Prediction of Self-Ignition Delay of Different Liquid Diesel Fuels

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ABSTRACT

The determination of autoignition delay of hydrocarbon fuels is of invaluable interest, as this value defines the pressure increase in the premixed flame in diesel engine combustion. Based on experimental analysis, a simple correlation law enabling prediction of autoignition delay is proposed in this study. Among the different formulations used to model this delay (1-2), the relationship chosen here is based on the Wolfer's law (1). In its initial formulation, this law can only be applied to a given diesel fuel. The proposed correlation law is applicable to all fuels on the condition that their cetane number is known. The relationship, determined through experiments performed in a constant volume combustion chamber, in which ten different hydrocarbon fuels were tested, gives very satisfying results, for an injection pressure of about 230 bar in the ranges of chamber pressure from 15 to 40 bar and gas temperature from 570 to 770 K.

INTRODUCTION

The autoignition of hydrocarbon fuels is an essential parameter in diesel engine combustion. It plays an important role concerning the level of kinetic reaction rate of pollutants because it defines the maximum temperature reached in the first stage of combustion. Therefore, the ignition delay prediction is of particular interest. In order to model this delay, it is necessary to know its dependence on the gas physical and chemical characteristics on one hand, and on the fuel's chemical composition on the other. The Wolfer's law has often been used in previous studies (1-10) to model the delay. This law only offers limited interest in its initial form as it is only useful for a given fuel. The objective of this study is to determine, from experimental results obtained in a constant volume combustion chamber, a general law enabling prediction of the autoignition delay of a diesel fuel as a function of its chemical composition and the experimental conditions. This law both generalizes and enhances Wolfer's law (1).

EXPERIMENTAL APPARATUS

The experimental apparatus consists of a constant volume, cylindrical combustion chamber equipped with two diametrically opposed Pyrex windows, which allow optical diagnostics (Fig. 1). The combustion chamber is filled with air from an accumulator and it is preheated (up to 500 °C) by electrical resistance heaters imbedded in the walls. A single-shot injection pump supplies the fuel by a one-hole injector. The injection pressure and the needle lift signal are measured in order to determine the injection conditions. Temperature and pressure in the bomb are measured respectively with a thermocouple probe and a piezoelectric transducer. This transducer and the injector are cooled by circulating water.
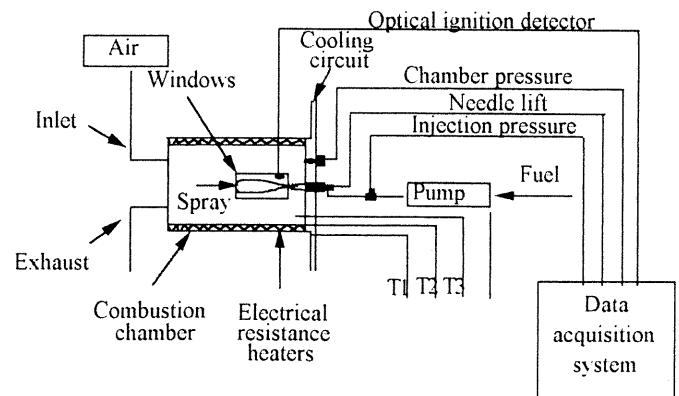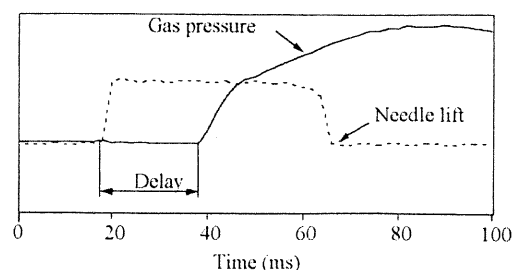

Fig. 1 Experimental apparatus

Fig. 2 Determination of autoignition delay

The experimental apparatus enables the measurement of the ignition delay of different hydrocarbon fuels at high temperature and pressure. The ignition delay is the period from the start of injection to the time at which ignition is detected.

If the start of injection is easily detected by the needle lift signal, it is more difficult to determine the start of combustion and various concepts have been used in previous works (pressure rise delay, luminous delay ...). In this work, the start of combustion is defined as the instant where the gas pressure recovers its initial value before injection, after its decrease due to droplet evaporation (Fig. 2).

