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Energy Procedia 148 (2018) 336-343



www.elsevier.com/locate/procedia

73rd Conference of the Italian Thermal Machines Engineering Association (ATI 2018), 12–14 September 2018, Pisa, Italy

Experimental and Numerical Analyses of a Spark-Ignition Engine Firing with N-Butanol-Gasoline Blends

at High Load Operation

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Abstract

In this paper, the potential of alcohol-gasoline blends as fuels for spark-ignition engines has been evaluated. The general purpose of the work is to verify the possibility of incrementing the bio-fuels penetration in the market of transportation fuels. As it is well known, bio-mass derived fuels, in fact, could significantly reduce the CO_2 emissions of energy thermal systems.

The behavior of a small, turbocharged spark-ignition engine, firing with gasoline-butanol blends, has been analyzed. Analyses have been carried out by means of both experimental tests and numerical simulations. In previous works, engine main performances have been illustrated and discussed. Here, experimental tests have been carried out in order to compare the engine knock resistance and the obtainable fuel conversion efficiency when the engine is fueled by pure gasoline or gasoline-butanol blends at high load operation. Furthermore, one dimensional numerical analyses have been utilized in order to compare the engine behavior, at different operating points, when it is firing with pure gasoline or pure butanol.

In general, the obtained results seem to indicate that butanol (produced by bio-masses) is a viable alternative to fossil fuels in the way of CO_2 emission reduction.

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Keywords: biobutanol, spark ignition engine, knock, experimental analysis, numerical analysis

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Introduction

Today, the world energy demand continues to grow while the fossil fuel reserve gradually diminishes. Focusing on the transportation sector, this accounted for about 25% of total world delivered energy consumption in 2012, and transportation energy use is expected to increases by 1.4% per year from 2016 to 2040 [1]. Furthermore, considering the greenhouse effect produced by fossil derived hydrocarbons, more and more attention is paid to the potential of biofuels. In order to avoid competition between energy cultivation and food production, today great attention is deserved especially to the so called second-generation biofuels [2]. The liquid biofuels such as ethanol, methanol, bio-diesel or raw vegetable oil [3, 4] are of particular interest for the transportation sector. They can be used as pure fuels or blended with traditional fuels. Among these, today great attention is addressed to bio-butanol due to both the potential of its production [5, 6] and the potential of its utilization [7–13].

In previous works, the authors widely discussed the properties of n-butanol by investigating the behavior of a spark ignition engine operating at part load [14,15]. In these papers, also an in-depth literature review has been reported. It was highlighted how every researcher, in general, investigated just some features of the behavior of engines fueled with this alcohol. In particular, pollutant emissions have been widely observed. And a lot of study are relative to carbureted engines. Sometimes, conflicting results are reported in the technical review, as it has been highlighted in [12]. Even the value of n-butanol Octane Number has not yet been precisely determined. As an example, results reported in [10,16] seem to prove that n-butanol lowers the knock resistance of the engine. Again, dealing with the knock resistance of the n-butanol/air mixtures, different values of the Octane Number are mentioned in the technical literature. In [11,13] a RM ON value equal to 113 is reported, while in [10,12] values lower than 100 have been indicated.

The aim of this paper is to investigate about the behavior of a downsized spark ignition engine firing with butanol/gasoline blends at high load. In this operating conditions, knock phenomena could occur so the knock resistance of the charge is very important. Investigations have been made by means of both experimental and numerical tests. Experimental tests have been carried out considering the engine fueled by a particular n-butanol/gasoline blend (hereinafter named B40). A 1-D numerical model has been used to evaluate the performance of the engine fueled by neat n-butanol when it runs at tolerable knock conditions.

Experimental analyses

Steady state tests have been performed on a turbocharged, port injected, spark-ignition engine. This engine has been developed to run with straight regular grade gasoline fueling. Engine main characteristics are reported in Table 1.

Model	4 Cylinders, 16 Valves Turbocharged SI
Displacement	1368 cm ³
Bore / Stroke / Con. Rod	72 / 84 / 129 mm
Compression Ratio	9.8
Max Power (ISO Conditions)	110.3 kW @ 5500 rpm
Max Torque (ISO Conditions)	230 Nm @ 3000 rpm
Turbocharger group	IHI RHF3

Table 1 - Engine main characteristics

References [14] and [17] widely describe the experimental set-up. Briefly, the engine was coupled to an eddy current dynamometer. In-cylinder pressure curves have been measured by means of a pressure transducer mounted flush to the combustion chamber. The engine emissions have been measured by an AVL Digas device.

Two different fuels have been compared: B0 (pure gasoline) and B40, a n-butanol/gasoline blend, (60% gasoline and 40% n-butanol, mass percentages). Table 2 shows the main characteristics of these fuels compared to those of straight n-butanol (B100). Blends have been prepared in a fuel tank; they are introduced upstream to the inlet valves by means of the standard engine injectors.

