International Master 2 Atmospheric Sciences: Research Training 2021-2022

Laboratory: PC2A

Supervisor: FENARD Yann and TRAN Luc-Sy

Tél : 03.20.43.49.78, E-mail : yann.fenard@univ-lille.fr and luc-sy.tran@univ-lille.fr

Collaborator:

Eventually,

CaPPA Work Package: WP-1 or WP-2 or WP-5

Combustion chemistry of saturated cyclic ethers

More than 90% of fuels consumed worldwide today are petroleum-based. Greenhouse gas emissions and the exhaustion of their reserves are currently main concerns of the uses of petroleum-based fuels. A view to the next three decades shows that the demand for energy for transportation will rise by approximately 70%. Cyclic ethers, which are being considered as promising biofuels and can be produced from non-food plants, such as lignocellulosic biomass (agricultural waste, forest residues, wood, dedicated plants, etc.), are of increasing interest as alternatives to petroleum-based fuels. These biofuels offer the long-term promise of fuel-source regenerability and now provide opportunities to extend the petroleum era, as blending agents with petroleum-based fuels or as complete replacement. A good understanding of the combustion chemistry of the cyclic ethers is essential in development of reliable kinetic models for predicting the combustion and emissions of these biofuels. However, the ring size effects of the three to six membered saturated cyclic ethers are still not well understood and will be explored in this internship using modelling approaches.

Concretely, the master student will first be trained in the use of the modelling tools necessary to achieve the project's objectives. In parallel, he/she will carry out bibliographical studies on the project's theme. Under supervisors' support, he/she will establish a single kinetic model for the studied cyclic ethers and test the model by comparing model simulations with literature experimental data. These numerical simulations will be carried out with the Chemkin-PRO software, under different reactor conditions (flame, jet-stirred reactor, flow reactor, etc.). The expected results will be used to analyze the combustion chemistry of the studied cyclic ethers and the influence of the ether ring size on fuel reactivity and product emissions.

Key words: Biofuels, kinetic model, cyclic ether, alternative fuels, Chemkin-PRO.