CFD simulations of Rapid Compression Machines using detailed chemistry for iso-octane

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Rapid Compression Machines (RCM) have been extensively used in the past decades and are still today to investigate auto-ignition phenomena [1]. Although many research groups contribute to the pool of experimental data and to the development of kinetic mehanisms, two key questions related to experimental data remain pending and limit all the valuable information that could be extracted from the RCM experiments. The first point concerns the comparability from machine to machine: as illustrated by Fig. 1, the auto-ignition delays measured for the iso-octane on different RCMs exhibit a significant variability, especially in the range of end-compression temperatures relevant for internal combustion engines. The second question is about the shot-to-shot repeatability for a same machine. The first question is addressed by fundamentally understanding the physical and the chemical phenomena arising within RCMs, as well as their interactions. High fidelity computational fluid dynamics (CFD) simulations (i.e., wall-resolved RANS) coupled to detailed mechanisms are suited for such a study.

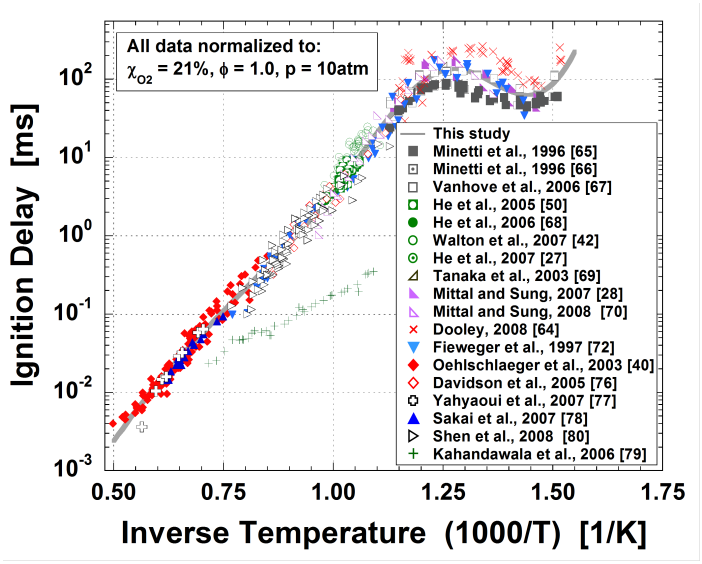

Figure 1: Iso-octane auto-ignition delays as a function of the adiabatic core temperature (i.e., the supposed temperature at the end of the compression stroke) for different RCMs. All data have been normalized to Y_{O2} = 21%, ϕ = 1 and p = 10 atm [2].

As including detailed chemistry into classic CFD simulations is very prohibitive in terms of computational cost, it is requested to resort to speed-up techniques. Such strategies essentially can act on two aspects: the reduction of the mechanism [3,4] or the tabulation of previously computed results [5,6]. We take advantage of those two approaches by using the TDAC (Tabulation of Dynamic Adaptive Chemistry) algorithm, respectively mitigating the impact of the number of species and of the number of cells on the computational cost [7].

Reactive simulations for the iso-octane combustion using a very detailed mechanism (i.e., more than 1000 species) will be presented and compared to the experimental results of two different rapid

compression machines. The basic reasons explaining discrepancies between different machines will be highlighted. Essentially, the impact of the machine design (e.g., the piston geometry and the piston stroke) is significant on the auto-ignition delay that is finally measured. Hence it is believed that results from different RCMs should not be compared without taking into account properly the geometrical and the design specificities of each machine.

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