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An NTC zone compliant knock onset prediction model for spark ignition engines

Emiliano Pipitone[a], Giuseppe Genchi[a], Stefano Beccari[a]*

[a]*University of Palermo, Viale delle Scienze edificio 8,90128Palermo, Italy*

Abstract

Pollutant emissions reduction and energy saving policies increased the production of Spark Ignition (SI) engines operated with gaseous fuels. Natural Gas (NG) and Liquefied Petroleum Gas (LPG), thanks to their low cost and low environmental impact represent the best alternative. Bi-fuel engines, which may run either with gasoline or with gas (NG or LPG), widely spread in many countries thanks to their versatility, high efficiency and low pollutant emissions: gas fueled vehicles, as example, are allowed to run in many limited traffic zones. In the last years, supercharged SI engines fueled with either gasoline or gaseous fuel, spread in the market. Thermodynamic simulations, widely used to reduce costs during engine development and optimization process, require proper combustion and knock onset prediction models. In particular the fuel knocking resistance is a crucial issue in supercharged engines development. Starting from these considerations the authors developed and calibrated an original knock onset prediction model for knock-safe performances optimization of engines fueled by gasoline and gaseous fuels. The proposed model, despite its very simple formulation, takes into account the Negative Temperature Coefficient (NTC) behavior exhibited by many hydrocarbons fuels such as gasoline, propane and methane. The knock prediction model has been calibrated by a great number of light-knocking pressure cycles sampled using a Cooperative Fuel Research (CFR) engine. The engine Compression Ratio (CR), inlet mixture temperature and spark advance have been varied to obtain very different operative conditions for model calibration; as a result the model can be used in the development of different kind of engines, i.e. naturally aspirated or supercharged. Five fuels have been tested: gasoline, LPG, NG, propane and methane. The calibrated model showed a very high reliability with a maximum knock onset prediction error of only 4 crank angle degrees (CAD) and an overall mean absolute error lower than 1 CAD, that are negligible quantities from an engine control point of view.

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Keywords: SI engines; knock prediction model; NTC zone.

* Corresponding author. Tel.: +3909123897254; fax: +3909123860840.
E-mail address: stefano.beccari@unipa.it.

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1. Introduction

Natural Gas (NG) and Liquefied Petroleum Gas (LPG) are a valid alternative to gasoline for SI engines thanks to a lower cost, lower pollutant emissions and higher engine efficiency. These results are obtained through better mixing capabilities and higher knocking resistance that in turn allow the engine to run with stoichiometric fuel mixture also at full load. On the contrary gasoline operated engines need rich mixture at full load thus producing higher hydrocarbon and particulate emissions and high specific fuel consumption. Bi-fuel engines fed by gasoline or gaseous fuel spread in many countries in the last decades and some car makers put in production engines fueled only with NG. Moreover the engine downsize process led to an increasing production of supercharged SI engines (also in Bi-fuel version).Numerical simulations are a fundamental tool during engine development process as they allow a strong reduction of times and costs. Combustion is the most important phase of engine operation and a reliable combustion simulation is essential to correctly predict engine performances. As far as SI engines are regarded, and in particular supercharged engines, knocking phenomena must be taken into consideration by using proper knock onset prediction sub-models. In this paper the authors propose an innovative knock onset prediction model, based on the classical knock integral approach[1], which takes into account the Negative Temperature Coefficient (NTC) behavior exhibited by many fuels such as gasoline, methane and propane. Five fuels has been tested: commercial gasoline, NG, LPG, methane and propane. The first three were chosen because they are commonly available commercial fuels; however both NG and LPG are gas mixtures whose composition influences knocking resistance. Engine development and optimization process usually involves numerical simulations and experimental tests performed using reference fuels, whose fixed properties allow to draw repeatable and comparable results; for these reasons methane and propane, often used as reference fuels, have been tested. The model has been calibrated using light knocking pressure cycles obtained with a CFR engine[2] in different operative conditions.

