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CALIBRATION OF A KNOCK PREDICTION MODEL FOR THE COMBUSTION OF GASOLINE-NATURAL GAS MIXTURES

Emiliano Pipitone
Dipartimento di Meccanica, University of Palermo
Palermo, Italia
pipitone@dima.unipa.it

Stefano Beccari
Dipartimento di Meccanica, University of Palermo
Palermo, Italia
s.beccari@dima.unipa.it

ABSTRACT

Gaseous fuels, such as Liquefied Petroleum Gas (LPG) and Natural Gas (NG), thank to their good mixing capabilities, allow complete and cleaner combustion than normal gasoline, resulting in lower pollutant emissions and particulate matter. Moreover natural gas, which is mainly constituted by methane, whose molecule has the highest hydrogen/carbon ratio, leads also to lower ozone depleting emissions. The authors in a previous work (1) experienced the simultaneous combustion of gasoline and natural gas in a bi-fuel S.I. engine, exploiting so the high knock resistance of methane to run the engine with an "overall stoichiometric" mixture (thus lowering fuel consumption and emissions) and better spark advance (which increases engine efficiency) even at full load: the results showed high improvements in engine efficiency without noticeable power losses with respect to the pure gasoline operation. With the aim to provide a knock prevision sub-model to be used in engine thermodynamic simulations for a knock-safe performance optimization of engines fuelled by NG/gasoline mixtures, the authors recorded the in-cylinder pressure cycles under light knocking condition for different engine speed, loads and natural gas fraction (i.e. the ratio between the injected natural gas mass and the total fuel mass), and used the gas pressure data to calibrate a classical knock-prediction model: as shown, the results obtained allow to predict the onset of knocking in a S.I. engine fuelled with a gasoline-natural gas mixture with any proportion between the two fuels, with a maximum error of 5 CAD.

INTRODUCTION

Gaseous fuels, such as Liquefied Petroleum Gas (LPG) and Natural Gas (NG), thank to their good mixing capabilities, allow complete and cleaner combustion than normal gasoline, resulting in lower pollutant emissions and particulate matter. Moreover the use of natural gas, which is mainly constituted by methane, whose molecule has the highest hydrogen/carbon ratio, leads also to lower ozone depleting emissions. Some of the automobile producers already put on the market "*bi-fuel*" vehicle, which may be fed either with gasoline or with a gaseous fuel (NG or LPG). These engines, endowed of two separate injection systems, are originally designed for gasoline operation, hence they do not fully exploit the good qualities of both NG and LPG, that is their high knocking resistance, which would allow higher compression ratios. Moreover, when running with gasoline, at medium-high loads the engine is often operated with rich mixture and low spark advance in order to prevent from dangerous knocking phenomena: this produces both high hydrocarbon and carbon monoxide emissions (also due to the low catalyst efficiency caused by the rich mixture) and high fuel consumption. Starting from these considerations, the authors experienced, in a previous work (1), the simultaneous combustion of gasoline and natural gas in a bi-fuel S.I. engine under several operative conditions of load and speed and for different natural gas fraction (i.e. the ratio between the injected natural gas mass and the total fuel mass). The high knock resistance of methane allowed to run the engine with an "overall stoichiometric" mixture (thus lowering fuel consumption and emissions) and better spark advance (improving further on the engine efficiency) even at full load: a substantial increase in indicated and effective efficiency was observed, without noticeable engine torque loss. With respect to the to the pure gasoline operation, effective efficiency increments up to 27% were obtained at full load with a natural gas fraction of 50%, maintaining engine power loss under the 4% (which is better then the 12% loss caused by the pure CNG operation). These encouraging results lead to consider the double-fuel combustion a valid alternative to pure gasoline operation in bi-fuel engines. This third running mode could require a further effort in the engine development process. The design and calibration of engines running on double-fuel

