International Master 2 Atmospheric Sciences: Research Training 2021-2022

Laboratory: PC2A

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Eventually,

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

Kinetic modelling of the formation and decomposition of OPAHs 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. Recent studies have shown that the combustion of oxygenated biofuels produces lower amounts of large-sized soot particles than conventional petroleum fuels. However, the biofuels could potentially generate higher amounts of small-sized soot particles and these particles contain a significant fraction of oxygenates including oxygenated polycyclic aromatic hydrocarbons (OPAHs) which are generally more toxic than classic PAHs. These small-sized particles can penetrate our respiratory system and trigger health problems.

Due to the presence of oxygen atoms in the chemical structure of biofuels, the reaction mechanism involved during soot formation processes is expected to be much more complex as compared to conventional fuels. Understanding this mechanism is therefore very challenging, but it is a prerequisite step towards developing cleaner combustion technologies of biofuels. PAHs were proven to be the origin of soot formation, while the role of OPAHs and their chemistry are still less understood and 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 OPAHs 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 formation chemistry of OPAHs and related PAHs, which will provide a solid basis for developing a long-term proposal on the mechanism of soot formation in biofuel combustion.

Key words: Biofuels, kinetic model, OPAHs, soot, alternative fuels, Chemkin-PRO.