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Assessment of the Ignition Delay Times Criteria for Hydrogen Combustion

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Extended Abstract

The MDO and REgulations for Low-boom and Environmentally Sustainable Supersonic aviation (MORE & LESS) is a research project pursued by a consortium of European government and academic institutions including both the Italian Aerospace Research Centre (CIRA) and the University of Lund and coordinated by Politecnico di Torino under the EC Horizon 2020 financial support.

MORE & LESS was conceived to develop the enabling technologies aimed to make feasible and eco-friendly civil, supersonic, and air-breathing aviation. This challenging objective is carried out using a holistic approach based on a synergic coupling between low and high-fidelity modelling of several processes e.g., aerodynamics, jet noise, sonic boom, propulsion, and above all pollutant and climate-changing chemical emissions.

In this framework, hydrogen is esteemed to be a promising candidate as fuel for supersonic, air-breathing, trans-atmospheric, long-term passenger transportation aircraft, because it possesses the highest energy density and the shortest Ignition Delay Times (IDT) among the several available fuels. Moreover, it can be burned efficiently and reliably in supersonic combustion engines and it is a clean fuel with lower greenhouse gas emissions compared to hydrocarbons, since the overall product of its complete oxy-combustion is only water, even if, when reacts with air, it produces also NOx, due to the very elevated flame temperatures reached during combustion.

Nowadays, the design and development of air-breathing ramjet engines rely above all on numerical modelling ranging from Computational Fluid Dynamics (CFD) 3D Large Eddy Simulations (LES) to detailed 0D chemical/kinetic analysis of autoignition phenomena, combustion and afterburning. For this purpose, the assessment of several available kinetic mechanisms is usually accomplished through the comparison between the 0D numerical predictions and the experimental shock tube's measurements. IDT are combustion parameters of paramount importance in the kinetic analysis of every fuel since they can be accurately computed by uncoupling the chemical sub-model from the fluid dynamic and mixing interactions, thus allowing a deeper understanding of the oxidation behaviour in homogeneous, perfectly stirred closed reactor conditions.

Therefore, the implementation of the best-suited IDT computational and experimental determination criterion to identify the time instant corresponding to the formation of a radical pool concentration able to activate the exothermic combustion process, and start the autocatalytic chain branching reactions, is a valuable effort. This allows for improvement in the kinetic assessment and the selection of the most reliable and accurate kinetic schemes at given operative conditions.

In the work here reported, several kinds of IDT criteria were analysed and discussed. The first is the thermal/mechanical one associated with the abrupt increase of the reacting ideal gaseous mixture's temperature and consequently pressure, due to the stepwise heat release produced by the exothermic combustion process. Instead, the second criterion is defined as the time elapsed between the injection of the reactants within the combustion chamber and the achievement of the maximum concentration of the key radical species i.e., OH or its excited version OH*, which is the flame marker responsible for the light emissions and the flame chemiluminescence observed during hydrogen/air combustion.

For this reason, several atmospheric and medium-high pressure experimental datasets were analysed as reference measurements to compare with computational values calculated using Cantera/Python [1] 0D simulations of Perfectly Stirred Reactors (PSR) in closed, adiabatic, isochoric conditions using the Z22 kinetic mechanisms, formulated and developed by Zettervall and Fureby [2] according to the two above mentioned IDT criteria.

Preliminary results show the existence of a significant spread in the matching between the computational and the experimental IDT values in function of the followed criterion and, consequently, highlight the importance to select the most suited numerical definition of IDT based on the specific experimental facility set up and the installed diagnostic techniques.

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References

[1] D. Goodwin, H. K. Moffat, R. L. Speth. (2022). "Cantera: An Object-oriented Software Toolkit for Chemical Kinetics, Thermodynamics, and Transport Processes, [Online]. Available: http://www.cantera.org.

[2] N. Zettervall, C. Fureby, "A Computational Study of Ramjet, Scramjet and Dual Mode Ramjet/Scramjet Combustion in a Combustor with a Cavity Flameholder", in Proceedings of AIAA Aerospace Science Meeting Kissimmee, Florida (U.S.A.), 2018, 8-12th January.