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# A new method to predict high and low-temperature ignition delays under transient thermodynamic conditions and its experimental validation using a Rapid Compression-Expansion Machine

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ABSTRACT

A new procedure to predict both high-temperature stage and cool flames ignition delays under transient thermodynamic conditions has been developed in this paper. The results obtained have been compared with those obtained from the Livengood & Wu integral method, as well as with other predictive methods and with direct chemical kinetic simulations and experimental data. All simulations have been performed with CHEMKIN, employing a detailed chemical kinetic mechanism. The simulations and predictions have been validated in the working range versus experimental results obtained from a Rapid Compression-Expansion Machine (RCEM). The study has been carried out with *n*-heptane and iso-octane, as diesel and gasoline fuel surrogates, under a wide range of initial temperatures (from 358 K to 458 K), initial pressures (0.14 MPa and 0.17 MPa), compression ratios (15 and 17), EGR rates (from 0% to 50%) and equivalence ratios (from 0.3 to 0.8). The experimental results show good agreement with the direct chemical kinetic simulations and with the new predictive method proposed. In fact, the mean relative deviation between experiments and simulations is equal to 1.719% for *n*-heptane and equal to 1.504% for iso-octane. Besides, the new method has shown good predictive capability not only for the high-temperature stage of the process but also for cool flames, being the mean relative deviation versus the experimental data lower than 2.900%. Better predictions of the ignition delay have been obtained with the new procedure than the ones obtained with the classic Livengood & Wu expression, especially in those cases showing a two-stage ignition pattern.



## 1. Introduction, justification and objective

Advanced combustion modes based on the autoignition of a premixed mixture with a certain degree of homogeneity, such as Homogeneous Charge Compression Ignition (HCCI), Premixed Charge Compression Ignition (PCCI), Reactivity Controlled Compression Ignition (RCCI) and others, have been studied for the simultaneous reduction of soot and $NO_x$ [1]. Their working principle is based on Low Temperature Combustion (LTC) by avoiding the soot and $NO_x$ formation peninsulas, which can be seen in equivalence ratio – temperature diagrams [2] and their effectiveness has been widely proved in previous studies [3,4]. These modes show virtually zero emissions of soot and $NO_x$, but high emissions of unburned hydrocarbons (UHC) and carbon monoxide (CO) that can be easily eliminated with well-known after-treatment techniques. The lack of control over the autoignition process and over the heat release rate are the main challenge to implement these new combustion strategies in commercial reciprocating internal combustion engines [5].

Ignition is controlled by the chemical kinetics of the charge in these new combustion modes [6]. This control entails higher complexity because of the absence of an explicit ignition-controlling event, such as a spark or an injection process when very reactive conditions are reached in the combustion chamber (near top dead center). The reactivity of the mixture can be modified by adjusting the engine operating parameters, such as the Exhaust Gas Recirculation (EGR) rate and the inlet temperature. Therefore, improving the capability of predicting the autoignition is mandatory to properly modify the operating conditions of the engine and to control the heat release.

The autoignition event can be reasonably well predicted by using advanced CFD codes with detailed chemistry. However, the required computing time is too long to be solved in real time. Simple numerical methods with very short computing time are the only ones that can be implemented in an engine control unit. If

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**Notation**

| | |
|---|---|
| *BDC* | Bottom Dead Center |
| *CC* | Chain Carriers |
| *CFD* | Computational Fluid Dynamics |
| *CI* | Compression Ignition |
| *CR* | Compression Ratio |
| *EGR* | Exhaust Gas Recirculation |
| *Fr* | working equivalence ratio |
| *HCCI* | Homogeneous Charge Compression Ignition |
| *ICE* | referred to data obtained from CHEMKIN using the internal combustion engine reactor |
| *Int* | referred to data obtained from the new integral proposed in this paper |
| *LW* | referred to data obtained from the Livengood & Wu integral method |
| $LW-mod$ | referred to data obtained from the predictive method proposed by Hernandez et al. [19] |
| *LTC* | Low Temperature Combustion |
| *max* | referred to a maximum concentration of chain carriers |
| *NTC* | Negative Temperature Coefficient |
| $P_i$ | initial pressure |
| *PCCI* | Premixed Charge Compression Ignition |
| *PRF* | Primary Reference Fuels |
| *PSR* | Perfectly Stirred Reactor |
| *RCCI* | Reactivity Controlled Compression Ignition |
| *RCEM* | Rapid Compression-Expansion Machine |
| *SI* | Spark Ignition |
| $T_i$ | initial temperature |
| *TDC* | Top Dead Center |
| $t_i$ | ignition delay under transient conditions |
| $t_{i,CC}$ | ignition delay referred to the critical concentration of chain carriers |
| $t_{i,1}$ | ignition delay referred to the maximum pressure rise of cool flames |
| $t_{i,2}$ | ignition delay referred to the maximum pressure rise |
| *UHC* | unburned hydrocarbons |
| $X_{O_2}$ | oxygen molar fraction |
| $\epsilon$ | percentage deviation in ignition delay between experimental and simulation or predicted results |
| $\lvert\bar{\epsilon}\rvert$ | mean absolute deviation between experimental and simulation or predicted results |
| $\tau$ | ignition delay under constant conditions of pressure and temperature |
| $\tau_{CC}$ | ignition delay under constant thermodynamic conditions referred to the critical concentration of chain carriers |
| $\tau_1$ | ignition delay under constant thermodynamic conditions referred to the maximum pressure rise of cool flames |
| $\tau_2$ | ignition delay under constant thermodynamic conditions referred to the maximum pressure rise |