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mixtures could require in fact extensive experimental tests in order to obtain injection and spark timing maps. Computer simulations obviously represent a fundamental step in the design and performance optimization phase; engine models updated for the evaluation of in-cylinder pressure during double-fuel combustion may help to predict the performances attainable and give a valid first indication for fuel injection time and spark advance. However, since knocking is a crucial issue concerning SI engines, a reliable autoignition sub-model valid for double-fuel operation should be employed so as to safely maximize engine efficiency. This autoignition sub-model should estimate the onset of knocking with acceptable accuracy for each proportion between the two fuels used (natural-gas and gasoline or LPG and gasoline). The knocking occurrence prevision sub-models most encountered in literature can be grouped in two main categories: ignition delay models and detailed chemical kinetic models. Ignition delay models base their prevision on the unburned gas history of pressure and temperature and usually need some experimental data for the tuning of its constants (2, 4, 5, 6, 7, 9). Detailed chemical kinetic models, instead, take into account the elementary reaction steps that occur between the species involved in the combustion process (8, 10). Unfortunately, because of fuels complexity, some of the elementary reactions may be unknown; moreover, due to the high number of reactions to consider, chemical kinetic sub-models always require a great computational effort; for these reasons the first category is often preferred for the estimation of unburned gas autoignition time. Basically it rests on the concept that the knock resistance of a fuel, which can be expressed by its octane number, is proportional to the auto-ignition delay of the fuel-air mixture for given pressure and temperature levels.

The concept of ignition delay in spark ignited (SI) engines originates with experiments carried out in a rapid compression machine (2): it was defined as the time needed for autoignition to occur, starting from the end of compression stroke. For those machines, the ignition delay τ can be correlated with the constant fuel-air mixture pressure p and temperature T by means of an Arrhenius type equation:

$$\tau_{[\mathrm{sec}]} = A \cdot p_{[bar]}^{\ -n} \cdot e^{\frac{E}{R \cdot T}} \tag{1}$$

where E [J/mol] is the fuel activation energy, R [J/mol K] is the universal gas constant, while A and n are fuel dependent constants, which can be tuned by means of experimental data.

Since in S.I. engines the unburned gas pressure and temperature are far from being constant, the above correlation is employed with two different approach: the Livengood and Wu Integral approach (2, 3, 5, 6, 7, 9, 11) and the ignition delay approach (4). The first is based on the evaluation of the following Knock Integral (KI):

$$KI(t) = \int_{t_{IVC}}^{t} \frac{dt}{\tau} = \int_{t_{IVC}}^{t} \frac{dt}{A \cdot p^{-n} \cdot e^{B/T}} \tag{2}$$

where t_{IVC} represents the Intake Valve Closure time, while the constant B substitutes the ratio E/R.

According to this method, the knock onset time t_{KO} is obtained when the integral reaches the value of 1:

$$KI(t_{KO}) = \int_{t_{IVC}}^{t_{KO}} \frac{dt}{A \cdot p^{-n} \cdot e^{B/T}} = 1 \tag{3}$$

this condition corresponds to a critical concentration of the radical species needed for autoignition.

The second method, instead, evaluates the Ignition Delay ID with respect to the spark time by means of the unburned gas mean pressure p_M and temperature T_M (estimated during the combustion period):

$$ID = A \cdot p_M^{\ -n} \cdot e^{B/T_M} \tag{4}$$

EXPERIMENTAL TEST AND RESULTS

The purpose of the present work was to provide a knock prevision sub-model to be used in engine thermodynamic simulations for a knock-safe performance optimization of engines fuelled by CNG/gasoline mixtures in different proportions. This has been accomplished following the method of the knock-integral of equations (2) and (3), whose constants have been tuned by means of experimental data collected on the engine test bed. This knock prevision model can be easily implemented in numerical simulations involving the same fuel mixtures and different engines since the tuned constants should depend only on fuel type (6), while the engine is responsible for the pressure and temperature histories of the unburned gas.

In-cylinder pressure cycles have been acquired for various operative conditions (resumed in Table 1) on a FIAT four cylinders 8V 1242cc bi-fuel engine connected to a Schenck eddy current dynamometer W130. A Walbro-TDD ECU connected to a personal computer was employed to control in real time both gasoline injection time and spark timing, which was set to produce light knocking; about 20 knocking cycles were acquired for each operative condition, hence for each CNG mass fraction, a total of 160 knocking cycles were collected and employed for the calibration of the knock prevision model. The amount of natural gas injected (whose mean composition is reported in Table 2) was controlled through IGBT transistors connected to the GNG injectors and activated by digital pulses sent by a National Instruments Counter/Timer board PCI-6602 programmed and controlled under LabVIEW. The gasoline mass flow was measured using an Endress+Hauser Coriolis effect PROMASS 80A flowmeter,

while the natural gas mass flow was deduced through the previously determined injector flow chart.