During the tests, the injection timing, the ignition timing and the waste gate opening have been opportunely controlled by an on-line programmable ECU.

Three engine operating points have been considered, (Table 3).

		B0	B40	B100
Mass percentage of n-Butanol	[kg/kg]	0	40 %	100%
С-Н-О		7.9 - 14.8 - 0	6 - 12.4 - 0.5	4-10-1
Stoichiometric Air to Fuel ratio	[-]	14.6	13.2	11.1
Lower heating value	[kJ/kg]	43500	40544	33100
Latent heat of vaporization	[kJ/kg]	350	438	569

Table 2 - Butanol/gasoline blend characteristics. For regular gasoline, a conventional mean composition has been considered

Table 3 - Test cases. Air excess is α/α st where α is the actual air to fuel ratio and α st is the stoichiometric air to fuel ratio.

	Speed [rpm]	Manifold absolute pressure [bar]	Air excess [-]
Case 1	1500	1.11	1.0
Case 2	2500	1.22	1.0
Case 3	3000	1.10	1.0

In each point, the engine speed and the manifold absolute pressure have been kept constant. The injection timing has been tuned so to feed the engine with a stoichiometric mixture, while the spark timing has been advanced from free knock operating conditions to audible knock operation. Similar trends have been measured for each case. As an example, Figure 1 shows the brake thermal efficiency measured for Test Case 2. When the engine is running with B40 mixture, the brake thermal efficiency is higher than that obtained with the pure gasoline fueling.

Figure 1 highlights how the engine efficiency continues to increase when the spark timing is advanced. Indeed, knock occurs before the spark advance optimizing the engine torque is achieved [18]. Knock intensity has been quantified by means of the KI1 index [17,19] based on the analysis of the in-cylinder pressure curves. Figure 2 shows the behavior of this index for Test Case 2. The knock intensity observed for B40 is lower than that found for B0. As a consequence, B40 allows to operates with spark timings more advanced than those characterizing the engine firing with B0. Assuming that a K11 value equal to 15 corresponds to allowable knock operation [17], the knock limited spark angle (KLSA) has been found for both B0 and B40. Table 4 shows the main values characterizing the engine operating at these tolerable knock conditions.



Figure 1- Measured engine overall efficiency. Test Case 2



B40 allows knock limited spark angle advanced of about one crank angle degree with respect to B0. As stated above, when the engine burns an alcohol-gasoline mixture the specific fuel consumption increases, mainly due to the smaller alcohol heating value. At the same time, engine torque is almost unchanged, while the engine efficiency increases with the mixture alcohol content. The combustion duration also changes very little, while the brake specific O_2 values tend to decrease when the engine runs with B40.

		Case 1		Case 2		Case 3	
		B0	B40	B0	B40	B0	B40
Knock Limited Spark Angle	[°]	-5.7	-7.1	-7.9	-10.2	-14.3	-14.4
Torque	[Nm]	111	109	133	140	118	118
Brake Thermal Efficiency	[-]	0.30	0.31	0.30	0.34	0.31	0.34
Exhaust Gas Temperature	[°C]	662	651	815	793	812	791
Combustion Duration	[°]	31.9	32.8	36.4	36.3	38.7	39.2
NO _x	[g/kWh]	12.5	11.6	14.1	10.4	14.4	12.8
CO ₂	[g/kWh]	890	840	866	761	826	791

Table 4 - Main values measured at knock limited spark angle. The combustion duration is given by 0-90% burnt fuel mass

Numerical analyses

In order to enlarge the investigation in the field of butanol potential as a transportation fuel, numerical simulations of engine operation have been performed. The objective of the numerical analysis is to obtain information on the influence of different alcohol percentage in the fuel mixture, even including neat butanol which has not been available for the experimental tests. A 1-D model reproducing the whole engine lay-out has been used in order to compare the overall performance of the engine firing with straight gasoline (B0) or pure n-butanol (B100). The numerical approach has been widely illustrated in [15]. Combustion is modeled by means of a two zone approach. According to an entrainment model, the calculated turbulent flame speed depends on both turbulent flow indices and laminar flame speed. Turbulent flow indices (i.e. the turbulent intensity and the turbulent length scale) have been derived by the flow field details provided by 3-D calculations [20]. The laminar flame speed has been calculated by means of Eq. 1 [21]:

$$S_l = S_l(\phi, p, T) \cdot (1 - 2.06 \cdot \gamma^{0.77})$$
(1)

where γ is the mole fraction of burned gas diluent. $S_l(\phi,p,T)$ is calculated by means of the Metghalchi-Keck relationship (Eq.2):

$$S_L = S_{L,0} \left(\frac{T_u}{T_0}\right)^{\alpha} \left(\frac{P}{P_0}\right)^{\beta}$$
(2)

Where T_u is the unburned gas temperature and p is the in-cylinder pressure, while $S_{L,0}$ (Eq. 3) approximates the laminar flame speed at reference conditions ($T_0 = 298$ K, $p_0 = 1$ atm):

$$S_{L0} = B_m + B_\phi (\phi - \phi_m)^2$$
 (3)

Table 5 summarizes the parameters for Eq. 2 and Eq. 3.

