M2 – engineer internship

Understanding and MOdeling NOx formation in Turbulent HYdrogen flames

Context

Hydrogen combustion is a promising energy source to reach the carbon neutrality in 2050 in many applications, including transport, industrial processes and energy conversion. This ambitious objective raises great scientific challenges in terms of combustion. Indeed, H_2-air flames do not emit CO_2 (a greenhouse gas) or carbon containing pollutants such as, carbon monoxide, unburnt hydrocarbons, or soot, but they are characterized by high-temperature regions, which promote the formation of nitrogen oxides (NOx). While the emission and the reduction of NOx in turbulent flames has been studied for hydrocarbon combustion, the physical and chemical mechanisms responsible of NOx formation in turbulent H2 flames remain unknown.

This work is part of the collaborative project MONTHY which aims for a better understanding and MOdeling of NOx formation in Turbulent HYdrogen flames. In particular, there are two main scientific challenges to address for modeling NOx formation in turbulent H2 flames:

- Even though hydrogen chemistry is much more simplified than hydrocarbon combustion, H2-air detailed mechanisms which account for NO pathways are expected to involve more than 30 species and two hundred of elementary reactions. For CPU time reasons, these schemes must be reduced before being coupled with a CFD solver dedicated to compute the large-scale burners encountered in practical industrial applications.

- NOx formation and consumption feature multiple time and length scales: prompt NO is formed in the thin flame front region at a characteristic time scale in the range [10–7s,10–3s]. Thermal NO formation is observed in a post-flame region where temperature and major species reach chemical equilibrium, time scales involved are much slower and included in [10-3 s, 1s]. Turbulent combustion modeling is therefore especially complex because the wide range of time and length scales covered by the chemistry will lead to strong local variations of the Damkhöler number. However, existing turbulent combustion model are only valid in a specific flame regime of the Borghi Diagram [1], where Damkhöler numbers have the same order of magnitude. The key modeling challenges of MONTHY are to develop a turbulent combustion model, adapted to the different regimes covered by the wide range of interactions between turbulence and NOx chemistry.

Internship objectives

This internship is the introduction to doctoral studies that will be carried out in the framework of the MONTH PEPR collaborative project. The objectives of the internship are to design and validate an accurate highly reduced chemical scheme for H2-air combustion based on the virtual chemistry method [2-6]. Example of simulations conducted with virtual chemistry are shown in Fig.1. Kinetics rate constants of virtual elementary reactions will be optimized through machine-learning algorithms to model complex NOx chemistry. In addition, transport properties of virtual species will be optimized to handle for differential diffusion phenomena. The impact

of heat losses on the pollutant formation will be also considered. 1-D detailed chemistry flame simulations will be conducted with the EM2C REGATH solver. The code MELOPTIM based on genetic algorithm will be retained for virtual scheme optimization and will target the database of 1D laminar flames generated with a detailed mechanism. The optimized reduced kinetic scheme will be then used to carry out CFD simulations of 1-D and 2-D premixed laminar hydrogen flames.

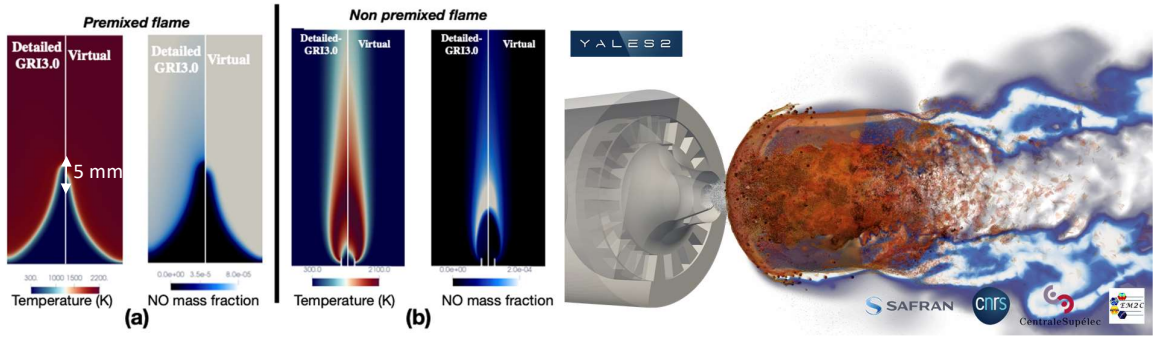

Figure 1. *Left: simulation of laminar CH4-air flame. Both temperature and NO mass fraction predicted by the reduced virtual scheme are compared against the GRI3.0 detailed chemistry solution. Right: LES of a turbulent spray n-heptane air flame with the virtual chemistry method.*

Skills required

Knowledge required in Numerical methods, Fluid Mechanics, Energetics, Heat transfer and Computational Fluid dynamics. This internship is adapted to Engineering school and/or Master's degree in research.

PhD perspective

The continuation of this research work through doctoral studies is strongly encouraged. Ph.D. funding opportunities are possible.

Location and supervision

The internship will take place at the EM2C-CNRS laboratory located at CentraleSupélec, Université Paris-Saclay (Gif-sur-Yvette, France).

Duration

6 months, beginning in Spring 2023

Application

Send a CV, transcript records and references to benoit.fiorina@centralesupelec.fr

References

[1] T. Poinsot, D. Veynante, Theoretical and Numerical Combustion, 3rd ed., R.T. Edwards Inc., 2011.
[2] M. Cailler, N. Darabiha, D. Veynante and B. Fiorina. Building-up virtual optimized mechanism for flame modeling. Proc. Combust. Inst. Vol 36 (1), pp 1251-1258 (2017)
[3] G. Maio, M. Cailler, R. Mercier and B. Fiorina. Virtual chemistry for temperature and CO prediction in LES of non-adiabatic turbulent flames. Proc. Combust. Inst. Vol 37 (2) 2591-2599 (2019)
[4] G. Maio, M. Cailler, A. Cuoci and B. Fiorina. A virtual chemical mechanism for prediction of NO emissions from flames. Comb. Theory and Modeling, pp1-31 (2020).
[5] H. Maldonado Colman, A. Cuoci, N. Darabiha and B. Fiorina. Reduced virtual chemistry models for soot prediction and radiative heat losses in hydrocarbon-air flames. Submitted (2021)
[6] G. Maio, M. Cailler, N. Darabiha and B. Fiorina. Capturing multi-regime combustion in turbulent flames with a virtual chemistry approach. Proceedings of the Combustion Institute, In Press (2021)