The CNG/gasoline mixture was kept in a stoichiometric proportion with air by means of an ECM AFRecorder 2400 connected to a UEGO sensor placed in the exhaust duct. The in-cylinder pressure was measured using an AVL GU13X piezoelectric pressure sensor, installed by means of its ZC32 spark plug adaptor. The Manifold Absolute Pressure (MAP) was measured by means of a DRUCK piezoresistive pressure sensor and it has been employed to compensate the acquired pressure cycles (12, 13).

Engine speed [rpm]	1500 – 2000 – 2500 – 3000
Manifold Pressure [kPa]	70 – 90
CNG mass fraction [%]	0 – 10 – 30 – 50 – 70
Overall A/F ratio	Stoichiometric
Spark Advance	Light knock condition

Table 1 - Operative condition used in the test

A fundamental aspect in indicating analysis is the precise determination of the TDC position (14) which has been accomplished by the use of a Kistler capacitive sensor 2629B, characterized by a 0.1 Crank Angle Degrees (CAD) precision.

All the quantities were acquired at 7200 sample per engine revolution by means of a high speed National Instruments DAQ Board PCI-6133.

Methane – CH_4	[%Vol]	88.539
Ethane – C_2H_6	[%Vol]	6.519
Propane – C_3H_8	[%Vol]	1.298
Carbon dioxide – CO_2	[%Vol]	0.925
Nitrogen – N_2	[%Vol]	2.176
Other	[%Vol]	0.543
Density	[kg/m^3]	0.7675
Lower Heat Value	[MJ/m^3]	35.795

Table 2 - Composition of the natural gas used in the test

The unburned mixture temperature was calculated, from the Inlet Valve Closure (IVC) to the spark ignition time, by means of the perfect gas law:

$$T = T_{IVC}\frac{p \cdot V}{p_{IVC} \cdot V_{IVC}} \tag{5}$$

where V is the in-cylinder volume, p_{IVC}, V_{IVC} and T_{IVC} are the pressure, volume and temperature at IVC.

The gas temperature T_{IVC} has been assumed to be 35°C higher than that measured in the manifold T_{MAN}:

$$T_{IVC} = T_{MAN} + 35°C \tag{6}$$

As from the spark ignition point, the unburned gas temperature has been assumed to vary with an isentropic law, hence:

$$T = T_{IGN}\left(\frac{p}{p_{IGN}}\right)^{\frac{k-1}{k}} \tag{7}$$

where T_{IGN} and p_{IGN} represent the unburned gas temperature and pressure at the ignition time, while k is the isentropic coefficient, function of the unburned gas temperature.

For each recorded pressure cycle the Knock Onset Position (KOP), and hence its time t_{KO}, was identified as the location of the first remarkable pressure oscillation on the band-pass filtered (3 kHz – 20 kHz) pressure signal. Figure 1 shows a typical light knocking pressure curve together with its band-pass filtered signal: the KOP is pointed out. The power spectrum of the band-pass filtered pressure signal is reported in Figure 2: as is clearly visible, on the engine tested, knocking produced pressure oscillation whose main frequencies are about 5 kHz and 13 kHz.

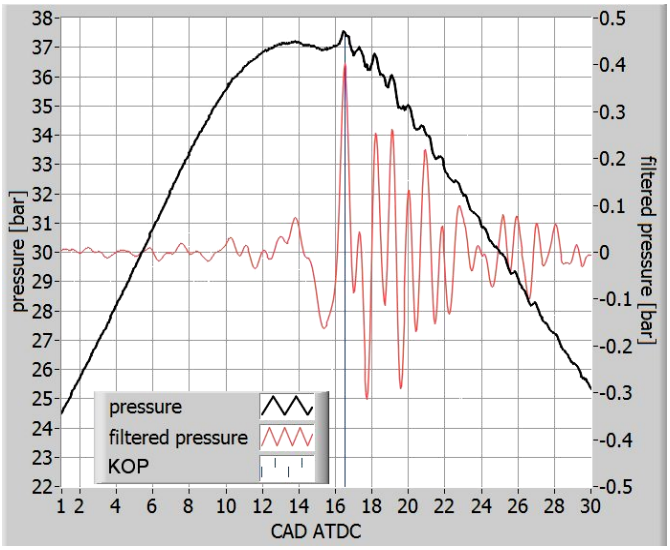

Figure 1 - An example of KOP evaluation, (pure gasoline, 2000 rpm, MAP=74 kPa)

