Model Predictions and Experimental Evidence of Detonation Characteristics in a Spark Ignition I.C.E.

M.Belli, S.Bova and P.Fragiacomo

Dipartimento di Meccanica Università della Calabria 87030 Arcavacata di Rende - Cosenza Italy

ABSTRACT

A simulation model, which uses the four-octane-number method, has been used for determining the knock-resistence of a generic fuel in a given engine.

In the meanwhile experimental data have been taken from a single-cylinder AVL engine. The cylinder pressure has been recorded for many consecutive cycles under different detonation conditions. The original data have been numerically filtered in order to obtain the pressure oscillations due to the detonation.

Finally the experimental results have been compared whith the numerical predictions, in order to check the capabilities of the proposed model.

INTRODUCTION

The aim of the present study is to predict (by means of simulation models) time and intensity of detonation of any given commercial fuel within an engine, for each operating condition.

In recent years this has been attempted by several researchers [1-7] using rather sophisticated detonation models.

The model employed by this study is a simple autoignition model [1] based on an induction time determined by a global kinetic theory. The governing equation is a simple Arrhenius-type equation:

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = \alpha \, \mathrm{A'} \, \mathrm{p^n} \, \mathrm{e^{-B}} \, / \mathrm{T} \tag{1}$$

Autoignition starts at the instant t_c , when a certain concentration value α_c has been reached. This concentration is independent of temperature and pressure, while it is dependent on the type of fuel. If pressure and temperature values are kept constant, equation (1) can be integrated directly, thereby expressing the autoignition delay, as:

$$\tau = t_c - t_o = A p^{-n} e^{B/T}$$
 (2)

In cases where temperature and pressure are not constant, as in spark ignition engines, this formula can be regarded as the instantaneous value of the autoignition delay. In this case, Livengood and Wu [1] call for an integral function:

$$I(t) = \int_{t_o}^{t} \frac{dt}{\tau}$$
 (3)

Detonation takes place at the instant t_{c} in which $I(t_{\text{c}})$ is equal to 1.

In order to evaluate the instantenous value of the induction period, it is necessary to know the A, n and B parameters (characteristic of the fuel) in addition to the pressure and the temperature data.

The main purpose of predicting the detonation of a given commercial fuel is fulfilled when parameters A, n and B are determined, once the composition and octane numbers are available.

These parameters are known for the Primary Reference Fuels (PRF) and have been obtained by means of an optimization procedure on the basis of a large number of tests of these fuels under various operating conditions.

The numeric values obtained are [5]:

$$A = 0.01869 \left(\frac{ON}{100}\right)^{3.4017}$$

$$n = 1.7 \tag{4}$$

$$B = 3800$$

(with p in kg/cm2 and T in Kelvin).

The general goal of the research reported in this paper is to achieve the prediction of detonation occurrence within an engine for any given commercial fuel.

To this aim three main steps were performed. The first one was to determine the detonation parameters of the fuel under test on the basis of its chemical composition and of its Octane Numbers. Then the previously mentioned delay time method was implemented in a phenomenological engine simulation model, in order to predict time and intensity of detonation. Finally data were taken from a single cylinder S.I. engine operated under detonation conditions to check the capabilities of the proposed model.

DETONATION-OCCURRENCE PREDICTION MODEL

For the present research a phenomenological two-zones model was used, which is characterized by a global application of the thermodynamic equations within the combustion chamber [8], while the phenomena to which combustion is subjected (turbulence, flame propagation, combustion kinetics and heat transfer) are modeled by means of empiric relations. Fig. 1 shows a typical result of the simulation.

In addition, a global kinetic model of pre-ignition reaction is used in order to determine the autoignition time. The I(t)

functional is computed during combustion and, in the event that this functional reaches the unit value before the completion of the combustion, it can be said that detonation occurs with an intensity which is proportional to the fraction of residual unburnt gas in the chamber at that time. Fig. 2 presents a case in which the occurrence of detonation is predicted.

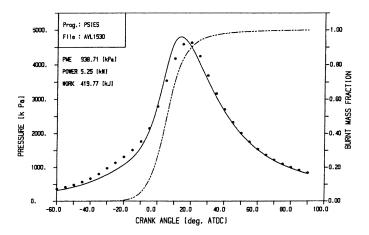


Fig. 1 - Pressure curve (solid line) and burnt mass fraction (dotted line) predicted by the model in the absence of detonation. Stars represent the experimental data.

