Energy Conversion and Management 152 (2017) 124–135

Contents lists available at ScienceDirect

Energy Conversion and Management

journal homepage: www.elsevier.com/locate/enconman

Correlations for the ignition characteristics of six different fuels and their application to predict ignition delays under transient thermodynamic conditions

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ARTICLE INFO

Keywords:
Autoignition
Ignition correlations
Ignition delay
Critical concentration

ABSTRACT

The ignition characteristics of six different fuels have been correlated as a function of the temperature, pressure, equivalence ratio and oxygen molar fraction in this investigation. More specifically, the ignition delay referred to cool flames, the high-temperature ignition delay and the critical concentrations and ignition times of HO_2 and CH_2O have been parameterized for n-dodecane, PRF0, PRF25, PRF50, PRF75 and PRF100. To do so, a wide database of ignition data of the aforementioned fuels has been generated by means of chemical simulations in CHEMKIN, solving a detailed mechanism for PRF mixtures and a reduced mechanism for n-dodecane. In fact, in-cylinder engine-like conditions reached in a Rapid Compression Expansion Machine (RCEM) have been replicated. The mathematical correlations have shown a relative deviation around 20% with the database in the low-temperature, low-pressure zone, which is the typical accuracy of usual correlations for the ignition delay. Finally, the ignition delay under transient conditions measured in the RCEM has been predicted by means of different integral methods coupled to both the proposed correlations and the generated database. I t has been found that deviations between the predictions obtained with the correlations or with the database are lower than 1%. This means that the correlations are accurate enough to predict the ignition time in spite of showing high deviation with the database, since the low-temperature, low-pressure zone has a minor contribution to the ignition delay.

1. Introduction, justification and objective

Autoignition is a combustion mode with high relevance in propulsive systems for transport media and, more specifically, in reciprocating internal combustion engines. Standard Diesel CI-engines base their start of combustion on the autoignition of a fuel spray, while autoignition is an undesirable combustion mode in SI-engines, resulting in unacceptable pressures rise rates that can damage the engine [1]. Furthermore, most of the new advanced Low Temperature Combustion (LTC) modes are based on autoignition [2]. These modes combine lean equivalence ratios and high Exhaust Gas Recirculation (EGR) rates to reach low-emission, high-efficiency engines [3]. Thus, nowadays, autoignition has become a really interesting topic in the frame of internal combustion engines [4].

Autoignition characterization is a key procedure in control engine models. Despite the fact that the ignition can be well predicted by means of numerical simulations with relatively low computational cost [5], the calculation time is too long to apply this methods in an Engine Control Unit (ECU) and, this way, controlling the engine in real time. Thus, the capability to characterize and even predict the ignition characteristics of different fuels is really interesting in the frame of engine control.

Mathematical correlations for the ignition delay are widely used in 0-D combustion models due to its simplicity and low calculation time. Pan et al. [6], for instance, correlated both ignition delays, referred to cool flames and referred to the high-temperature stage, for n-heptane and DME. Moreover, the NTC behavior and the temperature increment associated to cool flames were also parameterized. Besides, Desantes et al. [7] proposed expressions for the ignition delay of n-heptane and iso-octane in order to evaluate the chemical propagation velocity of a sequential autoignition process. Finally, it should be noted that the development of empirical correlations for the ignition delay is an extended methodology in rapid compression machine and shock tube studies, as the works of Kukkadapu et al. [8] and Weber et al. [9].

Furthermore, such mathematical correlations are usually linked to predictive methods to estimate the ignition delay under engine-like conditions. The most extended procedure is the classic Livengood & Wu integral method [10], which uses the ignition characteristics under

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http://dx.doi.org/10.1016/j.enconman.2017.09.030
Received 19 July 2017; Received in revised form 8 September 2017; Accepted 9 September 2017