Once known the real knock onset time t_{KO} for each of the pressure cycle sampled, the knock integral error ε can be evaluated for each fixed set of constants A, n, and B from the following equation:

$$\varepsilon = \int_{t_{IVC}}^{t_{KO}} \frac{dt}{A \cdot p^{-n} \cdot e^{B/T}} - 1 \tag{8}$$

Equation (8) can also be written in the crank angle domain, replacing the time variable t with the crank angle ϑ; hence:

$$\varepsilon = \int_{\vartheta_{IVC}}^{KOP} \frac{d\vartheta}{\omega \cdot A \cdot p^{-n} \cdot e^{B/T}} - 1 \qquad (9)$$

where ω represents the angular velocity (rad/sec or CAD/sec according to the unit used for the crank position ϑ).

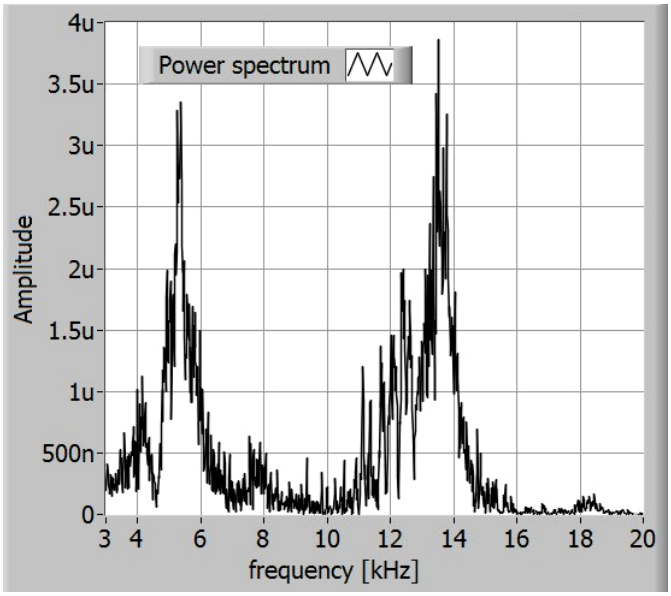

Figure 2 – Power spectrum of the filtered pressure signal (pure gasoline, 2000 rpm, MAP=74 kPa)

The set of constants *A*, *n* and *B* related to the pure gasoline operation has been determined employing a mathematical algorithm for the minimization of the root mean square error ε_{RMS} evaluated over the total number of pressure cycles N:

$$\varepsilon_{RMS} = \sqrt{\sum_{i=1}^{N} \varepsilon_i^{\,2} \Big/ N} \qquad (10)$$

The Downhill Simplex searching algorithm (also known as the Nelder and Mead method (15)) has been used for the absolute minimum evaluation of the objective function ε_{RMS} (*A*, *n*, *B*). The solution found is reported in Table 3:

fuel	A	n	B
Gasoline	2.233e-3	1.16	3477

Table 3 - Values of the model constant obtained for the pure gasoline mode

The same solution has been obtained searching, for a set of fixed values of the two constants *B* and *n*, the value of the constant *A* which minimizes the ε_{RMS}: the constant *B* was varied from 3000 to 4000, while *n* ranged from 0.9 to 1.4. This procedure allowed to trace the contour map of the minimum ε_{RMS}, reported in Figure 3, as function of *B* and *n*: the cross indicates the absolute minimum RMS error and corresponds to the three values reported in Table 3. It is worth to mention that in a previous work (6), the three constants *A*, *B* and *n* assumed, for a commercial gasoline, the values of 7.29 10^{-3}, 4341 and 1.685 respectively.