Nomenclature

A, n, B	calibration parameters of the model	T_{IGN}	unburned gas temperature at ignition
CAD	Crank Angle Degrees	T_{IN}	inlet mixture temperature
CFR	Cooperative Fuel Research	T_{IVC}	unburned gas temperature at IVC
CR	Compression Ratio	t_{IVC}	inlet valve closure time
IVC	Inlet Valve Closure	t_{KO}	knock onset time
KI	Knock Integral	T_{NTC}	lower temperature of the NTC zone
KOCA	Knock Onset Crank Angle	V	in-cylinder volume
LPG	Liquefied Petroleum Gas	V_{IVC}	unburned gas volume at IVC
m	the polytropic coefficient	ϑ_{IVC}	crank angle at IVC
NG	Natural Gas	$\vartheta_{KO,exp.}$	experimental KOCA
NTC	Negative Temperature Coefficient	$\vartheta_{KO,model}$	model evaluated KOCA
p	unburned gas pressure	ε	difference between estimated andexperimental KOCA
p_{IGN}	unburned gas pressure at ignition	ε_i	i^{th} KOCA error
p_{IVC}	unburned gas pressure at IVC	ε_{MA}	mean absolute KOCA error
SA	Spark Advance	ε_{max}	maximum absolute KOCA error
SI	Spark Ignition	ϕ	equivalence ratio
t	time	τ	auto-ignition time
T	unburned gas temperature	ω	engine angular velocity

1.1. Knock onset prediction model

Two main types of knock onset prediction models can be found in literature: auto ignition delay and detailed chemical kinetic models. The first is based on the unburned gas pressure and temperature histories and needs experimental data for its calibration[1][3][4][5][6][7]; the second takes in to account the elementary reactions that occurs between the species involved in the combustion process [8][9] and requires greater computational cost. Thanks to the lower computational effort and satisfactory results, the first type is often preferred. A fuel-air mixture, subjected to constant thermodynamic conditions, auto-ignites after a certain time τ which can be related to the pressure p and temperature T by the use of an Arrhenius type equation[1]:

$$\tau = Ap^{-n}e^{B/T} \tag{1}$$

where A, n and B are fuel dependent constants determined by statistical regression of the measured auto-ignition times [4][5][6][7].During combustion in a SI engine the unburned gas pressure and temperature are far from being constant so equation (1) cannot be directly employed and a Knock Integral (KI) must be evaluated as function of time t:

$$KI(t) = \int_{t_{IVC}}^{t} \frac{dt}{\tau} \tag{2}$$

being t_{IVC} the Inlet Valve Closure (IVC) time. According to this method[1], the knock onset time t_{KO} is obtained when the integral reaches the value of 1:

$$KI(t_{KO}) = \int_{t_{IVC}}^{t_{KO}} \frac{dt}{\tau} = 1 \tag{3}$$

This condition corresponds to the critical concentration of the radical species needed for auto-ignition. Equation (1) states that a pressure and temperature increase induces a reduction of auto-ignition time. This relation between temperature and auto-ignition time has a general validity in the lower and higher temperature range while, as stated by many authors [8][10][11][12], at intermediate temperatures (approximately between 650 and 900 K) many hydrocarbon fuels exhibit a reverse dependence, showing an increase of auto-ignition time for increasing temperature. This phenomenon, shown in Figure 1, is known as NTC behavior and its temperature range of existence depends on the fuel. For higher temperatures, the auto-ignition time shows again a decreasing trend (Figure 1). Equation (1) cannot model the NTC behavior of fuels: its representation in Figure 1would be a straight line. For gasoline, the NTC behavior has been found to exist for temperatures between 700K and 850K, as shown in Figure 1, regardless of pressure or equivalence ratio ϕ of the mixture [10].During combustion in SI engines the unburned gas temperature usually exceeds 700 K, in the present study the peak unburned gas temperature ranged from 600 K to 870 K depending on the fuel tested. A knock onset prediction model should take into account the fuel NTC behavior to give reliable and accurate results. From 720 to 800K the auto-ignition time of gasoline can be considered constant, as pointed out by the experimental data in Figure 1; a similar behavior has been observed with propane [11] and methane [12] whose auto-ignition times remain almost constant in the range 740-870 K and 850-1050 K respectively. With the aim to take into account the NTC behavior, the authors proposed a modified version of the Arrhenius type equation (1); the auto-ignition time is given by equation (1) until NTC behavior occurs (i.e. when $T \leq T_{NTC}$), while for higher temperatures the auto-ignition time is independent of temperature:

