Qualitative Analysis of a Knocking Prediction Model for Internal Combustion Engine Using Single-Zone Methodology

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ABSTRACT

The use of biofuels as alternatives to fossil fuels has been used because they are renewable energy sources. In Brazil, in particular, the use of ethanol is already widespread, but the maximum potential of this fuel is not extracted. The internal combustion engines used in the national territory adopt strategies that allow the consumer to choose between the ethanol or gasoline or a mixture of them, which limits the value of the engine compression ratio. However, the evaluation of the feasibility of developing combustion engines that use only ethanol as a fuel is very expensive to be carried out only with experimental tests, so it is convenient to use numerical methods in this task. Therefore, it is necessary that in the numerical methods used there are models for predicting the knocking phenomenon. The present work proposes to make a qualitative analysis of a knocking model used in conjunction with a single-zone type code. The study aim to evaluate if the behavior of the model phenomenon is compatible with the concepts found in the literature. These models were implemented in an in-house developed computer program that is able to simulate piston engine performance.

NOMENCLATURE

A	Calibration factor of the Single-Zone Knocking prediction method
B	Calibration factor of the Single-Zone Knocking prediction method
C_0	Constant of the Single-Zone Knocking prediction method
K_A	First coefficient of the Arrhenius formula
K_B	Second coefficient of the Arrhenius formula
K_C	Third coefficient of the Arrhenius formula
KIM	Knocking Integral Method
N	Rotational Speed
ON	Octane Number
P	Pressure
T	Temperature
T_{EQ}	Function of the Octane Number
X	Function of the Octane Number
n	Calibration factor of the Single-Zone Knocking prediction method
t	Time
β	Calibration factor of the Single-Zone Knocking prediction method
ε	Ignition time delay to the KIM method
κ_{PRESS}	Function of the Octane Number
μ	Constant of the Single-Zone Knocking prediction method
σ	Constant of the Single-Zone Knocking prediction method
τ	Auto-ignition delay time
ϕ	Equivalence ratio
ω	Function of the Octane Number

subscripts

1	Referent to the pre cool flame appearance
2	Referent to the ignition delay
CF	Referent to the cool flame appearance
IVC	Referent to the Intake Valve Close
end	Referent to the end of the combustion
i	Referent to the initial conditions
h	Referent to the cool flame time appearance

INTRODUCTION

Over the years, the simulation of internal combustion engines started to become increasingly important during the design and/or calibration process of these thermal machines. Today, it is a step that the automakers use to reduce the number of hours of experimental tests, which can also represent an economy of fiscal resources [1].

These simulations can be carried out using different types of numerical models, each of which will have advantages and disadvantages; however, for the interests of the automotive industry, it is extremely important that these models are able to provide results regarding operational characteristics in addition to the performance of these thermal machines. In the current scenario, one of the main characteristics that should be possible to be analyzed with these tools are the problems related to pollutant emissions, which is directly related to the type of fuel that will be used as an energy source [2].

Naturally, issues related to emissions will reflect on different alternatives that have emerged in recent years, with the intention of reducing the amount of agents that cause climate change, produced, in part, by vehicles. An alternative has been the insertion of electric and hybrid vehicles, which has been stimulated in different countries [3], but this measure has several problems related to the lack of knowledge about the real environmental impacts [4], or even due to economic problems related to fleet changes, indicated by different authors [5 - 7]. Another alternative that can be adopted is related to the use of biofuels to replace fossil fuels. In Brazil, this alternative seems more interesting, due to the actual experience of the current market with fuel, which has been used as an energy source since 1978 [8].

Even with these alternatives, however, it is necessary to be able to predict, with some level of precision, what will be the environmental impacts and what will be the benefits related to each one, and the result of these simulations will depend on the type of strategy chosen and the adopted model. Regarding the biofuel alternative, power generation is still carried out by an internal combustion engine. In this case, the model used to determining the thermodynamic parameters, as well as the submodels used to calculate the other parameters of interest, will have a great impact on the results.