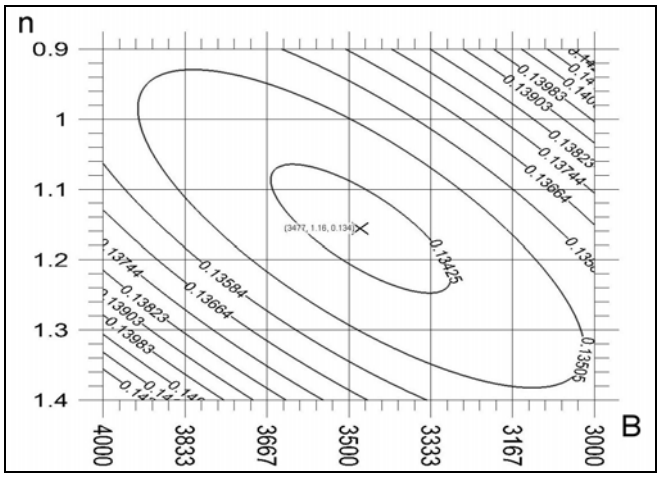

Figure 3 - Contour map of the minimum RMS error as function of *B* and *n*

As regards the simultaneous combustion of CNG and gasoline, the authors considered that in a mixture of two fuels with significantly different knock resistance (CNG has RON≈130 while for standard gasoline RON=95), it is always the less resistant to cause knocking to occur. Moreover, due to the relatively low compression ratio of the engine used in the test (i.e. 9.8), the authors never succeeded in causing knocking to occur in the pure CNG operation, even advancing the combustion at engine speed as low as 1000 rpm, full load and heating the inlet air to about 100°C. This fact confirms that the knocking phenomena which occur in the double-fuel operation are caused by the autoignition of the gasoline; hence, according to this concept, the three model constants should remain unchanged varying the proportion between CNG and gasoline in the mixture used. The empirical observation however showed that, for a fixed MAP and engine speed, increasing the CNG mass fraction (and maintaining the air-fuels mixture stoichiometric) allows to advance the combustion without knocking to occur: Figure 4, as example, shows the Knock Limited Spark Advance (KLSA) for different engine speed as function of the CNG mass fraction for the full load case. This means that the presence of CNG in the gasoline-air mixture increases the knock resistance. The hypothesis made by the authors to explain this phenomenon is that natural gas, due to

its high knock resistance, absorbs the heat released by the autoignition of the first gasoline nuclei without igniting, thus suppressing the propagation of heat and hence the knock onset; this implies that, for a given knocking condition of unburned gas pressure and temperature, the autoignition of the gasoline does not succeed in causing the same knocking effect which would cause in the pure gasoline operation; in conclusion, for a given condition of unburned gas pressure and temperature, the autoignition time of the fuel mixture results to be increased by the suppressing role of the natural gas, or, which is equivalent, the same knocking effect can be achieved by means of higher unburned gas pressure and temperature: this, in turn, is equivalent to an increase in the constant *A* of the autoignition time of equation (1).

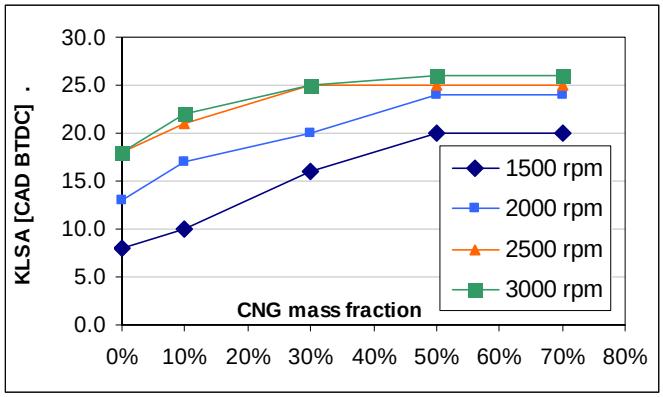

Figure 4 – KLSA as function of the CNG mass fraction at WOT

According to this hypothesis, for the simultaneous combustion of natural gas and gasoline, the authors considered the same constant *n* and *B* determined for the pure gasoline mode (i.e. the fuel sensitivity to pressure and temperature was supposed to remain unchanged), ascribing the increased autoignition time only to the constant *A*: the same procedure has been followed in (6) for the simultaneous combustion of n-eptane and isooctane. Hence, minimizing again the RMS error ε_{RMS} of equation (10), the authors determined the values of the constant *A* for each of the CNG mass fraction investigated, reported in Table 4.

% CNG	A
0%	2.233e-3
10%	2.505e-3
30%	3.004e-3
50%	3.401e-3
70%	3.920e-3

Table 4 - Values of the constant *A* obtained for each CNG mass fraction tested

The graph in Figure 5 reports the values determined for the model constant *A* as function of the CNG mass fraction: as can be observed, a clear linear regression can be drawn. This means that the autoignition time of the double-fuel mixture linearly depends from the CNG mass fraction. The authors consider this a very good property, since, by simple interpolation, it allows to determine the constant *A* of the knock prediction model for any CNG mass fraction in the range 0-70%. On the other hand, CNG mass concentration higher than 70% are not useful for the engine tested since, as already reported, a previous work (1) carried out by the authors shown the maximum efficiency to be reached employing a 50% CNG mass fraction, while the maximum power was achieved with CNG mass fraction around 30%.