$$\tau = \begin{cases} A\,p^{-n}e^{B/T} & T \leq T_{NTC} \\ A\,p^{-n}e^{B/T_{NTC}} & T > T_{NTC} \end{cases} \tag{4}$$

where T_{NTC} is the lower temperature of the NTC behaviour zone; it depends on the fuel considered and the following values can be assumed[10][11][12]:720 K (gasoline), 740 K (propane) and 850 K (methane). Since methane and propane are the main components of the tested NG and LPG respectively, the T_{NTC} value used for each pure gas has been assumed valid also for the corresponding gas mixture.

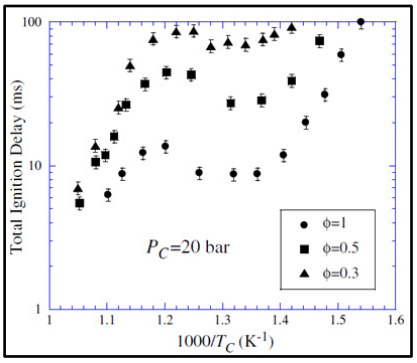

Figure 1 – NTC zone of gasoline (three equivalence ratio ϕ)[10]

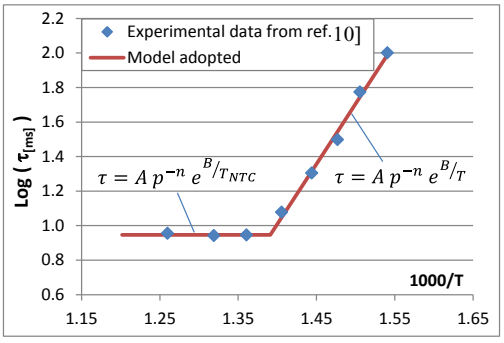

Figure 2 - Comparison between measured auto-ignition time [10] and model adopted in the present paper

Figure 2 graphically displays the adopted model compared with experimental data of reference [10]; the end of the NTC zone has not been taken in to account because, for all the tested fuels, the unburned gas peak temperature always remained below the higher temperature limit of NTC zone. In the present work equation (4) has been implemented in the KI of equation (3) and, after an accurate calibration procedure the model constants A, n and B have been determined for gasoline, propane, methane, NG and LPG.

2. Experimental setup and test method

Being the Knock Integral method based on the unburned gas pressure and temperature history, the authors aimed to determine the model's constants by means of experimental data in which these two parameters varied significantly. In this way, once calibrated with an heterogeneous set of pressure and temperature histories, the model can be used to predict knock occurrence in SI engines of different kind, naturally aspirated as well as supercharged. The experimental tests were performed using a CFR engine which, thanks to its particular arrangement[2], allows a great variation of CR and inlet mixture temperature thus producing a very differentiated collection of pressure and temperature histories. Figure 3shows the experimental setup: the CFR engine is endowed of two independent injection systems, one for gasoline and one for gaseous fuel; both fuel and air flows were measured with proper flow meters, while a personal computer has been employed both for ignition and injection systems control and for data acquisition(combustion chamber pressure, mass flows, inlet air temperature, intake duct pressure, etc.). Both data acquisition and engine control were performed by means of National Instruments DAQ Cards programmed in LabVIEW environment .Knock occurrence was monitored using a Kistler piezoelectric pressure sensor flush mounted in the combustion chamber, whose signal has been acquired at 160 kHz sample rate.

As already mentioned, five fuels were used in this study, and for each fuel, four different inlet mixture temperatures and three Spark Advances (SA) where tested; for each operative condition, 50 light knocking pressure cycles were acquired. Table 1 resumes the operative conditions used in the test together with the composition of the LPG and the NG employed.