The choice of these models and submodels have influence in the calculated parameters and, consecutively, how other properties will be calculated. For example, the models used to determine thermodynamic properties in a cycle of an internal combustion engine, can be of the Single-Zone, Multi-Zone or Multi-Dimensional type [9]. One of the main differences between the Single-Zone models for the others is the fact that there is no stratification of the thermodynamic properties, such as pressure and temperature, with no distinction of these properties for the burned and unburned mass present within the cylinder. These characteristics make the submodels used to predict the occurrence or not of Knocking, have different approaches [10]. Like Knocking, other characteristics of interest, such as the way in which the emissions of these thermal machines are calculated will be different for each of these models, with some using models based on chemical equilibrium and others using more complex methods, such as the use of chemical mechanisms [11].

It is notable that the current demands of the market, with the increase in new policies and the development of new strategies in Brazil, include the strengthening of the biofuels use, a fact that is proven due to successive increases in the percentage of ethanol in gasoline [12]. From this information, and knowing the application of the numerical models in the development process of internal combustion engines, it is necessary that the models used are able to predict, with relative precision, phenomena that have impact on the energy use of these new fuels. Among these phenomena, it can be mentioned the Knocking, which is perhaps the biggest power generated limiter in a spark ignition engine [13], and which is directly related to the fuel used.

In this work, an analysis will be made of a knocking prediction and a single-zone models for spark ignition internal combustion engines using numerical simulation. This approach becomes relevant, especially when the computational resources are limited, considering that, single-zone models have a lower computational cost, in addition to being relatively easier to implement [14].

INTERNAL COMBUSTION ENGINES MODELS

The classification of the models used for the simulation of internal combustion engines may vary from one literature to another, so that it is possible to adopt a certain division between the types of the models. In this work, as previously mentioned, the models are classified as Single-Zone, Multi-Zone and Multi-Dimensional, and each of them will be better explained in the following paragraphs.

The Single-Zone models are characterized by the fact that the only independent variable in their formulation is time [9]. Therefore, the thermodynamic properties, such as pressure and temperature, and the chemical composition, are always the same for any point of the cylinder where the analysis is being developed [15]. These models generally determine the rate of fuel consumption through an empirical relationship, such as a cosine function or the Wiebe curve [16]. One of the major disadvantages in the use of these empirical functions is the fact that some parameters related to combustion must be defined, such as the interval of combustion duration, and for that, it may be necessary to use the literature to find ways for these parameters to be determined.

One of the great advantages of Single-Zone models, however, is thelow computational cost required, in addition to the fact that it is relatively easy to implement. These models have great limitations, since there is no distinction of properties between the burned and unburned mass.

In the case of Multi-Zone models, the volume of the cylinder is divided into multiple regions, so that each of these regions maintain energy interactions with the others, so it is possible to determine the exchange of heat and mass between adjacent regions [17]. However, each of these regions has homogeneous properties; so that the stratification will be as sensitive as the number of regions discriminated in the model. Figure 1 is a representation of a division in a Multi-Zone model.

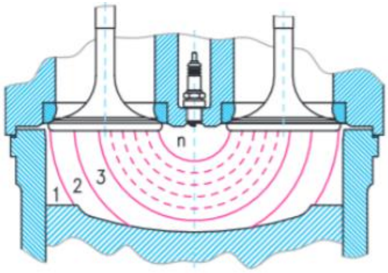

FIGURE 1. Representation of a Multi-Zone model [18].

The fact that each of these regions has its own properties represents a significant advantage, as it allows the use of more complex models to determine some important parameters. Citing as an example, the combustion process, in the case of a Multi-Zone model it is possible to use submodels, where the flame front propagation speed is calculated at each moment, so that it is no longer necessary to determine the combustion duration before starting the cycle calculation. Several studies use this strategy to model combustion [19, 20].

Among the Multi-Zone models, there is a particular class of these models, which are called Quasi-Dimensional. These are classified in this way because there is a division of the cylinder into two regions, one intended for the burned mass and other for the unburned mass, with a difference in thermodynamic properties and chemical composition between these two regions; however, this differentiation in two regions is made only during the combustion event [9]. During this event, the flame propagates as a spherical cap shape, which expands throughout the cylinder region, until there is no more fresh mass to be oxidized. The fact that, there is discrimination between regions, does not prevent combustion from being analyzed by an empirical formulation, as in the Single-Zone models, but it already allows using more complex approaches for this event.