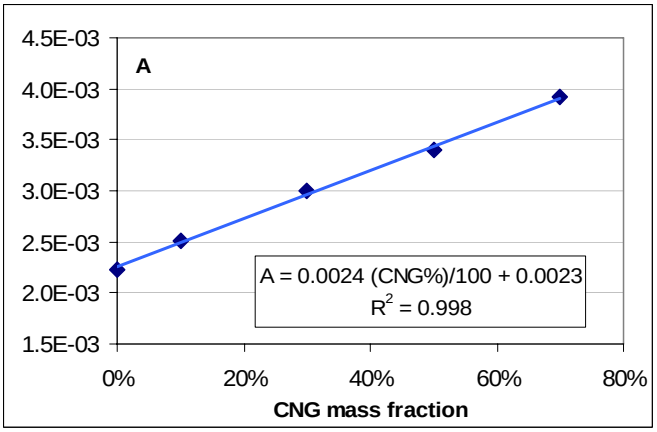

Figure 5 – Model constant *A* as function of the CNG mass fraction

It must also remarked that the linear regression in Figure 5 cannot include the 100% CNG mass fraction, because, as already described above, in the pure CNG operation it was not possible to cause knocking to occur, due to the high knock resistance of methane and the low engine compression ratio. Hence, for 100% CNG mass fraction, the three constants of the knock onset prediction model cannot be determined.

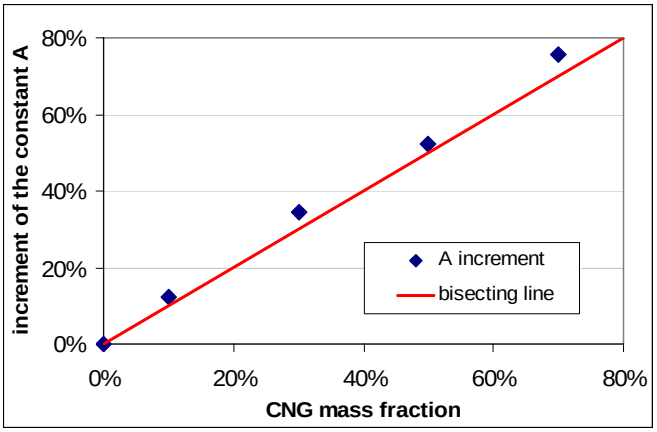

Figure 6 – Increment of the model constant *A* with respect to the pure gasoline operation

It is worthwhile to mention that, as clearly shown in Figure 6, the increment of the model constant *A* with respect to the pure gasoline mode, resulted to be almost equal to the CNG mass fraction: this further on facilitates the use of the model, since makes unnecessary the determination of the value assumed by the constant *A* for the double-fuel operation. It must be however pointed out that the results determined in this work may not have a general validity, since the end-gas thermodynamic state, and hence knocking occurrence, strongly depend on the engine geometry and on in-cylinder turbulent flow; moreover, in accordance with the hypothesis made on the suppressing role of the natural gas, this behaviour may change with the CNG composition, which in turn may vary from one district to another. Nevertheless the qualitative results remain valid, and the procedure followed by the authors may be applied to any other spark ignition engine fuelled with natural gas-gasoline mixtures.

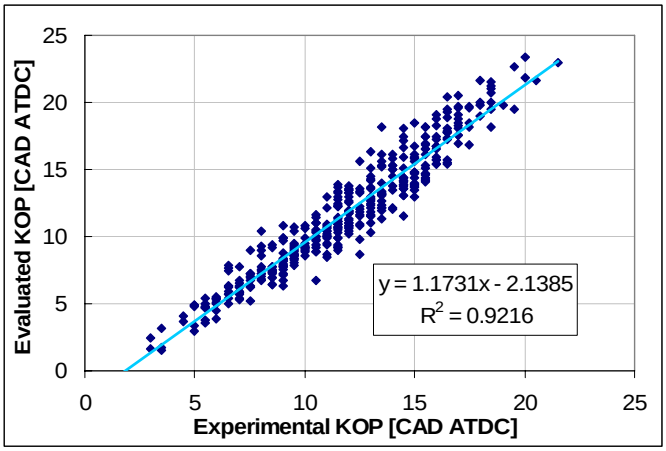

Figure 7 – Comparison between the estimated and the experimental Knock Onset Position (KOP)