Table 5 - Parameters for Eq. 2 and Eq.3. Data for B0 have been taken from Ref.[21], data for B100 have been derived from Ref.[22]. α and β values have been taken from Ref. [21].

	B0	B100
B_m	30.5	0.348
B_{ϕ}	-54.9	-0.788
ϕ_m	1.21	1.162
α	$2.4-0.271 \cdot \phi^{3.51}$	2.18-0.8· (φ -1)
β	-0.357+0.14 · $\phi^{2.77}$	-0.16+0.22·(\$\$ -1)

In order to take into account the knock occurrence, a knock model has been implemented in the 1-D model. Knock onset is calculated by means of a simplified approach proposed in [23]. This approach is based on two equations that describe the growth of a 'precursor' representing the auto-ignition delay. The kinetics of the precursor formation from the delay is calculated by using an exponential function where the precursor concentration x_p is calculated prior to the auto-ignition like:

$$\frac{\partial x_p}{\partial t} = x_{fu,u} F(\tau) \tag{4}$$

where $x_{fu,u}$ is the fuel mass fraction of the unburned gas phase, while the function $F(\tau)$ depends on the ignition delay (τ_{ID}) :

$$F(\tau) = \frac{1}{\tau_{ID}} \sqrt{\tau_{ID}^2 + 4(1 - \tau_{ID}) \frac{x_p}{x_{fu,u}}}$$
(5)

The model assumes that auto-ignition occurs when the precursor concentration reaches the unburned fuel mass concentration.

This model has been developed for regular grade gasoline for which the ignition delay is calculated by the AnB relationship (Eq.6):

$$\tau_{ID} = A \left(\frac{RON}{100}\right)^a p_{eff}{}^n e^{\frac{B}{T_u}}$$
(6)

For n-butanol, the same $F(\tau)$ function has been assumed, while the ignition delay is calculated by means of Eq. 7:

$$\tau_{ID} = 10^{A} [x_{O2}]^{a} [x_{n-but}]^{b} p_{eff}^{\ n} e^{\frac{B}{T_{u}}}$$
(7)

Table 6 summarizes the parameters assumed for Eq.6 and Eq.7. Both in these equations, the in-cylinder pressure is opportunely corrected to take in account the presence of diluents as suggested in [23]. Knock intensity is estimated as [24]:

$$KI = (1 - x_b)(\rho - 1)\sqrt{1 - \frac{\theta_k}{\theta_{ref}}} \frac{N}{N_{ref}}$$
(8)

Table 6 - Parameters for Eq. 6 and Eq. 7.

	B0 – Eq.6	B100 – Eq.7
A	0.0193	-8.5
а	3.402	-1.7
В	/	-1.4
Ν	-1.7	-1.5
В	3800	9730
RON	96	/

Where x_b is the mass of burned fuel, ρ is the compression ratio, θ_k is the knock onset crank angle and N the engine speed; θ_{ref} is the maximum crank angle for which knock is still audible and it is set to 50 CAD. N_{ref} is a tuning parameter that has been set equal to 1000 rpm. As in [25], it has been assumed that allowable knock corresponds to a KI level equal to 0.5.

The 1-D model has been extensively validated by the authors in previous papers [15,25]. As an example of model validation, some calculated data are compared to those measured for different engine operating points (Figure 3 and Figure 4). In particular, for each test case summarized in Table 3, a given spark angle has been considered. In each case, a good prediction accuracy has been reached. The difference between calculated and measured mean values is less than 5%. This encouraged the authors in utilizing the model when pure n-butanol is supposed to be fired. In the future, in order to model the combustion of butanol/gasoline blends, further considerations will be necessary.



Figure 3 - Comparison of calculated and measured mean values. Engine firing with straight gasoline.

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Figure 4 - Comparison of calculated and measured in-cylinder pressure curves. To consider the cyclic variation, minimum, mean and maximum acquired pressure curves are shown. Case 1, spark angle equal to -5.4° (left); Case 2, S.A.= -6.8° (middle); Case 3, S.A.=-9.8° (right). Engine firing with straight gasoline

The 1-D model has been used to estimate the knock limited spark timing by means of a controller that changes the spark angle until a target value of KI is reached. Figure 5 shows the comparison between measured and calculated knock limited spark-angles. Calculated KLSA corresponds to a KI level equal to 0.5, while measured data correspond to a KI1 level equal to 0.15.