Engine speed 1500 rpm; spark advance -30 deg ATDC; stoichimetric mixture.

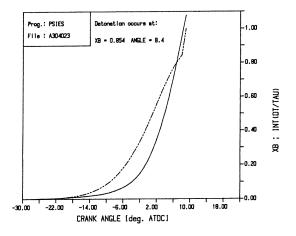


Fig. 2 - Case of detonation occurrence as results from the model. Solid line I(t); dotted line burnt mass fraction.

Engine speed 925 rpm; spark advance 30 deg.

ATDC; stoichimetric mixture.

Knowing the values reported in (4) for the A, n, B parameters of a PRF, the detonation time and intensity can be fixed for the case of the operating conditions relative to an Octane Number test. The assumption is that, in a particular test (e.g. in a "Motor" test) the unburnt mass fraction at the detonation time is the same in both the case of the gasoline under analysis and in the PRF representative of that Octane Number (e.g. MON). By running the simulation program in the operating condition of a given standard test (e.g. "Motor"), one first determines the unburnt gas mass

fraction at detonation time using the PRF, then the fuel under analysis is substituted with the PRF, and the pressure and temperature data $p_{\mbox{MON}}(t)$ and $T_{\mbox{MON}}(t)$, and the detonation time $t_{\mbox{cMON}}$ - i.e. the instant at which the unburnt gas mass fraction is the same that in the case on the PRF - are computed. Therefore the following equation can be written:

$$\int_{t_0}^{t_c_{\mathsf{MON}}} \frac{dt}{A_t \, P_{\mathsf{MON}}(t)^{-n_t} \exp\left[\frac{B_t}{T_{\mathsf{MON}}(t)}\right]} = 1 \quad (5)$$

in which the unknowns are A_t , n_t and B_t .

This equation can be set down for different operating conditions. Douaud and Eyzat [5] proposed to use 4 different operating conditions: the two classic "Motor" and "Research" tests, and, in addition, two other ad hoc defined "Motor-prime" and "Research-prime" conditions, which derive from the previous two by exchanging the intake mixture and intake fuel conditions. The problem of determining the detonation parameters A_t , n_t and B_t is then solved by the minimization of

$$\min_{\mathbf{A}_{\mathsf{C},\mathsf{R}_{\mathsf{C}},\mathsf{R}_{\mathsf{C}}} \left[\mathbf{F}_{\mathsf{MON}}^2 + \mathbf{F}_{\mathsf{RON}}^2 + \mathbf{F}_{\mathsf{RON}}^2 + \mathbf{F}_{\mathsf{RON}}^2 \right] 6)$$

where

$$F_{j_{ON}}(A_t, n_t, B_t) = \int_{t_0}^{t_{oj_{ON}}} \frac{dt}{A_t p_{j_{ON}}(t)^{-n_t} \exp\left[\frac{B_t}{T_{j_{ON}}(t)}\right]} - 1$$

$$j_{ON} = MON, RON, MON', RON'.$$

More details about the method can be found in ref [9].

EXPERIMENTAL APPARATUS AND DATA ANALYSIS

The engine used during the tests was a four-stroke single-cylinder AVL model 530, characterized by an Heron type combustion chamber.

The engine was coupled to a 20 kW electodynamic dynamometer. A water cooled AVL quarz transducer and a Kistler amplifier were used to measure the pressure in the combustion chamber. The signal from the pressure measuring system was recorded by a HP-9817H computer by using an A/D converter. The sampling rate was 55kHz and the data acquisition was triggered by the BDC signal. Ignition and injection were provided by a Marelli electronic ignition system and by a Bosch injector respectively, driven by home made circuits.

The gasoline was injected in a heated mixing tank, which was positioned in the intake duct.

The engine was operated at 925 and 1850 rpm, full load, with stochiometric mixture and different spark advances and for each operating conditions 50 individual cycles were recorded with a resolution of 0.1 c.a. deg at 925 rpm and 0.2 at 1850.