Nomenclature

Notation

CAD	Crank Angle Degrees
CC	referred to chain carriers
$[CC]_{crit}$	critical concentration of chain carriers
CI	compression ignition
CFD	Computational Fluid Dynamics
Ea	activation energy for the Arrhenius expression
ECU	Engine Control Unit
EGR	Exhaust Gas Recirculation
f	correlation function
$[F]$	fuel concentration
HCCI	Homogeneous Charge Compression Ignition
k_i	specific reaction rate
LLNL	Lawrence Livermore National Laboratory
LTC	Low Temperature Combustion
N	number of samples
NTC	Negative Temperature Coefficient
P	pressure
PRF	Primary Reference Fuel
PSR	Perfectly Stirred Reactor
R	universal gas constant
R^2	Pearson's coefficient of correlation
RCEM	Rapid Compression-Expansion Machine
SI	spark ignition
t	time
T	temperature
T_a	activation temperature
t_i	ignition delay under transient thermodynamic conditions
$t_{i,2}$	ignition delay referred to the high-temperature stage of the process
$t_{i,CC}$	ignition delay referred to a critical concentration of chain carriers
x_i	input variables vector
X_{O2}	oxygen molar fraction
y	data vector from the chemical kinetic database
β	calibration constants vector
δ	β variation
$\overline{\xi}$	mean relative deviation between database and correlation results
ϕ	working equivalence ratio
λ	Marquardt parameter
τ	ignition delay under constant conditions of pressure and temperature
τ_{LTHR}	ignition delay under constant conditions referred to cool flames
τ_{HTHR}	ignition delay under constant conditions referred to the high-temperature stage
τ_{CC}	ignition delay under constant conditions referred to a critical concentration of chain carriers
$\dot{\omega}$	global reaction rate

constant thermodynamic conditions to predict the time of ignition under transient conditions as follows:

$$1 = \int_0^{t_i} \frac{1}{\tau} dt \tag{1}$$

where t_i represents the ignition delay of the process, while τ represents the ignition delay under constant conditions for each successive thermodynamic states reached in the process.

Several authors have used the Livengood & Wu integral method coupled to τ correlations to predict the ignition delay in combustion models for engine simulation and control. Hu et al. [11], for instance, used the Livengood & Wu integral method as a reaction progress variable to determine the instant and location of ignition for heterogeneous mixtures in CFD calculations. Furthermore, the integral method can be applied not only to SI-engines, but also to CI-engines. In fact, on the one hand, Zheng et al. [12] used the Livengood & Wu integral as the method to predict knock in 1-D engine cycle simulations. Experiments under knocking conditions were carried out in a turbocharged gasoline SI engine with cooled EGR and the knocking time were properly estimated by Eq. (1). On the other hand, Shahbakhti et al. [13] used the integral method as the way to control the ignition under HCCI conditions. The predictive method was validated by comparison to experimental data from a single cylinder engine in HCCI operation, in which the equivalence ratio, EGR level, engine speed, and intake temperature were varied for three different PRF blends with octane number values of 0, 10 and 20.

Different databases have been used to solve Eq. (1). For example, Choi et al. [14] trained an artificial neural network to predict ignition delays under constant thermodynamic conditions, τ, by means of the data obtained in a perfectly stirred reactor solving a detailed mechanism. The artificial neural network was linked to the Livengood & Wu integral method to predict ignition delays under HCCI conditions.

However, the easiest way to implement Eq. (1) is by using mathematical correlations for the ignition characteristics under constant thermodynamic conditions. Rausen et al. [15] proposed a mean-value model to control HCCI engines, in which the start of combustion is given by the Livengood & Wu integral method. Empirical correlations were used to parameterize the ignition delay under constant conditions, while the model was validated using steady-state tests data from a gasoline engine. Besides, Zhou et al. [16] proposed mathematical correlations for the ignition delay under constant conditions, τ, based on simulations solving detailed chemical kinetic mechanisms for different fuels. The authors used these correlations to solve the Livengood & Wu integral method and predict the ignition under engine conditions. The comparison of predictions to 0-D simulations with detailed chemistry showed that the Livengood & Wu integral method is able to accurately reproduce the ignition characteristics at an insignificant computational cost, leading to a method to control the ignition in real time. Similar correlations have been proposed by Del Vescovo et al. [17] for PRF mixtures. The authors tested their correlations using the Livengood & Wu integral method and comparing the predictions to experimental HCCI heavy-duty engine data, obtaining a mean deviation of 1.5 CAD between predictions and experimental results. Finally, Hillion et al. [18] proposed an open-loop control strategy to improve the stability during transients of a conventional CI Diesel engine. The Livengood & Wu integral method was used coupled to Arrhenius-type correlations to adjust the injection time and avoid too violent ignitions. This strategy was implemented in a real engine, which was tested on a test bench and on-board in a vehicle, and showed promising results in terms of combustion stability, pollutant emissions and noise.

The Livengood & Wu correlation has been recently used as an autoignition model for alternative fuels. Amador et al. [19], for instance, used the integral method to predict knock in an internal combustion engine fueled with Syngas. Their results showed that knock appears earlier if the methane number of the fuel increases. Besides, Kalghatgi et al. [20] tested the Livengood & Wu integral with five fuels that have different octane number values, sensitivities, and compositions, including ethanol blends. Predictions were compared to experiments in a single cylinder engine over a wide range of operating conditions, confirming that knock can be accurately predicted.

Desantes et al. [21,22] proposed an alternative integral method to predict both ignition delays, the one referred to cool flames and the