Influence of temperature heterogeneities on self-ignition process of methane-air mixtures in a Rapid Compression Machine.

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1 Introduction

Homogeneous Charge Compression Ignition (HCCI) is an advanced mode of engine operation providing both high thermal efficiency and low NOx and soot emissions thanks to the combustion of lean homogeneous mixtures. The onset of ignition for such engines cannot be easily controlled since it results from both mixing processes and chemical kinetics. So it depends strongly on temperature fluctuations or fuel equivalence ratio stratification. In particular the problem of non-uniform temperature distribution is far from being straightforward: aerodynamics inherent to engines enhances heat transfers, leading to strong temperature gradients. Such temperature heterogeneities have also been observed on several occasions in RCM [1].

The sensitivity of ignition process on temperature heterogeneities depends also on the fuel: while one-stage ignition chemistry exacerbates initial temperature fluctuations, negative temperature dependence of reaction rate can smooth out the temperature distribution inside the reaction chamber [2]. Turbulent mixing can also play a non negligible role on the HCCI combustion process since it affects both temperature and concentration fields.

The present work focuses on the influence of temperature heterogeneities on the self-ignition process. Self-ignition of methane/air mixtures has been performed with a flat piston RCM, and it has been simulated in conditions relevant to HCCI engines (high pressure, low/intermediate temperature). Methane has been chosen and it does not exhibit cold chemistry, revealing the effect of temperature fluctuations on the ignition process.

Experimental device

Rapid Compression Machines (RCM) are well suited to perform self-ignition of homogeneous mixtures in conditions relevant to HCCI engines. Indeed, initial conditions (pressure, temperature, mixture composition…) and boundary conditions (closed vessel) are better defined or stabilized in these ‘single shot’ devices than in real engines. As shock tubes, it can provide useful information about the overall response of chemical kinetics mechanism through the measurement of the ignition delay.

Compression of reactive mixtures is carried out as follows: a hydraulic jack sets a cam in motion. The horizontal translation is transformed into a vertical motion thanks to a guided wheel. The total time of compression is about 38 ms. In this study, the compression ratio is set to ε=18. The RCM is fitted with a heating system of chamber walls to vary the initial temperature of gases at Bottom Dead Centre (BDC) between 293 and 358 ± 1.5 °K. The piston position is recorded thanks to a laser device during the experiment. Simultaneously, time pressure evolution is followed by a piezoelectric transducer. These two signals are sampled at a frequency f=100 kHz. The RCM features a square section piston (50x50 mm), so a flat window is mounted on a lateral side of the chamber, enabling measurements in the whole dead volume. Moreover the RCM features an important stroke (S=420 mm), providing a wider window at top dead centre (TDC) for a given compression ratio. A fast camera Photron APX RS-3000 is also used to provide direct visualisation of the combustion process, with a focusing on the whole dead volume and a resolution of 512 x 512 pixels. Reactive mixtures are obtained from methane with a purity of 99.95 %, and compressed air.

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Numerical model

Numerical simulations of self-ignition within the RCM have been performed with a 0D model including detailed chemistry. Indeed, the consideration of such chemical description remains out of reach for practical use in 3D turbulent reactive flow simulation.

Most RCM self-ignition simulations just aim at quickly compare the experimental data with complex chemistry results. Typically, homogeneous temperature in an adiabatically compressed core zone is assumed and heat transfers are determined thanks to experimental pressure signals. In this respect, Lee and Hochgreb [3] proposed an improved two-zone model, with an adiabatic core zone and a closure for heat transfers in a secondary zone. The model agrees well with experimental pressure traces for a creviced piston. In an attempt to validate the adiabatic core hypothesis, Mittal and Sung [1] performed fluid dynamic simulations: the adiabatic core temperature deduced from the computed pressure evolution agrees well with the maximum computed temperature for a creviced piston RCM, but this hypothesis fails early after TDC with a flat piston.

Otherwise, a lot of study deals with simulation of self-ignition in HCCI engines with complex chemistry [4]. Some of them take into account temperature (or fuel equivalence ratio) heterogeneity using multi-zone models thanks to an initial temperature profile, but mixing is not modelled. Such fluctuations can also be taken into account in other models assuming a homogeneous probability density function of temperature and species within the vessel [4,5]. Fluctuations can also be introduced in the simulation thanks to the initial temperature distribution. Then, their evolution is driven by chemical kinetics and molecular mixing. This approach can be coupled to a stochastic heat transfer model, likely to induce additional temperature fluctuations [6].

The RCM used for this study is fitted with a flat piston, and the important stroke leads to high piston velocity and also high velocity gas motion. Heat transfers are enhanced and the adiabatic core assumption is expected to fail fairly early after TDC. As a result, models relying on this assumption are probably not well suited. Therefore the PDF approach is chosen to take into account temperature heterogeneities.

