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A PREDICTIVE MODEL FOR KNOCK ONSET IN SPARK-IGNITION ENGINES USING HYDROUS ETHANOL

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Abstract. *A model for knock prediction in the thermodynamic cycle simulation is vital for the development of spark-ignition engines. In this study, a knock model was implemented in a zero-dimensional simulation. The simulation was then calibrated with experimental data obtained from an engine fuelled with ethanol operating at stoichiometric condition. For each speed condition, two tests were performed. One in which the engine presented the knock occurrence and the other one in which the engine did not present the knock occurrence. The model was then calibrated to indicate both knock and no-knock conditions in an engine simulation operating in the same conditions. The results demonstrate that a calibrated knock model with experimental data gives an acceptable prediction of knock onset for several different conditions.*

Keywords:SI engines simulation, Knock prediction, Experimental test of engines.

1. INTRODUCTION

Knock consists in a rapid and violent combustion caused by auto-ignition of an air/fuel mixture inside the cylinder. The main causes of such abnormal type of combustion are the thermodynamic conditions of the air/fuel mixture summed to hot spots in the surface of cylinder or the non uniformities of the unburned gases (Ganestam (2010) and Konig and Sheppard (1990)). The herein called end-gas (air/mixture unburned during the combustion) is compressed by the expansion of burnt gasses while simultaneously heat is transferred to the end-gas, increasing pressure and temperature. Once the gasses undergo through certain thermodynamic conditions, it will auto-ignite after a period of time (Qi *et al.* (2015)), called delay of auto-ignition.

Depending on the severity of this spontaneous combustion, it will generate pressure waves that oscillates inside the cylinder, producing a characteristic sound (Boretti (2010)). Moderate knock increases vibration an noise that reduces engine durability while heavy knock will bring breakage of pistons rings, cylinder head erosion and will lead to engine failure (Tougri *et al.* (2017), Zhen *et al.* (2012) and Topinka (2003)).

Since knock is an undesired phenomena, it is avoided at all costs, from the project and design of the engine to its real-time operation. The effect of knock concern in the development of an engine reflects in the limitation of the compression ratio, with the objective to avoid an excessive compression of the air-fuel mixture, what would lead to knock. During the operation of the engine, the electronic control unit (ECU) is at all time monitoring the signal from a sensor to verify whether the engine is presenting knock. In a positive case, the ECU retards spark, reducing pressure in the combustion chamber. Also, the electronic control can enrich the air-fuel mixture, obtaining a shorter combustion and, thus, avoiding knock occurrence.

Once the strategies used to suppress knock are described, it is clear to perceive why it is stated in the literature that knock restrains efficiency improvement. One strategy is the compression ratio, which is directly linked to thermal efficiency. Higher values of compression ratio would provide a higher efficiency, however, the efficiency is limited by the maximum compression ratio established to avoid heavy knock. Another strategy is spark advance, which is related to torque generated. There is an optimum value that lead to the MBT (Maximum Brake Torque). If the engine cannot operate at MBT because of knock, the efficiency is sacrificed by the spark retarding. Also, there is the strategy of mixture enrichment, which is related to consumption. As the engine operates at normal condition with stoichiometric mixture, enrichment of the mixture increases fuel consumption and decreases efficiency.

Therefore, studies on knock are fundamental to predict in which conditions it will occur and how it would be possible to avoid it. Most times, the development of an internal combustion engine initiate with simulations on computer, implementing mathematical models. For knock, there are three forms of modelling:

- Detailed chemical kinetic mechanism for pre-flame reactions;
- Simplified chemical kinetic mechanism for pre-flame reactions;
- Phenomenological models based on Arrhenius expression.

The two first categories have a huge computational cost and becomes infeasible when applied to multi-variables and multi-objects optimization based on engine cycle simulation (Topinka (2003)). Phenomenological models typically use a one step reaction instead of detailed chemical kinetics, and auto-ignition delay is described as the Arrhenius equation. This is the method implemented in this study for the aforementioned reasons. The selected model allows the adjustment of its coefficients with experimental data.