EXPERIMENTAL RESULTS ·

In order to determine the influence of fuel characteristics on ignition delay, the experimental study has been carried out with different hydrocarbon fuels, for various gas temperatures and pressures in a constant volume combustion chamber. Ten fuels have been used (Table 1). This set of fuels consists of three reference fuels (n° 1, 2 and 3) and seven blends obtained from these reference fuels alone or with different additives in varying quantities (n° 4 to 10). The blended fuels are obtained by blend of two reference fuels in the same proportion.

Fuel	CN	t_{arom}	Observations
n° 1	20.1	0.703	
n° 2	42.8	0.310	
n° 3	60.1	0.182	
n° 4	32.2	0.5065	n° 1 + n° 2
n° 5	50.7	0.246	n° 2 + n° 3
n° 6	41.1	0.4425	n° 1 + n° 3
n° 7	44.3	0.4425	n° 6 + 0.1 % alkyl nitrate
n° 8	52.8	0.246	n° 5 + 0.1 % t-butyl peroxide
n° 9	53.1	0.246	n° 5 + 0.03 % alkyl nitrate
n° 10	55.0	0.246	n° 5 + 0.1 % alkyl nitrate

Table 1 Fuels tested in the combustion bomb

Figures 3 to 6 show the evolution of the logarithm of the delay, versus the inverse of the absolute temperature, for different variables such as absolute gas pressure (Fig. 3), cetane number (Fig. 4) or additives (Fig. 5 and 6).

Figure 3 represents the evolution of autoignition delay of fuel n° 1 versus the gas temperature for different initial pressures. The role played by the pressure is relatively small compared to those of temperature. Figure 4 shows the decrease of ignition delay with increasing cetane number.

Figures 5 and 6 show the influence of the quantity and the nature of additives on the autoignition delay.
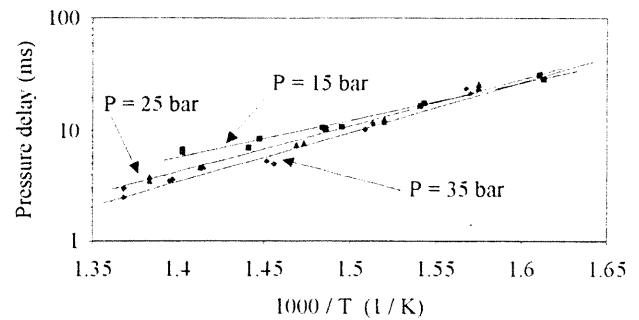

Fig. 3 Effect of initial pressure on ignition delay (fuel n° 1)
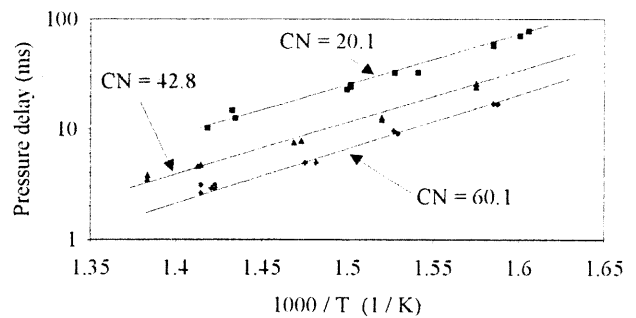

Fig. 4 Effect of cetane number on ignition delay
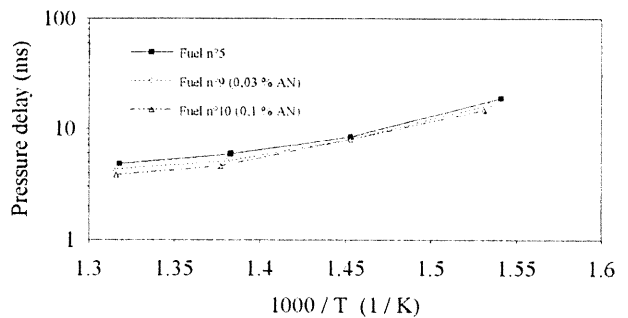

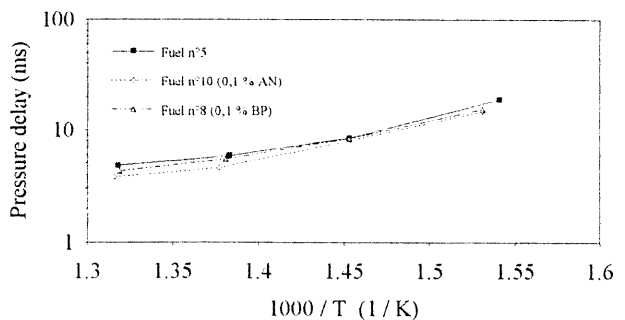Fig. 5 Effect of alkyl nitrate amount on ignition delay