Table 1 – operative conditions tested

Engine speed	900 [RPM]
Inlet temperature (T_{IN})	50, 80, 110, 140 [°C]
Engine load condition	full load
Compression ratio (CR)	determined to cause light knocking
Overall air/fuel ratio	stoichiometric
Spark advance (SA)	15, 25, 35 [CAD BTDC]
Fuel tested	gasoline; methane; propane; LPG (80% propane, 20% propylene); NG (86% methane, 8% ethane, 1.6% propane, 1% CO_2, 3% N_2, 0.4% others)

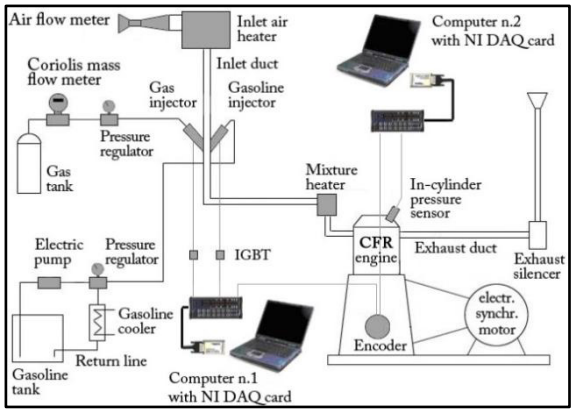

Figure 3 – experimental layout

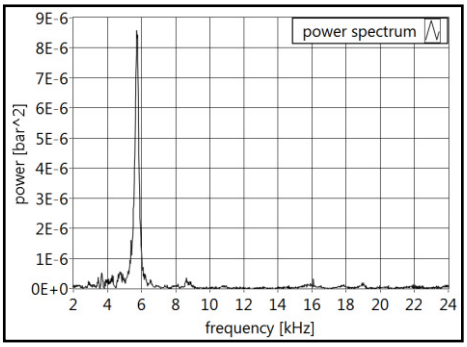

Figure 4 – Power spectrum of the raw pressure signal (NG, SA=25 CAD BTDC, T_{IN}=80 °C).

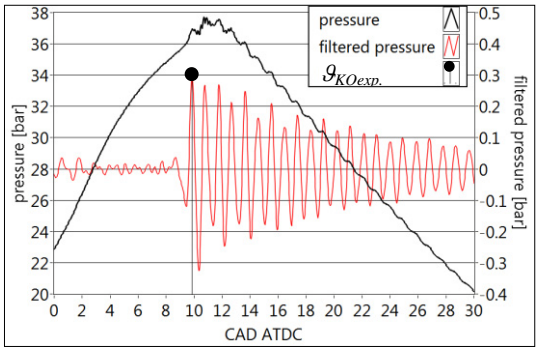

Figure 5 – Raw and filtered pressure with $\vartheta_{KO,exp.}$ evaluation, (NG, SA=25 CAD BTDC, T_{IN} =80 °C)

Figure 4 reports the power spectrum of a raw pressure signal, showing the main frequency of the knocking pressure oscillations to be around 6 kHz. Hence, with the aim to remove unwanted noise and highlight knocking pressure oscillations, each pressure trace has been filtered by means of a second order, zero-phase shift, 3-20 kHz band-pass Butterworth filter. The result is reported in Figure 5 which shows the raw and filtered pressure signals; a pressure cycle has been identified as "light knocking", and then saved for subsequent analysis, when the peak to peak value of the filtered signal resulted higher than 0.2 bar; this threshold is based on previous experimental experience [6][7].For each recorded pressure trace, the experimental Knock Onset Crank Angle (KOCA) $\vartheta_{KO,exp.}$ (showed in Figure 5) has been identified as the location of the first oscillation with peak to peak value higher than 0.2 bar. The use of light knocking cycles for model calibration allows to define the boundaries of the knock safe zone for a given fuel mixture; these boundaries will help engine designers and testers to safely optimize engine performance, since a slight reduction of spark advance with respect to light knocking condition completely suppress any knocking phenomena.