The modelled PDF transport equation is solved by a Monte Carlo method featuring operator splitting. In the framework of this study, the compression is simulated using experimental position or pressure signal, with a compression ratio measured in the RCM. The specific heat ratio ($\gamma=C_p/C_v$) of the mixture and the instantaneous reaction rates are computed from Chemkin subroutines library [7]. The chemical scheme of Huang et al [8] is used, since it includes both high and low temperature chemistry relevant to HCCI combustion. In particular, it is validated against high pressure shock tube ignition delays, for stoechiometric methane-air mixtures. The simulation is started before compression (BDC), so the initial temperature is assumed to be homogeneous. A stochastic heat transfer model is then used to create temperature fluctuations. Like some multidimensional transported PDF methods [9], it is based on a Wiener diffusion process within the chamber, but with a turbulent viscosity estimated by a 0D simplified k-epsilon equation. Simultaneously fluctuations are decreased by molecular diffusion i.e. the micromixing term in the PDF transport equation, with the IEM [10] model.

2 Experimental results

Self-ignition of stoechiometric mixtures of methane-air is performed in the RCM at high pressure P=40 bars. The aim of these experiments is first to compare ignition delays in RCM to data available in the literature. Indeed, Huang et al [8] performed shock tube experiments at P=40 bars with the same mixture. In parallel of pressure measurements, direct visualisations are carried out to assess the development of the ignition process.

As methane is very resistive to self-ignition, relatively high conditions of temperature and pressure must be reached to perform self-ignition. Therefore experiments with this fuel must be done with care since impurities (dust, grease…) can perturb the ignition process by producing hot spots leading to early ignition. This behaviour must be avoided, since it is not representative of chemical kinetics of the reactive mixture.

Figure 1 shows two pressure traces obtained in the same conditions: an initial temperature T_0=353 °K and an initial pressure P_0=0.92 bars. As the pressure drop is fairly steep during ignition process, the ignition delay can be defined as the time between TDC and the occurrence of the maximum temporal derivative of pressure. The adiabatic core temperature is deduced from pressure traces thanks to the expression: $\int_{T_0}^{T} \frac{\gamma}{\gamma-1}\frac{dT}{T} = \ln\left[P(t)/P_0\right]$ (1)

On figure 2 are depicted ignition delays measured by Huang et al [8] for similar conditions but at higher temperatures: CH_4-Air, Φ=1, P=40bars, 1000<T<1300°K. The temperature corresponding to our experimental data are based on the adiabatic core temperature at TDC, Tc. The ignition delay measured in the RCM agrees reasonably well with the shock tube experiment. However, one must notice that choosing the adiabatic core temperature at TDC consists in neglecting the cooling after TDC: in particular the adiabatic core temperature before ignition Tci (when dP/dt=0) is lower. This temperature also seems to agree well with shock tube experiments. Nevertheless, higher temperatures must be reached within the RCM to make a quantitative comparison of the measurements with available data. Moreover, the evolution of temperature should also be taken into account to improve this comparison.

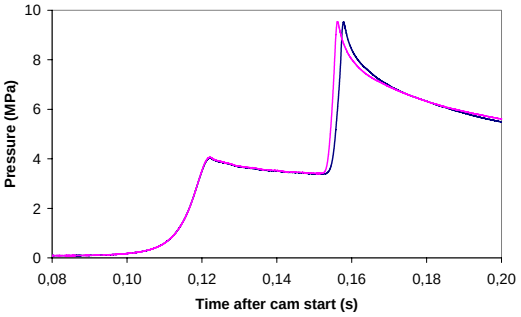

Figure 1: Pressure traces of two consecutive methane-air self-ignition experiment within the RCM in the same conditions.

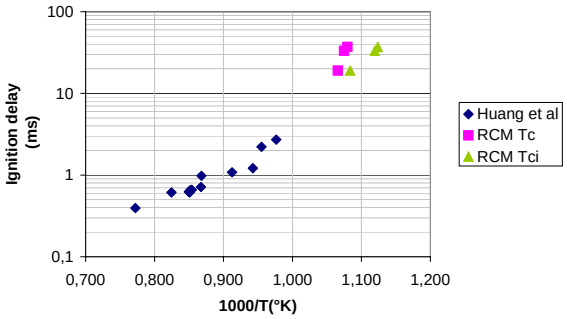

Figure 2: Ignition delay measurements in shock tube [8], and in RCM.
Tci: adiabatic core temperature at the onset of ignition.
Tc: adiabatic core temperature at TDC.

