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Full Length Article

Interpretation of auto-ignition delays from RCM in the presence of temperature heterogeneities: Impact on combustion regimes and negative temperature coefficient behavior

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HIGHLIGHTS

- Large temperature heterogeneity is demonstrated in a flat piston RCM.
- Adiabatically compressed region is impacted by heat transfer 30 ms after compression.
- Reaction fronts regime is demonstrated during the auto-ignition of n-hexane/air.
- With temperature heterogeneity, NTC underestimation is demonstrated.
- Ignition delay plots depend on the spatial and temporal variations of temperature.

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ABSTRACT

Rapid compression machines (RCMs) have often been used to study auto-ignition phenomena and to validate chemical kinetic models at conditions relevant to engines. Many RCM designs were historically used for the latter purpose. First, the flat piston configuration was extensively used and contributed to valuable ignition delay data. Temperature heterogeneity in these devices was later addressed, and new designs were proposed. In particular, creviced piston configurations have been demonstrated to enhance the temperature homogeneity in the bulk volume of RCM chambers. Nevertheless, data from flat piston RCMs are still used in the community. Thus, additional understanding of experimental results from such devices is still useful, and it also helps to enhance the understanding of temperature stratification effects on auto-ignition phenomena.

This paper addresses the interpretation of measured ignition delays from a flat piston RCM (without a circumferential crevice in the piston). First, we characterize local and temporal temperature evolution with a toluene planar laser induced fluorescence (PLIF) technique applied in oxygen-free gas under different test conditions. At a compression pressure (P_c) of 11 bar and an adiabatic core temperature (T_c) of 750 K, we find that the maximum measured temperature is very close to T_c up to 30 ms after the compression stroke. In the second step, we qualitatively compare temperature fields with chemiluminescence images during the auto-ignition of n-hexane and an n-heptane/methyl-cyclohexane (MCH) blend for a fuel-air equivalence ratio of 0.4, P_c values of 11 bar and 16 bar and T_c values of 700–900 K. The chemiluminescence results of n-hexane show a fast sequential auto-ignition which strongly suggest that the combustion propagation regime is mainly a reaction fronts regime. In the n-heptane/MCH case, the tracking of ignition kernels demonstrates that the auto-ignition initiates in the cold vortex at T_c values of 787 K and 834 K and in the adiabatically compressed region at T_c values of 742 K and 900 K.

In this study, flat piston RCM experiments demonstrate temperature heterogeneities with ranges up to 120 K and gradients of approximately 160 K/mm. This significantly influences the ignition delay measurement in the negative temperature coefficient (NTC) range. Through the example of n-heptane/MCH auto-ignition, it seems that despite temperature heterogeneities, the lower limit of the NTC range is well detected, whereas the higher limit is over-estimated. The determination of temperature thresholds in which ignition delay data may be confounded highly depends on the stratification level and on complex thermo-kinetic interactions. Outside these thresholds, when combustion is dominated by

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auto-ignition in regions at the adiabatic core temperature, the experimental data are easier to compare with simulation frameworks assuming a homogeneous hypothesis. In chemical kinetics-oriented studies, temperature heterogeneity should be considered when flat piston RCMs are used and when the piston crevice is not adequate.

1. Introduction

Rapid compression machines (RCMs) are experimental devices used to study combustion phenomena at low to intermediate temperatures and pressures. These facilities are often used to investigate the auto-ignition process of highly premixed and diluted lean fuel/air mixtures, commonly called the homogeneous charge compression ignition (HCCI) mode [1–4].

One of the specific uses of RCMs is in the study of chemical kinetics [5]. Currently, auto-ignition delays are measured at reference conditions (compression temperature/pressure, composition fuel/oxidizer/diluent) and then compared to simulations to validate chemical kinetic models. Often, the simulation framework implies homogeneous conditions to reduce the complexity, particularly when detailed chemistry is considered. However, heat losses and internal aerodynamics in flat piston RCMs induce important temperature stratification. Indeed, when the piston head is not designed to avoid the formation of a roll-up vortex, the colder shear layers are entrained into the center of the combustion chamber [6]. Although it was demonstrated in the literature that an adiabatic core region exists within the reaction chamber of flat piston RCMs under a range of conditions [7], the direct comparison of ignition delay data to these 0D models is still questionable [8]. In fact, temperature heterogeneities in the combustion chamber raise two problems. First, the way the chemistry interacts with local temperature variations is not well understood. Second, in some cases the temperature taken as a reference condition for delay time measurements is not relevant. This paper sheds light on these two issues. It also brings additional understanding of these complex phenomena that are relevant to the real engine case. Indeed, turbulence in automotive engines creates temperature heterogeneities that influence the auto-ignition process, particularly under HCCI configurations.