Finally, the Multi-Dimensional models are models where, as in the Multi-Zone models, the cylinder is also divided into different regions, however, these have more than one physical dimension. Generally, these models are not used to determine the performance parameters of the internal combustion engine, since the computational cost associated with these simulations is extremely high [21]. These types of models are used in specific studies, such as the movement of the air mass that passes through the intake valve.

KNOCKING

Knocking is a combustion anomaly found in spark-ignition internal combustion engines. This is an unwanted phenomenon that can cause the engine damage if not quickly controlled. However, it is necessary to understand some other aspects of the operation of combustion engines in order to understand how this anomaly appears.

In a spark-ignition internal combustion engine, as the name implies, combustion will start at the moment in which a spark is provided, this moment is called the ignition point.

The ignition point can be seen as the beginning of the first of the three phases that make up the combustion event in a spark ignition engine. This first phase is characterized by the development of a first core, which will start the combustion. The second phase is defined as occurring during the spread of the flame, until it meets the cylinder wall. This spread is proportional to the turbulence intensity within the cylinder [22].

Naturally, there will be criteria that must be respected in order to define the best time for this spark to be provided. This parameter is perhaps one of the most important in the operation of the engine, as it will strongly influence the performance parameters of the thermal engine, so this choice must be made carefully.

As the advance of the ignition point increases, the point where the maximum pressure of the cycle occurs changes, also changing the module of this maximum pressure. It is extremely important that this peak pressure be positioned after the Top Dead Center (TDC), in order to maximize the work produced during the cycle expansion event. However, it should be noted that not only the expansion work will be increased by increasing the ignition advance, but also the compression work, which is undesirable, so that there must be an optimum point where it is possible to maximize the work produced. Figure 2 shows a representation of the ignition point influence on an internal combustion engine.

Note that as the ignition advance increases, the maximum pressure reached during the cycle increases, and this characterizes a more severe pressure and temperature condition inside the combustion chamber. These more severe conditions will favor the knocking phenomenon.

This phenomenon can be explained as follows. With the start of the combustion event, and consecutively with the increase in pressure and temperature inside the cylinder, the mass of air-fuel mixture that has not yet been reached by the flame front, will also begin to experience these new thermodynamic conditions. As these conditions become more and more severe, different points inside the cylinder, in the region of the unburned mass, can start the oxidation process of this mass, that is combustion. Each of these points can be seen as a nucleus, similar to that generated by the spark, and starts other combustion process. Just like the nucleus generated by the spark, from these other different nucleus inside the cylinder, the propagation of a flame front will start, and at a certain moment these different flame fronts met, causing an oscillation in the pressure inside the cylinder, which is the characteristic of the knocking phenomenon. This type of pressure oscillation check can be done experimentally through the use of accelerometers.

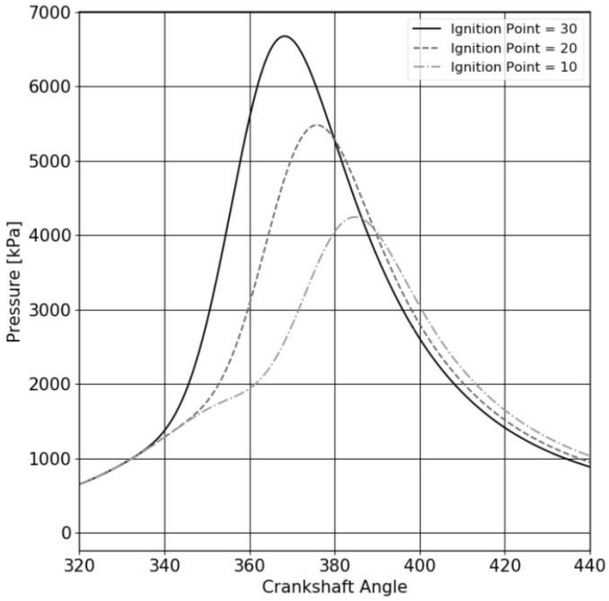

FIGURE 2. Ignition point effect under the indicated pressure.

This characteristic of the Knocking phenomenon is shown in Figure 3 [16]. As shown in Figure 3, the pressure oscillation will be more intense the more severe the pressure and temperature conditions in the cylinder.