On Figure 3, direct visualisations of self-ignition clearly show the heterogeneity of self-ignition process. Pictures correspond to experiments reported figure 1, 1.4 ms after detection of the onset of ignition by direct visualisation, which is synchronised with the onset of pressure rise (the gap is less than 0.5 ms). Both experiments show several ignition zones, developing across the whole chamber. As self-ignition process is far from being homogeneous, it is very important for the numerical model to take into account such non homogeneous temperature distributions.

Figure 3: Direct visualisation, 1.4 ms after the onset of ignition, for the first (left) and the second experiment (right). Lateral window.

3 Numerical simulation results

The influence of temperature evolution on the ignition delay is first studied in homogeneous situation. In a second step attention is focused on temperature heterogeneity.

Homogeneous temperature distribution: The ignition process depends strongly on the temperature field. In particular, in heterogeneous situations, the maximum temperature generally determines the onset of ignition. This temperature is compared to several homogeneous temperature calculations:

1 - Adiabatic compression based on experimental volume evolution: For given conditions (P_0, T_0, ε), the computed temperature exceeds the maximum experimental temperature within the combustion chamber.

2 - Compression with heat transfers deduced from volume and pressure signals of inert experiment, thanks to the ideal gas law: The computed temperature equals the mean temperature within the combustion chamber, and so exceeds its maximum temperature. The cooling following top dead centre is taken into account.

3 - Adiabatic core compression: Before ignition, temperature of the adiabatic core zone is deduced from the experimental pressure signal thanks to the relation (1). In the experiment, heat transfers within the combustion chamber decrease the pressure. The resulting cooling is applied to the simulated adiabatic core zone. Its temperature equals the maximum temperature within the experiment if the adiabatic core zone assumption is valid. It exceeds the maximum temperature within the RCM when this hypothesis fails.

The left part of figure 4 depicts previously described homogeneous calculations, for the shortest ignition delay experiment reported on figure 2. It appears that if adiabatic calculation clearly underestimates the measurement of ignition delay, the adiabatic core calculation of the ignition delay is closer to measurement. Finally, ignition does not occur for the simulation based on the mean experimental temperature: after TDC, it is lower than the adiabatic core temperature by more than 70 K.

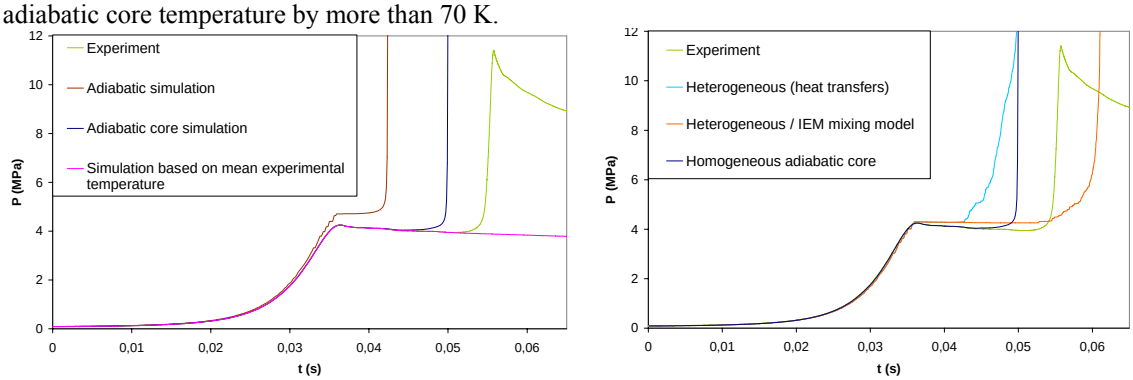

Figure 4: Pressure evolutions in homogeneous case (left), and heterogeneous case (right).

Heterogeneous temperature distribution: Heat transfers are modelled by a stochastic process, designed to reproduce experimental TDC pressure by adjusting exchange coefficient. Their level of heterogeneity is sensitive to the choice of the Wiener process time-step. A mixing time τ_t=40 ms and 200 stochastic particles have been used for the simulation.

Figure 4 also shows examples of pressure evolution in the heterogeneous case. The stochastic process reveals its ability to produce highly heterogeneous ignition process, with ignition delay value similar to the adiabatic core case. High sensitivity to micromixing can also be observed, since it moves the temperature distribution towards the mean, increasing thus ignition delay. The influence of micromixing and heat transfer models on both the temperature distribution and the ignition process will be reported in much more details during oral presentation. In particular the ability of the model to reproduce the adiabatic core hypothesis and its possible failure will be examined. The analysis will be also supported by heat transfers measurements within the RCM.

4 Acknowledgements

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