Once determined the values of model constants for each of the CNG mass fraction investigated, the authors verified the reliability of the model to estimate the onset of knock: to this purpose, for each CNG mass fraction (i.e. for each set of constants *A*, *n* and *B*), the knock onset position KOP has been determined solving the knock integral of equation (3) in the crank angle domain till it reached the value 1, as here reported:

$$\int_{\vartheta_{IVC}}^{KOP} \frac{d\vartheta}{\omega \cdot A \cdot p^{-n} \cdot e^{B/T}} = 1 \qquad (11)$$

The estimated values of the KOP has been then compared to those experimentally determined: the results, shown in Figure 7, revealed a good agreement, with a maximum difference of +4.7 CAD and a mean absolute difference of just 1.2 CAD. This means that the calibrated model succeed in predicting the knock onset position with a maximum inaccuracy of 5 CAD.

CONCLUSIONS

The authors already investigated in a previous work (1) the simultaneous combustion of natural gas and gasoline in a bi-fuel S.I. engine, achieving considerable improvements in engine efficiency (e.g. +27% at full load) with respect to the pure gasoline operation, keeping the power loss under the 4%, (which is better then the 12% loss caused by the pure CNG operation). Considering then the double-fuel mode a practical alternative in bi-fuel engines, the authors intended to study how a knock onset prediction model must be modified in order to be valid also for the double-fuel operation. To this purpose a wide experimental campaign has been carried out, recording in-cylinder pressure cycles under light knocking spark advance for many different operative conditions of speed, load and CNG/gasoline mixtures (always maintaining a stoichiometric proportion with air). The experimental data acquired have been used for the calibration of the three constants (*A*, *B* and *n*) of a classical knock onset prevision model, carried out through some hypothesis made on the autoignition of fuels mixtures; in particular, the authors gave an interpretation of the experimentally noticed increase in knock resistance of the CNG/gasoline mixtures when increasing the CNG mass fraction (i.e. the ratio between the injected natural gas mass and the total fuel mass). The hypothesis made allowed to fix two (*B* and *n*) of the three model constants to the values assumed for the pure gasoline operation. The successive calibration performed on the constant *A* of the model revealed a good linear correlation with the CNG mass fraction: this allows, through simple interpolation, to easily determine the model constant for each composition of the CNG/gasoline mixture in the range 0-70%. Moreover, the increment of the constant A due to an increasing content of CNG in the fuel mixture, was found to be almost equal to the CNG mass fraction itself.

The model, once calibrated, has also been verified in terms of reliability in the knock onset position prediction: the comparison made against the experimental data revealed a very good agreement, with a maximum error of 5 CAD.

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NOMENCLATURE

A: constant of the autoignition model
A/F ratio: Air to Fuel ratio
ATDC: After Top Dead Centre
B: constant of the autoignition model
BTDC: Before Top Dead Centre
CAD: Crank Angle Degree
CNG: Compressed Natural Gas
DAQ: Data Acquisition
ε: Knock integral error
ε_{RMS}: Root mean square value of the knock integral errors
E: Fuel activation energy
ECU: Electronic Control Unit
ID: Ignition Delay
IVC: Inlet valve closure
KI: Knock Integral
KLSA: Knock Limited Spark Advance
KOP: Knock Onset Position
KO: Knock Onset
LPG: Liquefied Petroleum Gas
MAP: Manifold Absolute Pressure
n: constant of the autoignition model
N: number of pressure cycles for a given CNG mass fraction
NG: Natural gas
ω: engine angular velocity
p_{IGN}: Gas pressure at the spark ignition point
p_{IVC}: Gas pressure at the IVC
p_M: mean unburned gas pressure during combustion
R: Universal gas constant
RON: Research Octane Number
ϑ_{IVC}: Crank position at IVC
τ: autoignition time
TDC: Top Dead Centre
T_{IGN}: Gas temperature at the spark ignition point
T_{IVC}: Gas Temperature at the IVC
t_{KO}: Knock onset time
T_M: mean unburned gas temperature during combustion
T_{MAN}: Gas temperature in the manifold
UEGO: Universal Exhaust Gas Oxygen
V_{IVC}: In-cylinder volume at the IVC
WOT: Wide open throttle (full load)