PhD position in PC2A (CNRS/Univ. Lille)

Etude de la formation des oxydes d'azote lors de la combustion de l'ammoniac

In order to reach the goal of carbon neutrality in 2030/2050, as announced by France in its "France 2030" investment plan and by Europe in its "Green Deal", the demand for electricity will increase significantly. Renewable energy resources such as wind and solar are considered as the main energy resources of the future. However, due to their intermittency and the need to ensure security of electricity supply, energy storage will be an integral part of the modern smart grid. One solution for storing excess electricity is electrofuels (e-fuels). For example, hydrogen (H_2) e-fuel can be produced by electrolysis of water and then stored as ammonia (NH_3) by a Haber-Bosch process or electrochemical methods. Unlike hydrogen, ammonia (which is already used worldwide for agricultural purposes) is easier to transport and store than hydrogen. NH_3 can be reduced to H_2 and N_2 (cracking). It can also be used directly in combustion devices. Thus, the use of ammonia is already effective in maritime transport (DNV-GL, C-JOB, MAN, ...) which must meet the obligation of the International Maritime Organization (IMO) to reduce CO2 emissions from shipping by 40% by 2030 and 70% by 2050, compared to 2008. However, ammonia has a very low heat release compared to fossil fuels, and its combustion can be affected by the occurrence of instabilities. These difficulties are mitigated when ammonia is used with a co-fuel, preferably hydrogen, in order to achieve the goal of zero carbon emissions.

While ammonia has the advantage of zero carbon combustion, the expected emissions of NOx, N_2O and unburned NH_3 must be controlled. The development of new burners, internal combustion engines relies on simulation codes of turbulent combustion for which it is important to have a good knowledge of the chemical kinetics of the oxidation of ammonia. Several detailed kinetic mechanisms representative of ammonia combustion are available today. Most of them have been validated by measurements of global parameters such as fundamental flame speeds and ignition delays. These mechanisms need to be consolidated from detailed data such as the evolution of chemical species as a function of combustion conditions. These can be obtained in low pressure stabilized premix flames which have the advantage of a flame front well detached from the burner surface.

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

Construction of an experimental database in laminar flames.

Different premix flames will be stabilized at low pressure; $NH_3/O_2/N_2$ with different equivalence ratio (NH_3/O_2), as well as flames where a small fraction of NH_3 will be substituted by hydrogen. 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, NH, 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). In order to complete the inventory of measurable species, the FTIR technique will be implemented to obtain the concentration profiles of NH_3, H_2O, NO_2 and N_2O.

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, as well as the conditions where unburned NH_3 emissions are critical. 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)
Funding: Labex CaPPA (WP1, https://www.labex-cappa.fr/), ADEME, University of Lille
Laboratory: PC2A https://pc2a.univ-lille.fr/
Supervisors: Nathalie Lamoureux, Pascale Desgroux
Duration: 36 months, starting in October 2022
Contact e-mail: Nathalie.lamoureux@univ-lille.fr, Pascale.desgroux@univ-lille.fr