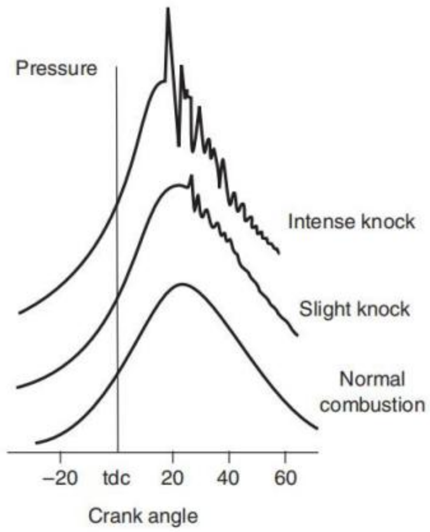

FIGURE 3. Pressure profiles for knocking conditions [16].

DIFFERENT KNOCKING METHODS

The methods to predict the Knocking phenomenon are different depending on the type of model used to determine the thermodynamic cycle.

Initially, considering the Multi-Zone models, a method widely used in scientific studies, known as Knock Integral Method (KIM). In this method, the calculation of the auto ignition delay (ε) can be done using an Arrhenius equation, which was developed through a series of experimental tests and is presented in Equation (1).

$$\varepsilon = K_A \cdot \left(\frac{ON}{100} \right) \cdot P^{-K_B} \cdot e^{\frac{K_C}{T}} \qquad (1)$$

The K coefficients of Equation (1) can be obtained from different literature [23 - 26].

The method consists of a manipulation and subsequent integration of Equation (1), between the intake valve closing (IVC) until the moment that all the fresh mass inside the cylinder is oxidized. Equation (2) presents the result obtained for this integration. Therefore, the behavior of the unburned mass inside the cylinder between this interval is monitored and the result of this integration is calculated. The method then assumes that, if the value of this integral is greater than one, then knocking occurs in the cycle.

$$KIM = \int_{t_{IVC}}^{t_{end}} \left(\frac{1}{\varepsilon} \right)_{P,T} \frac{dt}{N} \qquad (2)$$

Despite being very applicable in the scientific community, the methods that calculate the auto ignition delay using an Arrhenius equation need to know the thermodynamic properties of the unburned mass separated from the burnt mass, which makes its application not possible in Single-Zone models.

This work, however, will analyze the method proposed by Yates and Viljoen [27], which was later refined by Yates et al. [28], so that it is possible to determine the occurrence of Knocking in internal combustion engine simulations using Single-Zone models.

In the case of the method discussed in Yates and Viljoen [27] and Yates et al. [28], the only parameter that is obtained as a result is the ignition delay time, t_2, which indicates a minimum time where the combustion engine must remain in that given thermodynamic condition in order for the knocking occur. The internal combustion engines are thermal machines that operate in a continuous regime, so it is not real to think about a constant temperature and pressure condition, so that this isolated parameter does not provide enough information to determine the occurrence or not of knocking. It is necessary to have experimental data from some combustion engines, so that it is possible to determine what would be the minimum ignition delay in which, if this limit is exceeded, knocking will occur. An approach similar to that described can be found in Tougri et al. [29].

By the method described in Yates and Viljoen [27] and Yate et al. [28], the ignition delay is calculated using Equation (3).

$$t_2 = t_1 + \tau_{h,CF}\left(1 - \frac{t_1}{\tau_{h,i}}\right) \quad (3)$$

Since times t_1, $\tau_{h,CF}$ and $\tau_{h,i}$, are calculated using Equations (4), (5) and (6) respectively.

$$t_1 = \phi^{\beta_1} \cdot A_1 \cdot P^{n_1} \cdot e^{\frac{B_1}{T}} \quad (4)$$

$$\tau_{h,i} = \phi^{\beta_h} \cdot A_h \cdot P_i^{n_h} \cdot e^{\frac{B_h}{T_i}} \quad (5)$$

$$\tau_{h,CF} = \phi^{\beta_h} \cdot A_h \cdot P_{CF}^{n_h} \cdot e^{\frac{B_h}{T_i + X \cdot \Delta T_{CF}}} \quad (6)$$

