

## International Master 2 Atmospheric Sciences: Research Training 2021-2022

Laboratory: PC2A

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Eventually,

CaPPA Work Package: WP-1, WP-6

### **Insights in a better understanding of the atmospheric reactivity of pesticides**

Pesticides are semivolatile organic compounds emitted into the atmosphere by vapor shift during application, wind erosion from treated plants and soil and post application volatilization from the surface of treated soil and plants. The contamination of environment due to pesticides leads to several health problems and will disturb the balanced ecosystem. 80-90 % of pesticides are volatilized within a few days of application and there is a maximum probability for contamination in air and environment.

The primary route for the removal of pesticides from the atmosphere is by dry or wet deposition techniques. The chemical reaction initiated by atmospheric oxidants (OH, O<sub>3</sub>, NO, NO<sub>2</sub>) are responsible for the transformation of pesticides in the atmosphere. In the atmosphere, abiotic degradation of pesticides occurs mainly by photolysis and reactions with radicals in the atmosphere. The products formed from these reactions may be hazardous and may lead to several negative implications.

Recently, the French agency ANSES identified 32 pesticides for which more investigations are needed to better understand their environmental properties.

Molecular simulations will be performed to determine the thermochemical properties and kinetic parameters in both gas and aqueous phases for the reactions of OH with some pesticides for which no literature data exist. The fate of the degradation products after the primary reaction will be also studied.

This project will also aim to contribute to a larger research program devoted to the study of atmospheric processes (Labex CaPPA, CPER Ecrin). This work will be conducted in collaboration with different research groups worldwide (Comenius University in Bratislava, Monastir University).

The work will take place at PC2A laboratory, Lille University.

**Key words:** Atmospheric chemistry, reactivity, pesticides, molecular simulations