Firing with B0, the difference between predicted and measured data is less than 0.8 crank angle degree. Considering both the uncertainties inherent in the experimental quantification of knock and those related to the various submodels that influence the prediction of the end gas auto-ignition, the agreement between calculated and measured data seems to be satisfactory.

This encouraged the authors in using the model in order to predict the optimal values of the spark timing in the case of pure n-butanol fueling. Thus, Figure 5 shows also the predicted KLSAs of the engine firing with B100. Calculations show that B100 allows spark timings much anticipated than B0. Calculated results confirm that n-butanol improves the knock resistance of the engine. Differences between the ignition delay predicted for gasoline by eq. 6 and that predicted for n-butanol by eq. 7 do not seem to justify this result. Figure 6 shows the ignition delays calculated for B0 and B100 according to Eq. 6 and Eq. 7 respectively. The data reported in the pictures have been calculated considering a homogeneous air-fuel mixture and choosing, as an example, a given charge pressure equal to 30 bar. Calculated data show that the ignition delay of B100 is higher than that of B0 below about 800 K, while over this value the trend reverses. At the temperature characterizing the end-gas during the middle phase of the flame propagation, n-butanol seems to auto ignite more likely than gasoline.

Furthermore, simulations regarding the engine fueled by n-butanol, carried out using eq. 6 instead of eq. 7, predicted anywhere a considerable increase of the engine knock resistance with respect to the case of gasoline fueling. On the contrary, this result may be due mainly to lower temperatures characterizing the end-gas of the engine fueled by B100 (Figure 7). Operating at the same manifold absolute pressure, in-cylinder pressure during the intake phase practically do not change when B100 is used instead of B0. The latent heat of vaporization of n-butanol is higher than that of gasoline (Table 2), thus a slightly greater flow rate of cold air enters the cylinders of the engine fueled with alcohol. Furthermore, B100 has a stoichiometric air-to-fuel ratio lower than that of gasoline (Table 2), therefore more mass of fuel is trapped into the cylinder. Both these aspects contribute to lower the temperature of the incylinder charge during the compression phase and the subsequent combustion phase of the engine firing with n-butanol. Of course, lower temperatures determine a greater ignition delay of the end gas increasing the knock resistance of the engine.

At the end, Figure 8 reports some comparisons between calculated performance of the engine burning B0 and the engine firing with B100 at knock limited spark angle. B100 allows slightly higher indicated mean effective pressure, i.e. higher engine torque, and slightly higher indicated efficiency.

The indicated specific fuel consumption grows of about 28%, while the specific CO_2 emissions decrease of about 5%. This can be explained considering both the higher thermal efficiency of the engine running with n-butanol and the different chemical formula of the two fuels. In fact, when a stoichiometric air-butanol mixture is used, the



amount of CO_2 emitted per kWh of heat released is smaller than that produced by a stoichiometric air-gasoline mixture [14].

Figure 8– Calculated indicated performances at knock limited spark angle: Indicated Mean Effective Pressure; Indicated Conversion Efficiency; Calculated specific CO₂ emissions; Indicated Specific Fuel Consumption.

Conclusions

The behavior of a small, turbocharged spark-ignition engine, firing with gasoline-butanol blends, has been analyzed. A first interesting result, provided by the experimental analysis, is that at a given operating point, the overall engine efficiency does not significantly decrease when engine fueling is switched from pure gasoline to a butanol-gasoline mixture (60% gasoline, 40% n-butanol, mass percentage). Naturally, the specific fuel consumption increases, but this is almost exclusively due to the smaller heating value of butanol compared to that of gasoline. Another important feature of butanol-gasoline mixture fueling is represented by the optimal values for spark advance. The experimental tests have shown as the alcohol presence in the fuel mixture increases the knock resistance, thus allowing for greater spark advances. At high load operation, here investigated, this last circumstance favorites a slight recovery in terms of both delivered torque and fuel conversion efficiency. Both the experimental tests and the computations show n-butanol improves the knock resistance of the engine. As an example, at a given operating point, a more advanced knock limited spark timing (about 6 crank angle degrees greater) can be adopted when fueling is changed from pure gasoline to pure butanol. This tendency is confirmed by the measured data obtained with the engine firing with the B40 mixture. At high load operating points, greater values for spark advance have led to a gain of one percentage point in terms of engine indicated efficiency. At the same points, the ratio of CO_2 emissions to the indicated power value is decreased of about 5%.

At the end, the experimental and numerical analyses here presented confirm that n-butanol is an interesting transportation fuel. Main engine performances remain quite similar to those obtainable with gasoline fueling. In some operating points, even a slight improvement is observable. So, producing the alcohol fuel by biomasses could represent an effective way for the reduction of CO_2 emissions.

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