And the T_{CF} and ΔT_{CF} values, are calculated by Equations (7) and (8) respectively.

$$T_{CF} = T_i + 0.5 \cdot \left(X \cdot \Delta T_{CF} + \sqrt{(X \cdot \Delta T_{CF})^2 + C_0} \right) \quad (7)$$

$$\Delta T_{CF} = \omega \cdot \left(T_i - T_{EQ} \cdot P^{\kappa_{PRESS}} \cdot \phi^{\mu} \cdot \left(\frac{100}{99 + \phi} \right)^{\sigma} \right) \quad (8)$$

RESULTS

The results presented in this work were obtained through a Single-Zone computational model, developed by the lead author of this article, within the Turbomachinery Department of the Aeronautics Institute of Technology.

The simulations performed were developed using the following parameters with input data for the computational model: bore of 8.6 cm, stroke of 6.7 cm, compression ratio of 9.2, and fueled with E100. As the analyzes made are only qualitative, in order to analyze the behavior of the detonation prediction method used, these geometric data, and the fuel used, have little relevance, however, they are provided to guarantee the reproducibility of the results. The values used for each of the parameters of the knocking models can be consulted in Yates and Viljoen [27] and Yates et al. [28]

The analyzes presented in this work were elaborated to observe the behavior of the detonation method used, considering those that are the situations that most influence this combustion anomaly. These situations are: variation of the ignition point; variation of the compression ratio; variation of the equivalence ratio; variation of the intake manifold pressure; and variation of the rotational speed. In each analysis, only the parameter studied was varied, while the others were kept constant.

VARIATION OF THE IGNITION POINT – Figures 4 and 5 show the results obtained for this analysis.

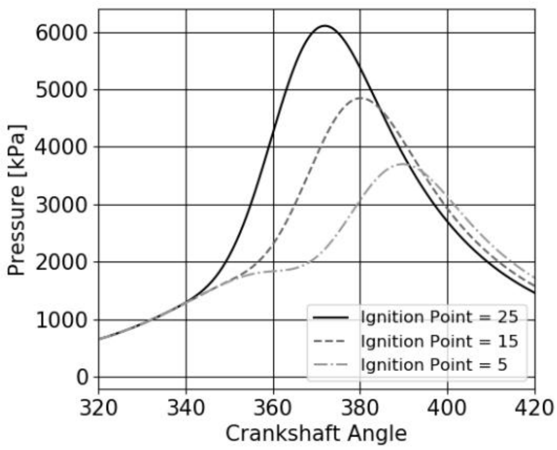

FIGURE 4. Effects of the ignition point variation on the indicated pressure.

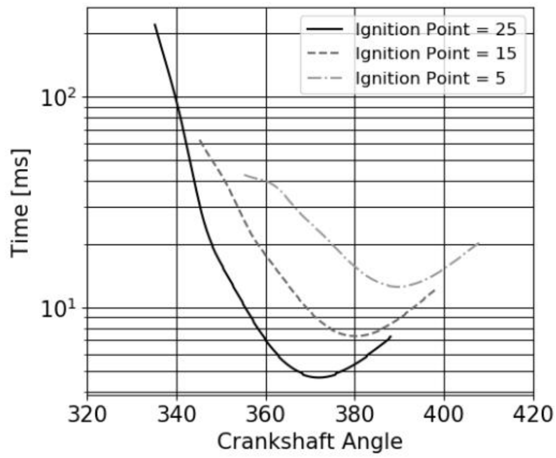

FIGURE 5. Effects of the ignition point variation on the Ignition Time Delay.

As can be seen in Figure 4, as the advance ignition increases, the pressure of the indicated cycle also increases, therefore characterizing a more severe thermodynamic condition. Figure 5 shows that, the minimum ignition delay time is shorter for situations where the thermodynamic condition found was more severe. This result is in fact the expected, since a shorter ignition delay time shows that the occurrence of Knocking was favored.

VARIATION OF THE COMPRESSION RATIO – Figures 6 and 7 show the results obtained for this analysis.