these low computing time methods have enough accuracy to properly predict ignition delays, the control of the engine can be improved since decisions in real time can be taken.

Moreover, the use of detailed chemical kinetic mechanisms coupled with CFD codes is limited by the physical discretization of the domain. The computational cost of solving detailed chemistry in cases with a high number of cells could be unacceptable, imposing the use of simplified mechanisms. The total computing time can be reduced by implementing predictive numerical methods to determine the ignition delay instead of solving the involved reaction rates.

The Livengood & Wu hypothesis [7], also known as the Livengood & Wu integral method, allows to obtain ignition delays of processes under transient conditions of temperature and pressure by using the ignition characteristics under constant thermodynamic conditions, which are much easier to obtain both experimentally and by simulation. The expression proposed by these authors is the following:

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

where $t_i$ is the ignition delay of the process and $\tau$ is the ignition delay under constant conditions of pressure and temperature for the successive thermodynamic states.

The Livengood & Wu integral assumes that the autoignition happens when a critical concentration of chain carriers is reached, being this critical concentration constant with pressure and temperature for a given air–fuel mixture. Besides, the oxidation process during the ignition delay is described by a single zero-order global reaction and, therefore, the reaction rate does not depend on time under constant thermodynamic conditions. The Negative Temperature Coefficient (NTC) behavior cannot be correctly modeled under these hypotheses.

This integral has been traditionally enunciated as a method to predict knock in SI-engines [8]. However, it has been extended to CI-engines as a way to predict the ignition delay of homogeneous air–fuel mixtures as the ones used in HCCI combustion modes [9]. Several authors such as Ohyama [10], Rausen et al. [11], Choi et al. [12] and Hillion et al. [13] studied the implementation of the Livengood & Wu integral in an engine control unit. These authors used the integral method to predict the start of combustion under HCCI conditions. This method can be combined with other simple models to obtain global parameters of the combustion process allowing the control of the engine in real time.

The integral method has been used in several CFD studies as the model to predict the autoignition delay. For example, Imamori et al. [14] coupled the Livengood & Wu integral with Star-CD and KIVA 3 to improve the performance of a low speed two-stroke diesel engine. And Li et al. [15] linked the integral method with the CFD code VECTIS to study the effects of heterogeneities on a two-stroke HCCI engine fueled with gasoline.

The validity of the Livengood & Wu integral when a two-stage ignition occurs has been wondered by several authors [16]. The integral method is not able to accurately predict the ignition delay because it is based on a single global reaction mechanism that ignores the cool flames. Some of these authors, as Liang and Reitz [17] or Edenhofer et al. [18], show the need to create simple algorithms, but more sophisticated than the integral method, to characterize the autoignition at low temperatures without using any chemical kinetic mechanism, since the integral method has great interest for the prediction of autoignition due to its simplicity and low computational cost. However, few alternatives to the Livengood & Wu integral can be found in the literature.

Hernandez et al. [19] analyzed the validity of the Livengood & Wu integral by simulations performed with CHEMKIN for several fuels and with various chemical kinetics mechanisms. They proved that the predictions of the method are accurate if the fuel do not show a two-stage ignition pattern. These authors also proposed two different alternatives, one with better and another with worse results than the integral method. However, most of the alternatives proposed to improve the integral method are based on the method itself or assume the same hypotheses, which are too simplified.