The individual cycles were numerically filtered in order to extract the pressure oscillations due to the detonation. Because of the relatively low sampling frequency of the A/D converter a 4th-order low pass filter was used and the high frequency components were obtained by subtracting the filtered data from the original

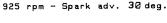
ones. In the time domain the filter is represented by the equation:

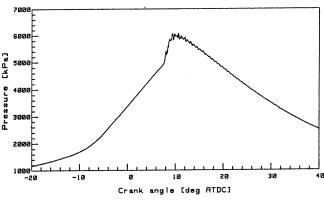
$$f(t) = \frac{t^3 e^{(-t/\tau')}}{\tau'^4 3!} \tag{7}$$

which was Z-transformed in order to be applied to the discreet data. A 5000 Hz cutting frequency was adopted. The results were corrected to compensate the inevitable phase delay and amplification due to the filter.

Figs. 3a, 3b and 3c show the original data, the filtered curve and the pressure oscillation in the case of 925 rpm and 30 c.a. deg. spark advance.

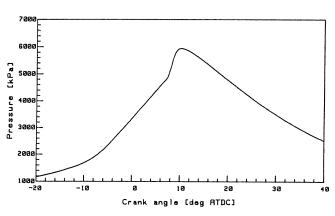
From fig. 3c, the crank angle at which the detonation occurs and the detonation intensity are easily identified. This procedure was applied to each single engine cycle and detonation timing and intensity for each operating conditions were obtained as ensamble average.



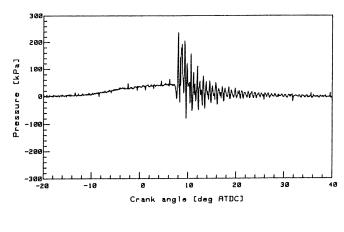


a)

925 rpm - Spark adv. 30 deg.



925 rpm - Spark adv. 30 deg.



c)

Fig. 3
a) Pressure time history recorded in the combustion chamber in the presence of detonation. Sampling frequency 55 kHz (resolution 0.1 c.a. deg.).

- b) Result of numerical filtering. Cutting frequency 5 kHz.
- c) Pressure oscillation due to detonation: difference between curve a) and b). Engine speed 925 rpm; spark advance 30 deg. ATDC; stoichiometric mixture.

RESULTS

The above described methodology was applied to a commercial European-type unleaded gasoline. A sample of this gasoline was analyzed in a gaschromatograph in order to obtain the hydrocarbons contents necessary to calculate its thermodynamic properties [10]. In addition, the 4 previously mentioned O.N. were measured by the CNR - Istituto Motori, Naples. The following detonation parameters were determined:

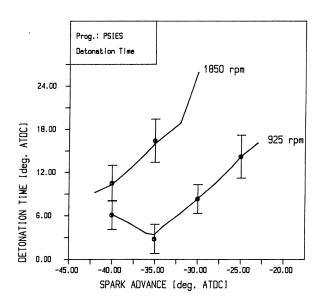
$$A = 0.00025 \text{ n} = 1.367 \text{ B} = 6317$$

and used in the simulation model, while the engine was operated with the same gasoline.

Fig. 4 summarizes the experimental results and the model predictions. The detonation timing is related to the spark advance, for the two different engine speeds. The model predictions match extremely well with the experimental evidence. However some caution should to be adopted. The experimental tests were carried out in sequence for the various engine speeds. As a consequence, both the mixture temperature and the cylinder wall temperature were varyng within a certain range during the tests. While the mixture temperature was measured, the cylinder wall temperature was unknown. Therefore, the simulation was done with the true mixture temperature but with a wall temperature qualitatively representative of the experiment conditions, chosen as the one which allowed the best fit of the data, as reported in Table I.

TABLE I

Engine speed	Spark advance	Inlet Temp. [K]	Wall Temp. [K]
925	-40	303	360
925	-35	318	450
925	-30	323	400
925	-25	323	380
1850	-40	338	420
1850	-35	330	400
1850	-30	323	400



Detonation time vs Spark advance: predicted (solid Fig. 4 line); measured (circules). Full load, stochiometric mixture. Inlet and wall temperatures reported in Table I.

