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CFD simulations of Rapid Compression Machines using detailed chemistry: Impact of multi-dimensional effects on the auto-ignition of the iso-octane

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Abstract

In Rapid Compression Machines (RCM), several phenomena can induce inhomogeneities inside the reaction chamber. The benefits of using a creviced piston have been largely demonstrated through good agreement with the widely used adiabatic core assumption. Still, temperature inhomogeneities due to wall heat transfer cannot be avoided. These induce spatial variations in terms of chemical composition, potentially affecting the auto-ignition process. Mass transfer to the crevices during two-stage ignition is also a phenomenon that can influence the ignition process. In this study, we quantify the impact of multi-dimensional effects on the auto-ignition of the iso-octane by comparing 0-D and RANS simulations of the Argonne RCM. A detailed kinetic mechanism is employed, which makes this study the first to couple an accurate description of both the physical and chemical phenomena in an RCM context for such a complex fuel. It is found that the influence of the inhomogeneities on the ignition delay is globally marginal except for the lowest temperature condition explored where the diffusive transport of intermediate species and radicals plays a key role. The effect of mass transfer to the crevices does not affect significantly the auto-ignition delay under the test conditions. The sensitivity of the results to the turbulence level is also assessed and the results indicate that turbulence

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may only exert a minor influence on the auto-ignition delay. Comparison with the experimental data is good, and RANS simulation results are similar to those of the 0-D simulations.

Keywords: Rapid Compression Machine; CFD; Detailed chemistry; Iso-octane

1. Introduction

Rapid Compression Machines (RCMs) have been extensively used in the past decades and are still nowadays to investigate auto-ignition phenomena. The RCM capability to maintain for a sufficiently long time high pressures and low to intermediate temperatures allows to acquire valuable information about the fuel decomposition and oxidation at engine relevant conditions. Specific behaviors such as two-stage ignition or the presence of a negative temperature coefficient (NTC) region can be evidenced by RCM experiments. For a review of RCMs' capabilities, the reader is referred to [1].

In addition to the large pool of experimental data gathered from RCMs, many research groups intend to develop detailed chemical kinetic modeling. The classic approach to validate kinetic mechanisms against experimental data consists of using a simplified model of the real RCM behavior. Most often, zero-dimensional modeling coupled to a method accounting for wall heat losses is used [2]. In this study, it is intended to evaluate whether multi-dimensional effects can affect the whole ignition process for the particular case of the iso-octane, as they would potentially fail to be reproduced by commonly used simplified models. Cool walls, non-uniform wall heat losses and heat release, or vortex generation in the boundary layer likely to roll-up can, non-exhaustively, induce spatial inhomogeneities inside the chamber, more specifically in terms of temperature. As it is the driving parameter for the kinetics, the consequences regarding the spatial variations of the chemical composition are potentially significant, therefore possibly impacting the auto-ignition delay as well. In order to address this question, a thorough and fundamental understanding of the RCM physics, of the chemical kinetics and of the interactions between both has to be achieved, especially in the case of iso-octane as it exhibits a NTC behavior. Solving the Reynolds-Averaged Navier–Stokes (RANS) equations while employing a detailed kinetic mechanism is suited for such a study.

One major source of temperature inhomogeneities was originally the roll-up of the boundary layer created by the rapid motion of the piston, bringing the cooler gases from the walls to the center of the chamber. Many earlier studies recommended the use of a creviced piston in order to absorb the thermal boundary layer and thus to avoid those undesirable inhomogeneities [3,4]. Mittal and Sung conclusively pointed out by numerical simulations and PLIF (planar laser-induced fluorescence) measurements the advantages of using a creviced piston regarding the homogeneity of the temperature field [5]. They also experimentally observed the significant differences between flat and creviced pistons in terms of auto-ignition delays. Würmel and Simmie studied extensively the influence of the piston geometry and ended up with an optimal crevice configuration [6]. The use of pistons with crevices is now almost generalized.

A less mitigable source of non-uniformities inside the reaction chamber is due to the wall heat transfer [7]. In situations where the temperature is close to the negative-temperature dependent domain, this can potentially lead to an enhanced level of reactivity in the cooler wall region. This effect has already been evidenced by Griffiths and Nimmo with some photographs of iso-butane ignition [8]; it has been further demonstrated with CFD simulations and experiments in the context of engine-knock investigations [9,10]. Recently, the more rapid reaction evolution for cyclohexane close to the boundary layer region has been numerically highlighted for temperatures entering the negative-temperature dependence domain [11]. Ignition has been observed to initiate in the boundary layer. However, some reservation has to be made regarding the relevance of directly comparing those results with experimental data: the simulation begins at top-dead center (hence missing all fluid dynamics effects due to the piston motion and possible chemistry initiation during the compression stroke), a constant wall heat flux is imposed (while heat losses are closely tied to in-cylinder physical conditions) and the employed mechanism has been reduced from 499 to 50 species and from 2323 to 143 reactions, thereby overlooking part of the comprehensive content of the initial detailed mechanism. Mittal et al. investigated by CFD simulations the behavior of the n-heptane using a skeletal mechanism (43 species, 185 reactions) [12]. They interestingly observed that in the presence of residual vortical motions inside the chamber, the NTC behavior of the n-heptane tends to smooth out the temperature inhomogeneities with a faster reaction rate in the cooler regions of the flow. Comparison with classic 0-D modeling was also carried out over the entire NTC regime, and ignition times were