2. COMPUTATIONAL MODEL

The Knock Integral Method Livengood and Wu (1955) was implemented in the work described herein. The use of this method in a thermodynamic simulation is justified by its simplicity and reliability which are based in the fact that it relies on basic calculation. Also, the parameters involved in the calculus process allow the adjustment with experimental data. When an air-fuel mixture is exposed to a level of pressure and temperature, it will take a certain amount of time to initiate the process of auto-ignition. This amount of time is called Delay of Auto-ignition (τ) and can be determined by the equation of Arrhenius:

$$\tau = f\left(ON\right) P^{-n} \exp\left(\frac{B}{T}\right) \tag{1}$$

in which n and B are empirical coefficients and $f\left(ON\right)$ is a constant defined as function of the Octane Number of the fuel adopted. As consequence, the knock is assumed to happen when the time of exposure t of the mixture at given Pressure P and Temperature T reaches the Delay of auto-ignition τ, i.e.:

$$t = \tau \tag{2}$$

or:

$$\frac{t}{\tau} = 1 \tag{3}$$

By the experiments carried out by Livengood and Wu, it was verified that a multiple stage compression between some levels of pressure and temperature would lead to conclusion that the auto-ignition occurs when:

$$\sum \frac{t_i}{\tau_i} = 1 \tag{4}$$

being i referred to one of the many thermodynamic states of the air-fuel mixture.

Extending this statement to a compression in which pressure and temperature level are varying constantly, which is the case that occurs in internal combustion engines, the condition for auto-ignition is:

$$\int \frac{dt}{\tau} = 1 \tag{5}$$

Note that the properties are related to conditions at the air-fuel mixture during compression and combustion, starting from the beginning of the compression, i.e., when the intake valve closes, to the fully consumption of the end-gas (portion of the gasses in the cylinder that were not burnt yet), at the end of the combustion. Therefore, it is fundamental to determine pressure and temperature of the end-gas, task that requires the implementation of a two-zone model simulation. This type of simulation ignores geometrical influence of the engine in the charge motion, considering a homogeneous charge and thus, its procedure consists in solving the differential equations that are given by the laws of energy conservation and the state equations.

In the developed two-zone model, the flame front is considered to be adiabatic and impermeable, dividing the end-gas and the burnt gas in two zones. During the process of combustion, both zones are at the same pressure P, since the burnt gas is assumed to be in mechanical equilibrium with the end-gas, while each zone has its temperature. For the end-gas, the energy conservation is given by:

$$\frac{dU_{eg}}{d\theta} = \delta Q_{eg} - \delta W_{eg} + h_{eg}\frac{dm_{eg}}{d\theta} \tag{6}$$

According to Zacharias (1967), the assumption of ideal gas is reasonable to be applied in internal combustion engine simulation. As result, the internal energy U can be determined as function of the temperature:

$$\frac{dU_{eg}}{d\theta} = f\left(\frac{dT_{eg}}{d\theta}\right) \tag{7}$$

The heat transfer term δQ_{eg} is given by the heat lost through cylinders wall by convection:

$$\delta Q_{eg} = \frac{hA\left(T_w - T_{eg}\right)}{\omega} \tag{8}$$

in which T_w is the temperature of the cylinder's wall, assumed to be constant. A represents the instantaneous area of the end-gas zone and h is the heat transfer coefficient, determined by a semi-empirical correlation, proposed by Hohenberg (1979). The factor ω is the angular velocity of the engine, which converts the heat transfer rate from time domain to crank position domain.

The term related to work is given by δW_{eg}. The only form of energy transfer through work interaction is the compression/expansion of boundaries, thus:

$$\delta W_{eg} = P\frac{dV_{eg}}{d\theta} \tag{9}$$

The burning effect is modelled by $h_{eg}\frac{dm_{eg}}{d\theta}$, assuming that the combustion can be interpreted as a mass transfer, associated with an upstream enthalpy.

Similarly, the same conservation equation is applied to the burnt-gas, leading to:

$$\frac{dU_{bg}}{d\theta} = \frac{dH_c}{d\theta} + \delta Q_{bg} - \delta W_{bg} + h_{eg}\frac{dm_{bg}}{d\theta} \tag{10}$$