Fig. 6 Influence of additive nature on ignition delay

The experimental results indicate that the ignition delay decreases with an increasing amount of additives. However, decrease of ignition delay is not proportional to the additive concentration. The additive nature also affects the ignition delay. At equal concentration, the alkyl nitrate seems to be more efficient to reduce ignition delay than the t-butyl peroxide. These results confirm those obtained by Clothier et al. (11) and Hoskin et al. (12).

All these results constitute a large data base which will be used to model the autoignition delay for each hydrocarbon fuel, taking into account the content of additives.

MODELING

Wolfer's Correlation Law (1)

To predict ignition delay of hydrocarbon fuel, several empirical laws have been proposed in previous studies (1-10). The most used formulation, in its initial form or modified for specific conditions, is that proposed by Wolfer (1) :

$$\tau = A \ P^{-n} \ \exp(E_a/RT) \tag{1}$$

where P and T represent respectively the average pressure and temperature of pressurized air in the combustion chamber during the ignition delay. In this work, the average temperatures and pressures during ignition delay are assumed to be equal to their initial values before the start of injection. In the original correlation law of Wolfer (1), A, n and E_a are constant. It has been shown (2) that these constants depend simultaneously on the fuel nature and on the experimental conditions. However it had never been formulated some relations between each of these constants and the above variables (fuel composition, injection conditions ...). So the values of A, n and E_a found in the literature are extremely spread. In this paper we assume that these constants depend on the fuel characteristics. Determination of these three parameters has been accomplished through their identification from the experimental results for fuels n° 1 to 6, using the least squares method.

Fuel	A	n	E_a (J/mol)
n° 1	3.63 10^{-4}	0.2440	66381
n° 2	2.04 10^{-5}	0.3275	78816
n° 3	7.07 10^{-6}	0.5258	85447
n° 4	7.58 10^{-4}	0.3774	64482
n° 5	9.87 10^{-5}	0.1799	68276
n° 6	3.41 10^{-5}	0.0870	75097

Table 2 Identification results

The parameters obtained are given in table 2. Figure 7, given as an example, enables comparison of computed and measured values of ignition delay using the data of table 2, for

fuel n° 2 at an initial gas pressure of 20 bar. A good agreement between experimental and predicted ignition delays for the other fuels is also observed.
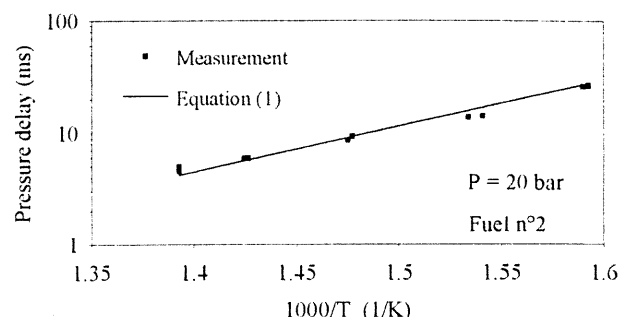

Fig. 7 Comparison between measured and computed (equation (1)) ignition delays

The data given in table 2 show that variations of the parameter A are in the range of 1 to 100 when the cetane number changes in the range of 1 to 3. The activation energy E_a remains in a relatively closed interval. Nevertheless, it may be kept in mind that the activation energy is the argument of the exponential term, and a little variation of this energy leads to an important variation in ignition delay. Finally, the parameter n represents the effect of partial pressure of oxygen, its variation is in the range of 1 to 6.

Proposed Correlation Law

The previous laws of Wolfer's type, used to predict ignition delay, can only be applied to one hydrocarbon fuel. To obtain a generalized law of ignition delay, we have correlated each parameter separately in the Wolfer's relationship, with the characteristics of fuels. We assume that the pressure exponent in equation (1) remains constant and characterizes the influence of oxygen concentration on ignition delay. Thus, the nature of the hydrocarbon must only affect the parameter A and the activation energy E_a. We have developed two different cases. In the first we assume that A is constant and E_a is function of fuel characteristics. In the second case the opposite. Each fuel is characterized by its cetane number, or more precisely by its aromatic content, these two characteristics being linked.