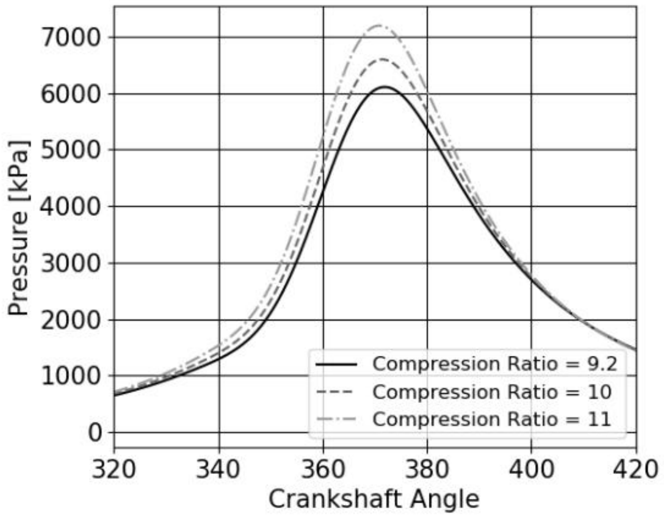

FIGURE 6. Effects of the Compression Ratio variation on the indicated pressure.

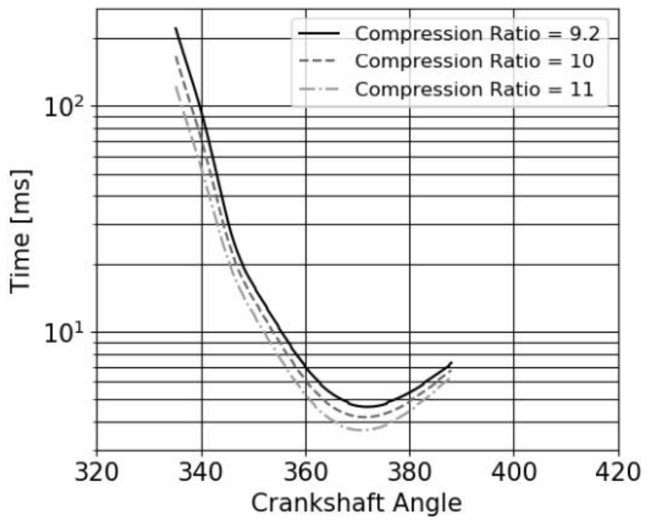

FIGURE 7. Effects of the Compression Ratio variation on the Ignition Time Delay.

Similar to what occurs for the variation of the ignition point, it can be seen from Figure 6 that, by increasing the compression ratio, the severity of the thermodynamic conditions in the cylinder is also increased. This result is expected by the knowledge about this parameter. Naturally, with this increase in the severity of temperature and pressure conditions, the minimum ignition delay time found becomes smaller and smaller, favoring the conditions of occurrence of Knocking. This result also corroborates what is found in the literature.

VARIATION OF THE EQUIVALENCE RATIO – Figures 8 and 9 show the results obtained for this analysis.

The variation of the equivalence ratio up to a certain value, causes the pressure and temperature conditions to become more and more severe, however, after a certain value of this parameter, the behavior is the opposite. This is confirmed by observing Figure 8, as the maximum pressure reached in the cycle for ϕ=1.3 is less than that experienced for a condition with ϕ=1.1. Part of this is due to the fact that, there is a combustion efficiency associated with changing the equivalence ratio [30]. However, it is noted that even with less severe conditions of temperature and pressure, the tendency for Knocking to occur increased with the increase in the equivalence ratio, when it changed from ϕ=1.1 to ϕ=1.3. This is because there is an influence of the equivalence ratio on the flame front speed, and this is accounted for in the calculation of the ignition delay time. Therefore, the presented trend is correct, however, there must be a limit where this behavior will change, since another important property that should be considered is the flammability limit of the mixture.