The study of thermo-kinetic interactions is often based on the experimental and/or numerical investigation of the temperature stratifications inside RCM chambers. Previous works have experimentally characterized the temperature distribution in the bulk volume of both flat piston and creviced piston RCMs. Sung and Curran presented a brief review [5] of non-intrusive temperature measurement methods used for this purpose. Two techniques were mainly used in flat piston RCMs: laser Rayleigh scattering [9,10] and laser induced fluorescence (LIF) [11] (acetone tracer), [12] (toluene tracer), [13] (anisole tracer). In creviced piston RCMs, LIF with acetone tracer [6] and a laser absorption technique [14,15] were used. These studies demonstrated the presence of important temperature heterogeneities in the combustion chamber of flat piston RCMs. However, it was demonstrated that the temperature is more homogeneous in creviced piston RCMs.

The temperature distribution in flat piston RCMs is mainly linked to the following two phenomena: (i) heat transfer to the wall that creates a colder shear area and (ii) the internal aerodynamics in the chamber. The piston motion induces a roll-up vortex that mixes the shear layer with an entrained warmer area [16]. These phenomena explain the non-adiabatic compression of the RCM, as the adiabatic compression pressure P_{ac} (see Eq. (3)) and temperature T_{ac} are not effectively reached. However, the presence of an adiabatic core region was demonstrated [7], and its temperature T_c is estimated based on the measured compression pressure P_c. Nevertheless, the size of this core region and the evolution of temperature heterogeneity in general still need more experimental investigations. In the present paper, the spatial and temporal evolution of temperature is experimentally investigated with the LIF technique (toluene tracer).

As a solution to suppress the roll-up vortex, a creviced piston design was first proposed by Park and Keck [17] to capture the shear layer in a crevice located at the piston head. Later, Lee and Hochgreb [18] further developed the idea with computational fluid dynamics (CFD) simulations and proposed recommendations for the crevice configuration. Mittal and Sung demonstrated in an experimental and numerical study [6] that the temperature inside the combustion chamber is drastically more homogeneous when a creviced piston is used. Nevertheless, this piston architecture brings additional issues that should be considered. A substantial gas flow between the crevice and the main volume of the combustion chamber was indicated [19,20]. This phenomenon could influence the auto-ignition process by lengthening ignition delays up to 25% in a multi-stage ignition case [20]. In addition, the crevice dimensions are optimized to suppress the roll-up vortex at a certain delineated operating range [21]. In all RCMs, the heat loss and shear layer effects on combustion are not fully controlled. Thus, the subsequent thermal variations could interact with chemical kinetics in a complex manner making it hard to interpret ignition delay experiments.

Griffiths et al. [22] studied the auto-ignition of di-*tert*-butyl peroxide and n-pentane in a flat piston RCM. n-Pentane showed NTC behavior in a temperature range of 750–850 K with ignition delays of approximately 10 ms. The authors used several diagnostic techniques (Schlieren, chemiluminescence, LIF of acetone and formaldehyde tracers) to investigate chemical interactions with local temperature heterogeneity. Their study [22] demonstrated that the ignition of di-*tert*-butyl peroxide initiates at the peak temperature zone in the combustion chamber. A similar combustion process was also observed with n-pentane at 765 K (lower limit of the NTC range). However, at 840 K (upper limit of the NTC range) the auto-ignition of n-pentane was initiated in a colder zone with a temperature estimated to be 40 K lower than maximum level. Griffiths et al. concluded that at temperatures outside the NTC range, the presence of temperature heterogeneities led to the onset of auto-ignition first in the highest temperature zones. On the other hand, the NTC behavior tends to smooth the temperature heterogeneity during the post-compression period and consequently leads to a fast and knocking combustion [11].

Mittal and Chomier [8] studied the auto-ignition of an n-heptane/O_2/diluent mixture through a CFD simulation of an RCM with a flat piston. First, the authors illustrated the importance of temperature heterogeneity in such a configuration. Then, they applied the kinetic mechanism proposed by Liu et al. [23] on both CFD and homogeneous models, followed by comparison of the results to experimental data performed with a flat piston RCM by Minetti et al. [24]. Surprisingly, the homogeneous simulation fit better with the experiments, especially in the NTC range. The authors explained that the chemical kinetic mechanism [23] was developed with the homogeneous hypothesis but using the same data from [24]. Thus, they concluded that such RCM configuration complicates the modeling of auto-ignition chemistry.