Again, the ideal gas hypothesis is assumed:

$$\frac{dU_{bg}}{d\theta} = f\left(\frac{dT_{bg}}{d\theta}\right) \tag{11}$$

The heat transfer is given by:

$$\delta Q_{bg} = \frac{hA\left(T_w - T_{bg}\right)}{\omega} \tag{12}$$

and the work done by the system:

$$\delta W_{bg} = P\frac{dV_{bg}}{d\theta} \tag{13}$$

The energy released by the combustion is presented in the term $\frac{dH_c}{d\theta}$ and can be determined by:

$$\frac{dH_c}{d\theta} = \eta_{comb} m_{fuel} \Delta H_c \frac{dX}{d\theta} \tag{14}$$

in which m_{fuel} is the amount of fuel admitted, ΔH_c is the enthalpy of combustion and η_{comb} is the efficiency of combustion, given as a function of the stoichiometry of the air-fuel mixture. The fraction of burnt mass is given by Wiebe's function:

$$X = 1 - \exp\left[\ln\left(1-\eta\right)\left(\frac{\theta-\theta_0}{\Delta\theta}\right)^{m+1}\right] \tag{15}$$

in which θ_0 corresponds to the start of combustion, η is the maximum fraction of burnt fuel, and m is the form factor, assumed to be 2 according to Heywood (1988). The Duration of combustion $\Delta\theta$ was determined experimentally, as explained in the next section "EXPERIMENTAL PROCEDURES".

With the presented equations, the hypothesis of ideal gas and the volume balance in the cylinder:

$$\frac{dV}{d\theta} = \frac{dV_{bg}}{d\theta} + \frac{dV_{eg}}{d\theta} \tag{16}$$

it is possible to solve for T_{bg}, P and T_{eg} using a Runge-Kutta method for differential equations. With T_{eg} and P it is calculated the delay of auto-ignition τ for each instant dt, allowing to evaluate the knock criteria, given by relations (1) and (5), respectively.

3. EXPERIMENTAL PROCEDURES

Experimental tests were conducted in order to provide information on knock occurrence. Summarizing, the experimental data indicates which conditions the engine will present knock. A dynamometer was used to brake and keep the engine at constant speed. For each speed of operation, the throttle was set to wide open throttle (WOT) position. The spark advance was initially determined by the original calibration of the ECU and the data related to the non-knock condition were acquired. Then, the ECU was set to manual and the spark advance values were overwritten for a more advanced spark value in order to force knock occurrence. After stabilization, data referred to knock condition were acquired. For each condition, it was obtained the average data for 300 cycles.

Other parameters measured in the test rig were used as input for the simulation model and consists in: Intake manifold pressure, exhaust manifold pressure and temperature, combustion duration, spark advance, and ambient conditions (relative humidity and atmospheric pressure). Besides the cited information, it is necessary to know the engine characteristics, such as geometry and valve synchronism.

3.1 Experimental set-up

The experiments were executed at IMT (Instituto Mauá de Tecnologia) facilities. The characteristics of the engine tested are given in Table 1:

Table 1. Engine technical data

Variable	Value
Displacement	1200 cm^3
Number of cylinders	3 in line
Cylinder diameter	75 mm
Stroke	90.473 mm
Compression Ratio	12.25:1

The engine tested was a flexfuel port fuel injection (PFI) engine. Hydrous Ethanol with 5% of water in volume, commonly known as E95h, was used as fuel in the tests. The Research Octane Number (RON) of this fuel was calculated as 109. The conditions in which data was generated vary from 1000 rpm to 3000 rpm, going from 1000 to 2000 rpm in steps of 100 rpm and from 2000 to 3000 rpm in steps of 200 rpm. At all conditions, the air/fuel ratio was kept at the stoichiometric condition.

3.2 Knock condition

It is necessary to stablish a criteria to determine whether the engine is at knock condition. At low speed, it is possible to verify the knock occurrence by its characteristic sound. However, this method is not reliable and it is imprecise for medium speed operation. In-cylinder pressure can indicate the phenomenon due to an observed oscillation of pressure that occurs after the peak of pressure, consequence of the knock. To quantify this oscillation, the Analysis software applies a low-pass filter, eliminating high frequency noise. Afterwards, a high-pass filter is applied to eliminate the pressure profile of the combustion. The remaining signal is composed basically by the pressure oscillation caused by knock. By measuring the amplitude of this oscillation it is possible to stablish a limit value to consider when the engine is at knock condition. The adopted criteria was an amplitude of 2.5 bar.

3.3 Combustion duration

Another fundamental parameter for knock modelling is the combustion duration. Since the auto-ignition is strongly dependant of the time in which the end-gas is submitted to high pressure and temperature conditions, slower combustion would favour the knock occurrence while faster combustion would minimize knock occurrence. Thus, to obtain reliable results in the simulation, it is necessary to determine the combustion duration in each case tested.

With the available pressure data, it is possible to generate the Apparent Rate of Heat Release profiles during the cycle. The combustion duration consists in the measured time between the start and the end of the Heat Release, which are approximately the beginning and end of the combustion, respectively.