Fig. 5 relates the mean value of the experimental pressure oscillation due to the detonation with the unburnt mass fraction predicted by the model at the detonation time. The trend is quite linear with the exception of the point relative to 925 rpm, 40 deg. spark advance, which was taken when the engine was relatively cold.

This figure validates the hypothesis that the detonation intensity is proportional to the unburnt mass fraction at the detonation time. Under thus conditions, the model can therefore predict predict not only the time but also the intensity of detonation.

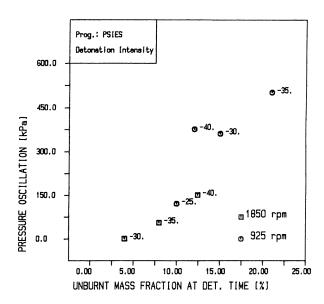


Fig. 5 -Measured pressure oscillations due to detonation vs unburnt mass fraction at detonation time predicted by the model.

CONCLUSIONS

A model is presented to predict detonation time and intensity within an engine which burns a commercial unleaded gasoline.

The comparison of the model results with experimental data taken in a single-cylinder research s.i. engine shows that the model predictions are quite reliable. However more detailed measurements seems to be necessary.

NOMENCLATURE

- pressure

 \mathbf{T} - temperature

- concentration of species in the autoignition reactions

A', A - constants in delay time formula

- pressure exponent in delay time formula - temperature constant in delay time formula

ON - octane number

PRF - Primary Reference Fuel

au - delay time f(t) - filtering function $1/\tau'$ - cutting frequence

subscripts

- values at detonation time

- values referring to the test fuel

- values at ignition time

MON- values referring to the "Motor" ON test operating contitions

RON- values referring to the "Research" ON test operating contitions

MON! values referring to the "Motor Prime" ON test operating contitions

RON'- values referring to the "Research Prime" ON test operating contitions

ACKNOWLEDGMENTS

The Octane Number tests were kindly performed by the CNR - ISTITUTO MOTORI, Naples. The research is supported by the Italian Ministry of Education in the frame of a national research program on optimization of the internal combustion engines.

REFERENCES.

- Livengood, J.C., Wu, P.C., "Correlation of Autoignition Phenomenon in I.C.E. and Rapid Compression Machines," 5th Int. Combustion Symposium, pp.34, The Combustion Inst., 1955.
- Halstead, M.P., Kirsch, L.J., Quinn, C.P., "The Autoignition of Hydrocarbon Fuels at High Temperature and Pressure-Fitting of a Matematical Model," Combustion and Flame, Vol 30, pp. 45, 1977.
- Trumpy, D.R., "The pre-knock chinetics of Ethane in a Spark Ignition Engine," SAE Trans., vol 78, Paper No. 690518, 1969.
- By, A., Kempinski, B., Rife, J.M., "Knock in Spark Ignition," SAE Paper No. 810147, 1981.
- Douaud, A.M., Eyzat, P., "Four-Octane-Number Method for predicting the anti-Knock Behavior of Fuels and Engines," SAE Trans., Paper No. 780080, pp. 294, 1978.
- Lignola, P.G., Reverchon, E., Piro, R., 20th Symp. Int. on Combustion, Combustion Institute, Pittsburgh, pp. 123, 1984
- Hu, H., "The Autoignition of Hydrocarbon-Oxigen-Diluent Mixtures in a Constant Volume Bomb," Ph.D. Thesis, M.I.T., 1987.
- Belli, M., Danieli, G.A., Amelio, M., Bova, S., Fragiacomo, P., "A Detonation Model in Spark-Ignition Engines. Preliminary results on Engine Octane Requirement," SAE Paper 841332, 1984.
- Belli M., Florio G., Fragiacomo P., Danieli G.A.,"A
 Technique to Determine the Octane Requirement for a
 Spark Ignition I.C.E. using the 4 Octane Number Method
 Coupled to a Phenomenological Simulation Model,"
 Congress on Modelling on I.C.E., Valencia, 1987.
- Belli, M., Bova, S., Danieli, G.A., Fragiacomo, P., "Propirieta' Termodinamiche di Benzine, Miscele Benzine-Aria e Prodotti di Combustione," Univ. Calabria, Dip. di Meccanica, 1984.