PhD position at PC2A

Study of the formation of nitrogen oxides (NO_x) during dihydrogen (H_2) combustion

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, as the chemical and physical properties of hydrogen are radically different from those of conventional hydrocarbon fuels, and high levels of NOx emissions are expected. The understanding and the modeling of NOx formation is mandatory to develop computing tools required by combustion engineers to design the future hydrogen combustion chambers.
Different kinetic pathways are responsible for the NO formation in combustion: the well-known thermal-NO at high temperature and NNH and N_2O pathways occurring at intermediate temperature and which are still uncertain.

The objective of the thesis is to reach a better understanding of NOx formation in H_2 flames by combining an experimental approach using high-performance laser diagnostics and numerical tools to validate a kinetic model. This project is part of a major national collaborative project “PEPR H2 décarboné”

The work of the thesis will be articulated around two axes:

- **Construction of an experimental database in laminar flames.**

Different $H_2/O_2/N_2$ premixed flames with different equivalence ratios (H_2/O_2) will be stabilized at low pressure. Laser spectroscopy techniques (Laser Induced Fluorescence, LIF and Cavity RingDown Spectroscopy, CRDS) will be used to measure in these flames the variations of the concentration profiles of species such as OH, NO, O and H, as well as the temperature profiles. These techniques are already well mastered in the PC2A laboratory (https://pro.univ-lille.fr/nathalie-lamoureux/publications/#descr) but never applied in $H_2/O_2/N_2$ premixed flames. The detection of other radicals like HNO could also be considered. In order to complete the inventory of measurable species, the FTIR technique will be implemented to obtain the concentration profiles of H_2O, NO_2 and N_2O. The impact of adding H_2O to reduce NO emissions will be studied.

- **Development of a detailed kinetic model.**

The kinetic simulation work will be carried out with calculation codes (Chemkin-Pro, LogeSoft, Cantera) using in a first step kinetic models from the literature. Based on the comparison between predictions and experiments, the kinetic analysis work will allow to identify the formation pathways of NOx and N_2O emissions.
At the end of the work, a detailed and validated kinetic model for emission prediction will be proposed.

Keywords: Combustion, Chemical kinetic, NOx emissions, laser based spectroscopic diagnostics

Academic requirements: Master's degree or engineering school in the field of chemistry, chemistry-physics, and a strong aspiration to perform experimental work are required. Knowledge in the field of combustion, laser techniques would be appreciated.

Doctoral school: Sciences de la Matière, du Rayonnement et de l’Environnement (https://edsmre.univ-lille.fr)
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Laboratory: PC2A https://pc2a.univ-lille.fr/
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