The three spark advances adopted have been fixed to avoid combustion ignition onset too different from that of practical interest in actual engines, while the four inlet mixture temperatures have been selected with the aim to include typical conditions of both naturally aspirated and supercharged SI

engines. As a result 12 test conditions have been explored for each fuel which means a total of 60 operative conditions.

From IVC to spark ignition time the unburned gas temperature T has been calculated by means of the perfect gas law, being both the in-cylinder volume V and gas pressure p known:

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

where p_{IVC}, V_{IVC} and T_{IVC} denote pressure, volume and temperature of the gas at IVC. T_{IVC} has been considered equal to the inlet temperature T_{IN} thus neglecting heat transfer during the intake stroke. Since combustion starts, the burned and unburned gas temperatures differ each other and their masses and volumes changes continuously during flame front propagation: this makes equation (5) no more valid. Hence, after spark ignition, the unburned gas temperature T has been evaluated on the basis of a polytropic law, as usually done in zero dimensional modelling of SI engines:

$$T = T_{IGN} \cdot \left(\frac{p}{p_{IGN}}\right)^{\frac{m-1}{m}} \tag{6}$$

where p_{IGN} is the unburned gas pressure measured at spark ignition time, T_{IGN} its temperature, evaluated by equation (5), while m is the polytropic coefficient. Once known the experimental location of knock onset ($\vartheta_{KO,exp.}$), for each of the pressure cycle sampled, the KOCA $\vartheta_{KO,model}$ estimated by the model has been determined by solving the knock integral of equation (3) in the crank angle domain:

$$\int_{\vartheta_{IVC}}^{\vartheta_{KO,model}} \frac{d\vartheta}{\omega \cdot \tau} = 1 \tag{7}$$

where ϑ_{IVC} is the crank position at IVC and ω is the engine angular velocity [rad/s]. The KOCA error ε can be then evaluated, for each single pressure trace, according to the set of model constants A, n, and B:

$$\varepsilon = \vartheta_{KO,model} - \vartheta_{KO,exp} \tag{8}$$

3. Results and discussion

The model was calibrated using the pressure cycles obtained with the different fuels tested. The optimal set of model constants A, n and B has been determined minimizing the mean absolute error ε_{MA} evaluated over the total number of pressure cycles N available for each fuel:

$$\varepsilon_{MA} = \frac{\sum_{i=1}^{N} |\varepsilon_i|}{N} \tag{9}$$

where ε_i is the KOCA error determined for the i^{th} knocking pressure cycle using equation (8).For a fixed set of n and B, the parameter A has been determined minimizing the objective function ε_{MA} (A, B, n) by the use of the Downhill Simplex searching algorithm [13]; this procedure has been repeated for B and n ranging inside predetermined intervals, obtaining, as a result, the surface and the contour plot of minimum ε_{MA} as function of B and n. As example, Figure 6 and Figure 7 show the surface and the contour plot obtained for methane: the cross in Figure 7 indicates the absolute minimum of ε_{MA} and allows to determine the best values of the three model parameters A, B and n.

Table 2resumes the optimum values of A, B and n obtained for all the fuels tested, together with the mean and maximum absolute error $|\varepsilon_{max}|$; it can be noted that the model parameters are quite different from each other due to the different knock resistance of the different fuels. As shown in Table 2 the mean absolute error of the model is always lower than 1 CAD and the maximum error always lower than 4 CAD: these are very satisfactory results considering the wide variety of pressure and temperature histories used for model calibration. For each of the fuel tested, the knock onset position evaluated by the model has been compared with the experimentally measured value; the results of these comparison are

shown in Figure 8: a very good correlation is found with a R^2 value of 0.986 and maximum error of ±3.5 CAD.