4. RESULTS AND DISCUSSION

For each experimentally tested condition, it was performed a simulation. In the simulation, the value of the integral (see Eq. 5) was calculated. So it was expected that for the condition in which it was observed knock, the value of the integral would be greater than 1. Otherwise, when it was not observed knock in the experimental test, the value of the integral calculated in the simulation would be expected to be less than 1.

By performing an adjustment *ad hoc*, starting from the values proposed by Douaud and Eyzat (1978), it was found that the following values fit the experimental data:

$$\tau = 17.13 \left(\frac{ON}{100}\right)^{3.402} P^{-1.7} \exp\left(\frac{3400}{T}\right) \tag{17}$$

being ON the RON of the fuel.

With the calibrated Delay of Auto-ignition equation (17), the results obtained are shown in Figures 1 and 2:

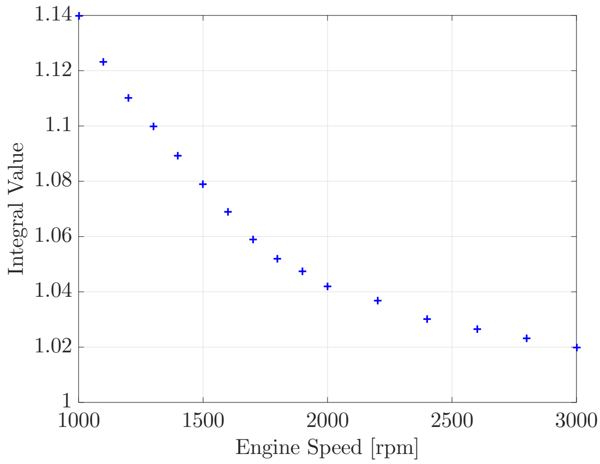

Figure 1. Value of the integral simulated for knock condition.

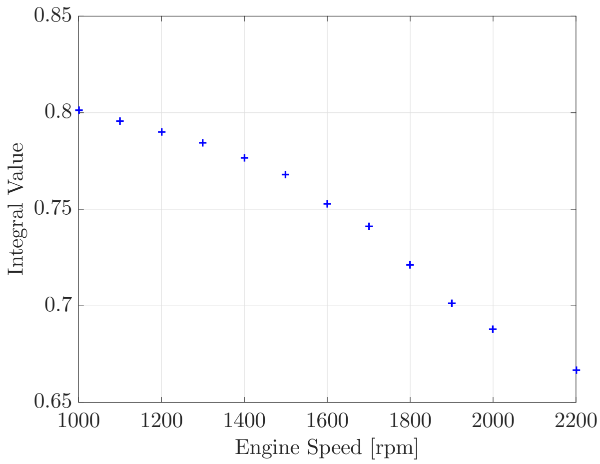

Figure 2. Value of the integral simulated for no knock condition.

Note that for the knock condition, presented in Figure 1, the integral resulted in values above 1 for all conditions of speed. On the other hand, for the no knock condition, presented in Figure 2, the value of the integral reached values less than 1, as expected.

5. CONCLUSIONS

This work has presented a calibrated model for prediction of knock occurrence in simulation of Spark ignition engines fuelled with ethanol. The chosen model implemented in zero-dimensional simulation is convenient because requires low computational cost and permits all the model parameters to be adjusted with experimental data. The method is performed by integrating the ratio between time and delay of autoignition of the end-gas until the end of combustion. Whenever the final value of the integral reaches 1, it means that the engine will present knock at those conditions.

With the objective of calibrating the model, simulated data was compared to experimental data. The conditions was going from a speed of 1000 rpm to 3000 rpm with a stoichiometric air/fuel proportion. For each condition, the spark advance was increased until the engine start presenting knock. The model was then successfully calibrated to indicate knock in the simulation with the same experimental conditions. For other conditions in which it was observed knock in experimental test, the simulation also presented values greater than 1 while for conditions in which it was not observed knock, the values were less than 1. Besides those results, it was observed a decrease in the value of the integral for higher speed. However, as the amplitude of the pressure oscillation caused by knock was kept constant during the tests, it was expected to obtain a constant value for the integral calculation in the same condition. Thus, we suggest that a better adjustment should include the effects of engine speed.

Further work aims the inclusion of speed on the correlation. Also, the verification of this model for other conditions of air/fuel ratio, considering lean/rich mixtures. Other types of fuel can also be analysed and define the influence of the mixture ethanol-gasoline on the correlation.

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