requirement in comparison with the conventional biogas (Biogas 1) consequently requiring less EGR rate. Boost pressure should also be adjusted in order to keep the imep constant.

Figure 3 shows the in-cylinder temperature (a) and pressure (b) traces versus the crank angle for Biogas 1, Biogas 2 and Biogas 3. The boost pressure, the intake temperature and the required EGR rates are also indicated for all fuels. The operating conditions were optimized for obtaining 8.4 bar imep with an optimal combustion phasing, keeping the ER at 0.4. The innovative biogases require less EGR rate (7 %) than Biogas 1 (9 %) for an optimized combustion phasing. The boost pressure also reduces with the presence of hydrogen in the fuel, 230.5 kPa for Biogas 1, 217.8 kPa for Biogas 2 and 216 kPa for Biogas 3. The in-cylinder gas temperature at the beginning of the compression stroke for the innovative biogases is also lower as it is related to the boost pressure.

Cycle averaged results are compared in Figure 4. The engine delivers the target imep (Figure 4a) with a lower peak pressure and a slightly reduced peak temperature (Figure 4c) for the biogases containing hydrogen. Engine efficiency does not change significantly (Figure 4b) while NOx emissions are drastically reduced, from 2.26 mg/kWh for Biogas 1 to 1.53 mg/kWh for Biogas 2 and 1.17 mg/kWh for Biogas 3, Figure 4 (d).

Figure 3. Temperature (a) and Pressure (b) traces versus crank angle for Biogas, Biogas 2 and Biogas 3. Boost pressure and EGR rate optimized for each fuel in order to obtain 8.4 bar imep with maximum engine efficiency
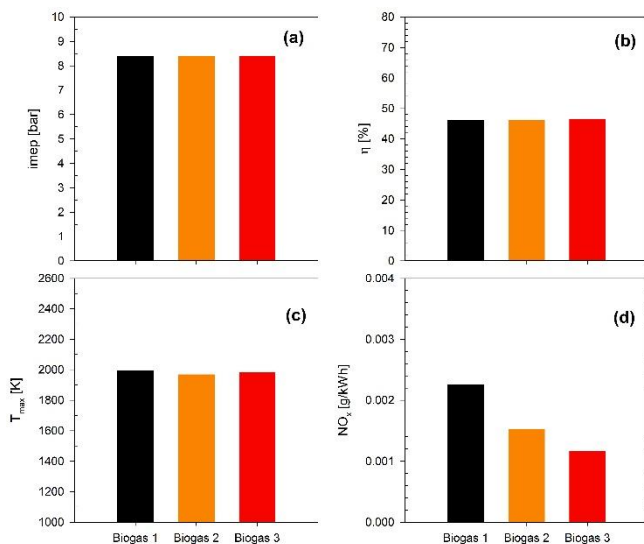
Figure 4. Effect of hydrogen on imep (a), efficiency (b), maximum temperature (c) and NOx emissions (d)

4. CONCLUSIONS

The paper describes a numerical study on a Controlled Auto

Ignition engine fed by a conventional biogas (Biogas 1) and innovative biogases containing hydrogen (Biogas 2 and Biogas 3). The model predicts indicated mean effective pressure, indicated efficiency and NOx emissions.

The engine was operated in order to obtain a reference imep value of 8.4 bar with an ER=0.4. The EGR rate was adjusted for each fuel in order to obtain an optimal combustion phasing.

The results show that hydrogen addition reduces the intake temperature requirement for the auto-ignition. As a consequence the innovative biogases require less EGR rate (7 % EGR for both Biogas 2 and 3) than Biogas 1 (9 % EGR required).

The boost pressure also reduces with hydrogen, from 230.5 kPa for Biogas 1, to 217.8 kPa for Biogas 2 and 216 kPa for Biogas 3.

Engine efficiency does not change significantly between tested fuels for the operating conditions considered. The fact that the presence of hydrogen does not bring an appreciable benefit in terms of engine efficiency can be explained taking into consideration the combustion characteristic of a CAI engine: it burns so fast (also without hydrogen) that any increase in the reaction rates due to the presence of hydrogen is not appreciable in terms of engine thermal efficiency.

The most important result is the potential benefit of innovative biogases in terms of NOx emission reduction. In fact, due to the lower boost pressure and EGR requirements Biogas 2 and Biogas 3 emit less NOx, respectively 1.53 mg/kWh and 1.17 mg/kWh, than Biogas 1, 2.26 mg/kWh for Biogas 1.

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NOMENCLATURE

imep	Indicated mean effective pressure, kPa
ER	Equivalence ratio
LHV	Lower heating value, MJ/kg
NOx	Nitrogen oxides emissions, g/kWh
p	Pressure, kPa
T	Temperature, K
V	Volume, l

Greek symbols

η	Engine efficiency

Subscripts

a	air
d	Displaced volume
f	fuel
Stoich.	stoichiometric