International Master 2 Atmospheric Sciences: Research Training 2022-2023

Laboratory: PC2A

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Collaborator:

Eventually,

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

## Chemical kinetics of oxygenated aromatics during biofuel combustion

Combustion process is the universal way to produce energy from fuels (>80% of the world's primary energy supply is currently generated via combustion in flame burners, car engines, airplane engines, etc.). Biofuels are considered as promising sources for renewable energy production to reduce $CO_2$ emissions. However, the presence of oxygen atoms in the chemical structure of biofuels complicates the reaction mechanism of oxygenated aromatics, e.g. oxygenated polycyclic aromatic hydrocarbons. These compounds are toxic, and together with soot particles, they can penetrate our respiratory system and trigger health problems. The formation mechanism of oxygenated aromatics will be explored in this internship. 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. Then, he/she will perform simulations on the formation/decomposition of oxygenated aromatics resulting from biofuel combustion using a kinetic model currently being developed in the laboratory. This can help us to validate the model using literature experimental data. These numerical simulations with complex chemistry will be carried out with the Chemkin-PRO software, under different reactor conditions (flow reactor, flame, etc.), temperature and pressure. The expected results will be used to analyse the chemistry of oxygenated aromatics and related non-oxygenated aromatics, which will provide a solid basis for developing a long-term proposal on the mechanism of soot formation in biofuel combustion.

Key words: Biofuels, alternative fuels, kinetics, oxygenated aromatics, Chemkin-PRO.