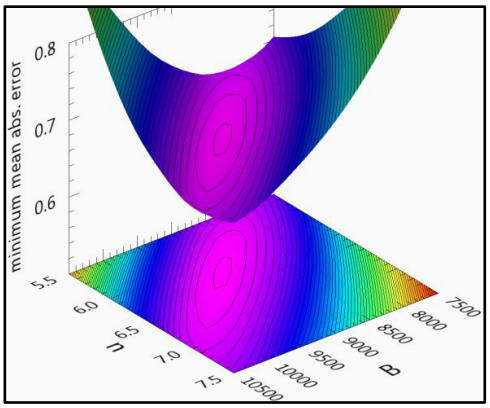

Figure 6 – Surface of the minimum ε_{MA} as a function of the model constants B and n (methane, T_{NTC}=850 K).

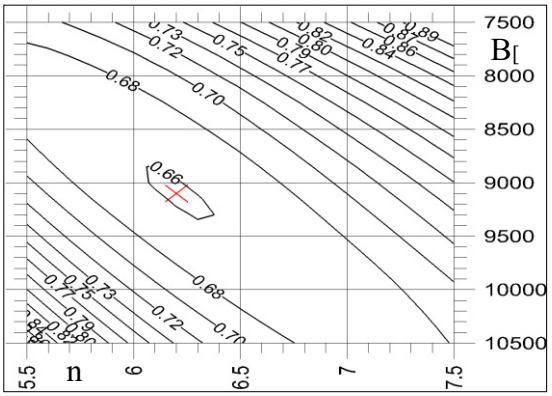

Figure 7 – Contour plot of the minimum ε_{MA} as a function of the model constants B and n (methane, T_{NTC}=850 K).

Table 2 – Model parameters

Fuel	A	n	B	ε_{MA} [CAD]	$\lvert\varepsilon_{MAX}\rvert$ [CAD]
Gasoline	0.122	4.2	5700	0.574	1.90
LPG	0.170	6.0	10500	0.523	1.86
Propane	0.0220	5.3	10500	0.540	2.98
NG	5.10	7.5	13800	0.640	2.52
Methane	90.0	6.2	9100	0.663	3.36

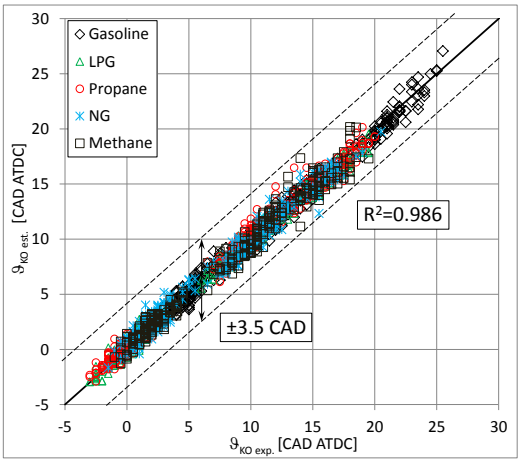

Figure 8 – Comparison between estimated and experimental knock onset.

4. Conclusions

The purpose of this work was to provide an NTC compliant knock onset prediction model to be used in engine thermodynamic simulations for a knock-safe performance optimization of SI engines fueled by gasoline or gaseous fuels (LPG and NG). The classical knock integral approach has been modified to take in to account for the NTC behavior featured by many hydrocarbon fuels. The model has been calibrated by using light knocking pressure cycles sampled on a CFR engine obtained with a large variation of initial temperature and compression ratio; this gives the model a general validity, allowing to predict knocking occurrence both in naturally aspirated and supercharged engines. The calibrated model showed very good

knock onset prediction abilities with mean absolute error always lower than 1 CAD and maximum error always lower than 4 CAD that are negligible quantities from an engine control point of view.

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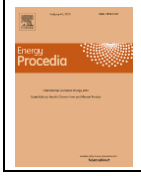

Biography

Stefano Beccari obtained his Ph.D. in Mechanical Engineering from University of Palermo (Italy) in 2005. He is currently a researcher there in the field of fluid machines. His main research interest is the spark ignition engines performance and efficiency optimization, with particular reference to the bi-fuel engines: gasoline-natural gas and gasoline-LPG.