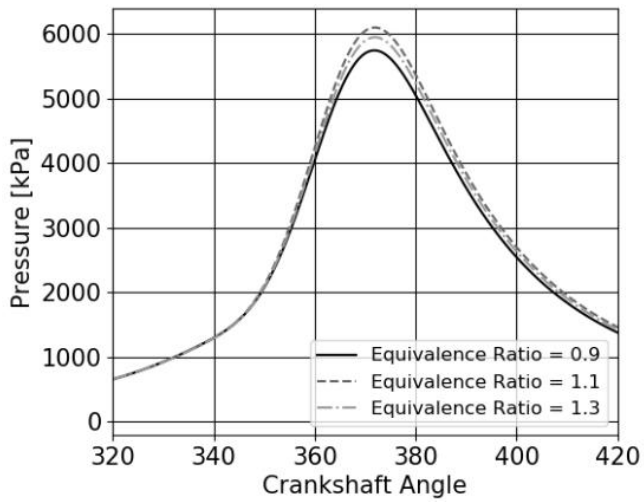

FIGURE 8. Effects of the Equivalence Ratio variation on the indicated pressure.

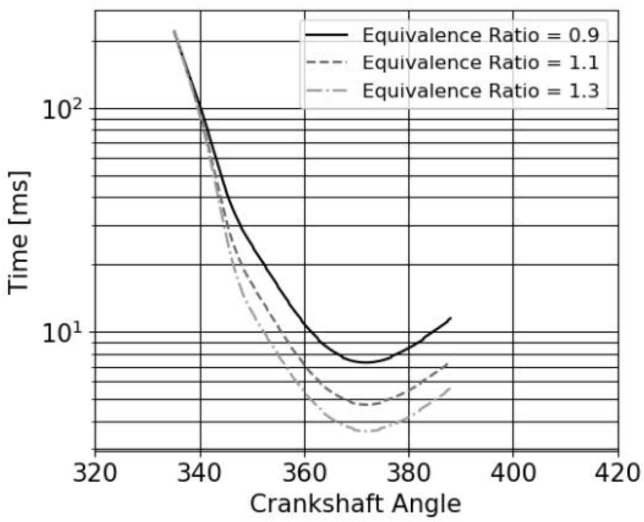

FIGURE 9. Effects of the Equivalente Ratio variation on the Ignition Time Delay.

VARIATION OF THE INTAKE MANIFOLD PRESSURE – Figures 10 and 11 show the results obtained for this analysis.

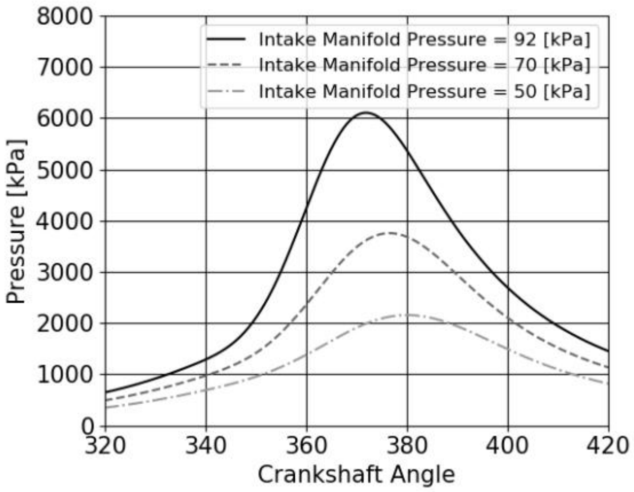

FIGURE 10. Effects of the Intake Manifold Pressure variation on the indicated pressure.

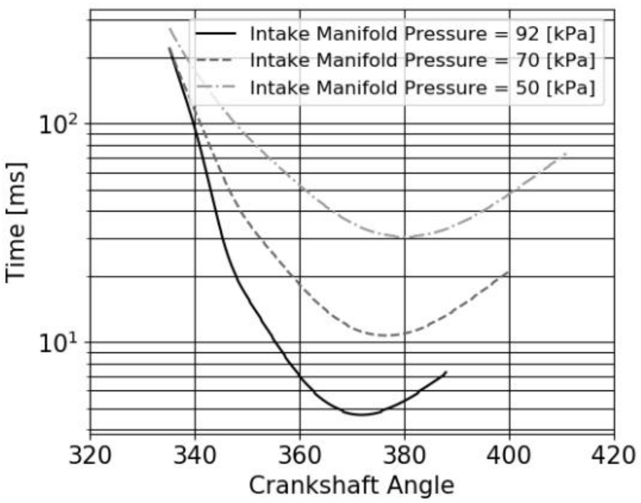

FIGURE 11. Effects of the Intake Manifold Pressure variation on the Ignition Time Delay.