Activation energy as a function of aromatic content. We assume in this section that there is a linear relationship between the activation energy E_a and the aromatic content :

$$E_a = a + b \ t_{arom} \tag{2}$$

Equation (1) becomes :

$$\tau = A \ P^{-n} \ \exp\left[(a + b \ t_{arom})/RT\right] \tag{3}$$

The identification of the constants A, n, a and b is obtained using the experimental results of fuels n° 1 to 6 simultaneously. Then, equation (3) can be written :

$$\tau = 1.052 \ 10^{-4} \ P^{-0.336} \ \exp\left[\left(66034 + 13921 \ t_{arom}\right)/RT\right]$$

(4)

Figure 8 shows a good agreement between the measured and the computed (by equation (4)) values of ignition delay.
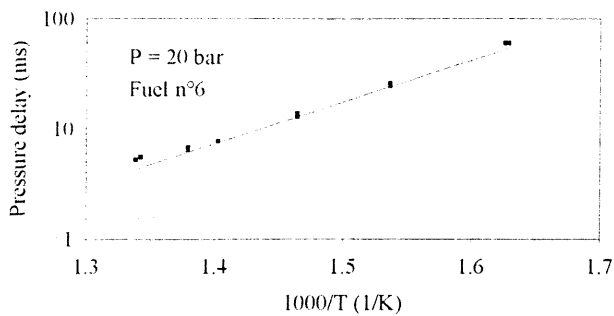
Fig. 8 Comparison between measured and computed (equation (4)) ignition delays

The identification of the constants a and b has allowed determination of the apparent activation energy of the fuels n° 1 to 6. The values obtained, given in table 3, are relatively close : the largest discrepancy between these activation energies is equal to +/- 4 %. Therefore, it seems that the apparent activation energy of different fuels could be considered as a constant. This remark is confirmed by the results given in figure 4, where the slopes of the curves for different cetane numbers (fuels n° 1, 2 et 3) are close to each other.

Fuel	E_a (J/mol)
n° 1	75820
n° 2	70350
n° 3	68568
n° 4	73085
n° 5	69459
n° 6	72194

Table 3 Apparent activation energies deduced from relationship (2)

Parameter A as a function of cetane number. The parameter A in equation (1) seems to be strongly related to the nature of the fuel. The determination of this parameter as a function of cetane number is obtained with two assumptions. The activation energy is assumed constant for all hydrocarbon

fuels. Its value is supposed equal to 71586 J/mol, the mean value obtained from the results shown in table 3. The exponent n of pressure in equation (1) is equal to 0.35, the mean value obtained from the identification using experimental results.

The results of the identification of parameter A, obtained by considering the hydrocarbon fuels separately, are shown in table 4.

Fuel	A
n° 1	2.008 10^{-4}
n° 2	0.790 10^{-4}
n° 3	0.508 10^{-4}
n° 4	1.945 10^{-4}
n° 5	0.922 10^{-4}
n° 6	1.483 10^{-4}

Table 4 Values of factor A of equation (1) for different fuels

Figure 9 shows the evolution of 1/A versus cetane number. We note from this figure that there is an exponential relationship between 1/A and cetane number. This relationship can be expressed as :

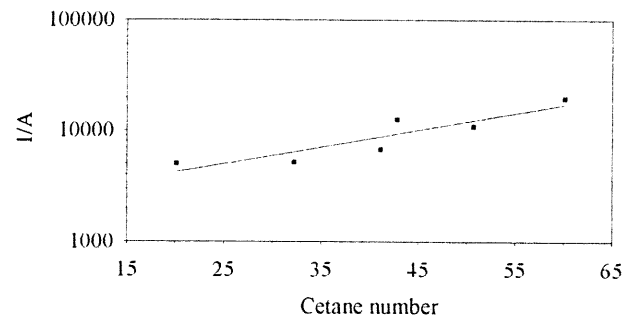$$A = \exp\left[-\left(3.55 \ 10^{-2} \ CN + 7.621\right)\right]$$

(5)

Fig. 9 Evolution of 1/A versus cetane number for the first six hydrocarbon fuels

Then, the relationship (1) takes the following form :

$$\tau = \exp\left[-\left(3.55 \ 10^{-2} \ CN + 7.621\right)\right] P^{-0.35} \exp(8610/T)$$

