Theoretical development of a new procedure to predict ignition delays under transient thermodynamic conditions and validation using a Rapid Compression–Expansion Machine

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ABSTRACT

An experimental and theoretical study about the autoignition phenomenon has been performed in this article. A new procedure to predict ignition delays under transient (i.e. variable) thermodynamic conditions has been developed starting from the Müller's chemical kinetics mechanism. The results obtained have been compared with those obtained from the Livengood & Wu integral method, as well as with direct chemical kinetic simulations. All simulations have been performed with CHEMKIN, employing a detailed chemical kinetic mechanism. The simulations 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 as a diesel fuel surrogate. The experimental results show a good agreement with the direct chemical kinetic simulations. Besides, better predictions of the ignition delay have been obtained from the new procedure than the ones obtained from the classic Livengood & Wu expression.

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1. Introduction, justification and objective

The potential of new combustion modes, such as Homogeneous Charge Compression Ignition (HCCI), Premixed Charge Compression Ignition (PCCI) and others based on Low Temperature Combustion (LTC), for the simultaneous reduction of soot and NO_x has been widely proved in previous studies [1,2]. These modes show virtually zero emissions of soot and NO_x, but high emissions of unburned hydrocarbons (UHC) and carbon monoxide (CO), by avoiding the soot and NO_x formation peninsulas, which can be seen in equivalence ratio – temperature diagrams [3]. 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 [4].

The ignition control is much more difficult under these conditions because of the absence of a 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). Thus, the ignition is controlled by the chemical kinetics of the charge [5], which can be modified by adjusting the engine operating parameters, such as the Exhaust Gas Recirculation (EGR) rate and the inlet temperature. Therefore, it is necessary to improve the capability of predicting the autoignition event to properly modify the operating conditions of the engine and control the heat release.

Although ignition can be reasonably predicted by using advanced CFD codes with detailed chemistry, the required computing time is too long to be solved in real time. In fact, simple numerical methods with very short computing time are the only ones that can be implemented in an engine control unit. Low computing time methods with enough accuracy to predict ignition delays allow improving the control of the engine, since decisions in real time can be taken.

The Livengood & Wu hypothesis [6], also known as the Livengood & Wu integral or, simply, the integral method, allows obtaining 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 τ is the ignition delay under constant conditions of pressure and temperature for the successive thermodynamic states.

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Nomenclature

a_{st}	oxygen-to-fuel ratio under stoichiometric conditions	SI	Spark Ignition
BDC	Bottom Dead Center	T_0	initial temperature
CFD	Computational Fluid Dynamics	TDC	Top Dead Center
CI	Compression Ignition	t_i	ignition delay under transient conditions
CR	Compression Ratio	t_{i,CH_2O}	ignition delay referred to the critical concentration of CH_2O
crit	referred to the critical concentration		
EGR	Exhaust Gas Recirculation	$t_{i,dP1}$	ignition delay referred to the maximum pressure rise of the cool flames
Fr	working equivalence ratio		
HCCI	Homogeneous Charge Compression Ignition		
ICE	referred to data obtained from CHEMKIN using the internal combustion engine reactor	$t_{i,dP2}$	ignition delay referred to the maximum pressure rise
		UHC	Unburned Hydrocarbons
Int	referred to data obtained from the new integral proposed in this paper	Y_{O_2}	oxygen mass fraction
		ϵ	percentage deviation in ignition delay between experimental and simulation results
k_i	specific reaction rate of reaction i		
LW	referred to data obtained from the Livengood & Wu integral method	$\bar{\epsilon^2}$	mean square deviation between experimental and simulation results
		ε	ignition delay prediction deviation
LTC	Low Temperature Combustion	$\bar{\varepsilon^2}$	mean square deviation of the predictive methods
NTC	Negative Temperature Coefficient	τ	ignition delay under constant conditions of pressure and temperature
P_0	initial pressure		
PCCI	Premixed Charge Compression Ignition		
PRF	Primary Reference Fuels		
PSR	Perfectly Stirred Reactor		

The Livengood & Wu integral assumes that the oxidation process during the ignition delay can be 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 modeled under this hypothesis. Moreover, the authors assumed 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.

Whereas this integral has been traditionally enunciated as a method to predict the occurrence of knock in SI-engines [7], 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 engines [8]. A new use of the Livengood & Wu integral is its implementation in an engine control unit. Several authors such as Ohyama [9], Rausen et al. [10], Choi and Chen [11] and Hillion et al. [12] 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 great interest for the prediction of autoignition due to its simplicity and low computational cost. This simplicity is just a consequence of the hypotheses assumed for its development.

The validity of the Livengood & Wu integral under certain conditions has been wondered by several authors [13]. When a two-stage ignition occurs, the integral method is not able to accurately predict any of both delays because it is based on a single global reaction mechanism that ignores the cool flames. Some of these authors, as Liang and Reitz [14] or Edenhofer et al. [15], 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. However, few alternatives to the Livengood & Wu integral can be found in the literature.

Hernandez et al. [16] analized 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 simple. Expressions based on more sophisticated autoignition models are needed in order to extend the range of validity of the methods.

In this study the validity of an alternative procedure to determine ignition delays under transient conditions is intended to be solved. The study has been done with n-heptane, the reactivity of which is very similar to diesel fuel. Despite the fact that more sophisticated surrogate fuels for diesel can be found in the literature, n-heptane was chosen because extended and fully validated chemical kinetic mechanisms are available for it. Moreover, n-heptane is a primary reference fuel (PRF) employed to define the octane reference scale and it is widely used in the literature as a diesel fuel surrogate under engine conditions [17].

Ignition delays and critical concentrations for n-heptane will be obtained under different conditions of pressure, temperature, equivalence ratio and oxygen mass fraction from calculations performed with the software of chemical simulation CHEMKIN. This software, which is developed by Reaction Design (ANSYS), is consolidated in the world of engineering investigations and the chemical kinetics mechanisms of several hydrocarbons are perfectly defined to be used with it. Finally, the numerical results are validated experimentally using a Rapid Compression–Expansion Machine (RCEM).

The structure of the paper is as follows: first, the experimental facilities involved in the study are presented. Then, a new expression to predict ignition delays under transient conditions is theoretically developed. Afterward, the methodological approach is described, including the experimental methods, the chemical kinetic simulations, the predictive methods and the parametric study performed. Next, the chemical kinetic mechanism is validated by comparison with experimental results. Thereafter, the predictive methods are validated with the chemical simulations, since they cannot be compared with the experiments due to they are referred to a different stage of the autoignition process. Finally, the conclusions of this study are shown.