Similar to what was demonstrated in the analysis involving the variation of the ignition point and the compression ratio, it is noted that with the variation of the intake manifold pressure, shown in Figure 10, the thermodynamic conditions are more severe as higher this parameter is, and therefore, the ignition delay is shorter.

VARIATION OF THE ROTATIONAL SPEED – Figures 12 and 13 show the results obtained for this analysis.

In the results presented in Figure 12 it is noted that, there is a small difference between the thermodynamic conditions experienced by the engine with the increase in the rotational speed. This difference is also seen in the results of the ignition delay in Figure 13. However, it is possible to notice that these differences are very small. The influence of the rotational speed should be greater, due to the experience using other simulation tools, such as the Diesel-RK® software, a Russian tool that has a free version for academic use [31].

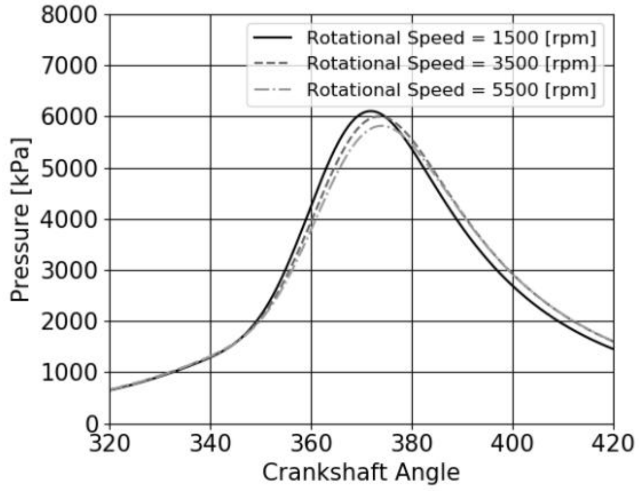

FIGURE 12. Effects of the Rotational Speed variation on the indicated pressure.

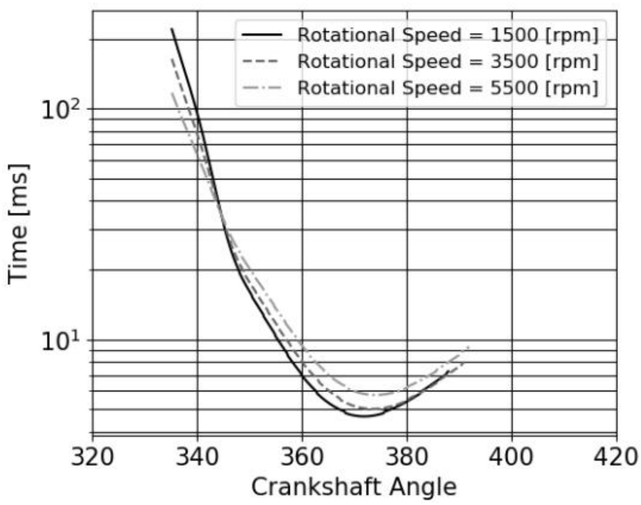

FIGURE 13. Effects of the Rotational Speed variation on the Ignition Time Delay.

CONCLUSIONS

From the simulation results obtained it can be noted that, the knocking prediction method studied has a behavior compatible with the concepts presented in the literature. It also seems to be compatible with the methods used in other software, as Diesel-RK® as a reference.

The method, however, has some limitations. One of them is the need to have experimental data where knocking occurs, in order to determine the minimum ignition delay required to foresee the occurrence of this anomaly. This information is not always available, so it will be necessary to develop another strategy to define this minimum value. Other methods, such as the *KIM* method, use other ways to determine this occurrence, which will not necessarily require experimental data to be available.

Despite this limitation, the method has as one of its main advantages, the fact that it is relatively easy to be implemented, since it is built, basically through empirical correlations that are applied directly. In addition, the low computational cost is also a major attraction for the method.

In general, the method seems to have the potential to be applied in some analysis of internal combustion engines, providing an indication of the occurrence of knocking. However, it is necessary for the user to have a reference value for the ignition delay, as this is the only output parameter of the method.

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