(6)

Figure 10, given as an example, allows comparison of the experimental results of fuel n° 5 with the computed values using relationship (6). We note that the discrepancy between measured and computed values is relatively small. However, the results obtained for high pressures are less satisfying.
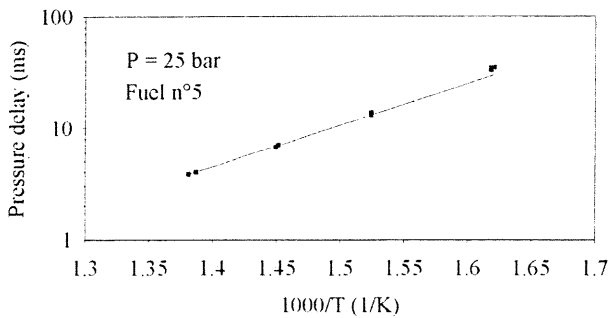
Fig. 10 Comparison between measured and computed
(equation (6)) delays (fuel n° 5)

VALIDATION

The validation was carried out with the experimental results obtained for fuels n° 7 to 10, which were ignored during the coefficients identification. Figure 11, given as an example, enables comparison, in the case of fuel n° 10, between the measured and computed ignition delays with equations (4) and (6).
It should be noted that this diagram shows the correctly predicted ignition delay of fuel n° 10 only. The results obtained for fuels n° 7 to 9 were just as successful.
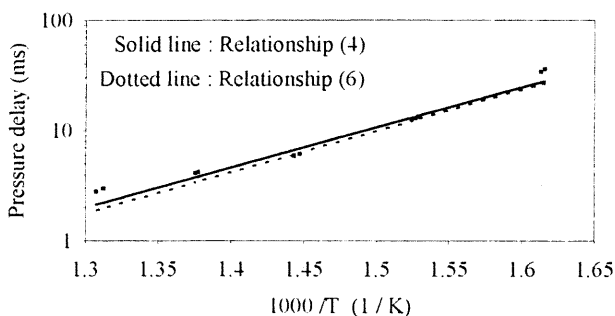

Fig. 11 Comparison between measured delay values
and those computed using the relationships (4) and (6)
(fuel n° 10, P = 20 bar)

The two approaches considered in this study seem to give very comparable results. Relationship (4) is better adapted to five of the ten fuels (n° 1, 2, 6, 7 and 10), while relationship (6) gives better results for the other five. Nevertheless, relationship (6) seems to be more suitable than relationship (4). As a matter of fact, fuels with the same aromatic content have different cetane number. Therefore, the aromatic amount can not be considered as a proper characteristic of the fuel, contrary to the cetane number. This observation is confirmed by the fact that relationship (6) gives the best results for fuels n° 5, 8 et 9, for which the only variable parameter is the cetane number.

CONCLUSION

The experimental studies performed in a constant volume combustion chamber have shown the effects of operating conditions and fuel characteristics on the ignition delay. With the set of experimental results from six fuels, a correlation law, based on the Wolfer's formulation, has been proposed to predict the ignition delay. Contrary to the formulation generally encountered in the literature (which is only useful for a given fuel), the proposed relationship (equation (6)) takes into account the cetane number and can be used to determine the ignition delay of different fuels. This law has been validated on 4 fuels. The ignition delay values obtained with this relationship are relatively accurate, and show good agreement with the measured ones.

In order to improve this relationship, we are presently looking to take into account other fuel characteristics such as aromatic and iso or n-paraffin content. The auto correlation of these parameters in the set of fuels used in this study has not yet allowed this improvement.

Alongside this empirical work, a reduced kinetic model of the autoignition is currently being developed. It consists of a chemically reduced mechanism, composed of 34 elementary reactions and using 19 chemical species. This model is elaborated from work by Sahetchian et al. (13-14) and has been inserted in three-dimensional code Kiva II.

NOMENCLATURE

A, a = constants
AN = alkyl nitrate
b = constant
BP = t-butyl peroxide
CN = cetane number
E = energy, $J.mol^{-1}$
n = constant
P = pressure, bar
R = perfect gas constant, $J.mol^{-1}.K^{-1}$
T = temperature, K
t = mass content
τ = autoignition delay, ms

Subscripts
a = activation
arom = aromatic

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