



Ecole Doctorale - 104

Sciences de la Matière, du Rayonnement
et de l'Environnement

ESTABLISHMENT : Université de Lille

Laboratory(ies) of affiliation : PhysicoChimie des Processus de Combustion et de l'Atmosphère (PC2A)

Scientific field, Speciality: **the speciality of the thesis must be one of those of the thesis (co)-director**

- DS2 Dense media, materials and components
- DS2 | Diluted media and fundamental optics
- DS3 | Earth and Universe Sciences
- DS3 | Earth, fluid envelopes
- DS4 | Theoretical, Physical and Analytical Chemistry
- DS4 | Organic, Inorganic and Industrial Chemistry
- DS4 | Materials chemistry
- DS5 | Molecular and Cellular Aspects of Biology
- DS8 | Energy, heat, combustion
- DS8 | Mechanics of solids, materials, structures and surfaces
- DS10 | Food Biotechnology, Food Science, Physiology
- DS10 | Biology of the environment, organisms, populations, ecology
- DS10 | agronomics sciences

Thesis director: LOUIS Florent, Associate Professor, florent.louis@univ-lille.fr

Co-director: SEGURA Pedro Alejandro, Professeur, pedro.alejandro.segura@USherbrooke.ca

Affiliate programme(s) : CDP AREA and CPER ECRIN

Planned (co)-funding (*mention: in progress/obtained*) : CNRS joint PhD Université de Sherbrooke (in progress), CDP AREA (in progress), ED SMRE (in progress)

Title of the thesis: Modelling of pesticide degradation and transport in rural environments

THESIS SUBJECT (ABOUT 1/2 PAGE)

In 2020, France consumed more than 64000 tons of pesticides, ranking first in Europe in terms of volumes sold. In the same year, Canadian consumption was estimated at more than 126000 tons. The effectiveness of these products for phytosanitary protection and the maintenance of a high level of agricultural productivity remains undeniable, however, many studies have highlighted the threat that pesticides pose to the biodiversity of terrestrial and aquatic ecosystems. The work conducted at the University of Sherbrooke by Professor Segura's group on the impact of organic contaminants, including pesticides, on the health of lakes in Canada, revealed the frequent presence of these compounds in lake waters and sediments, where they contribute significantly to ecotoxicological risks.

With a view to a more robust assessment of the risks of pesticide exposure and in order to prioritize mitigation strategies at the human population and ecosystem scales, it is essential to develop advanced predictive



Ecole Doctorale - 104

Sciences de la Matière, du Rayonnement
et de l'Environnement

models integrating the composition and properties of the particulate phase, in order to better characterize the persistence and atmospheric transport of pesticides. The originality of this innovative project lies in the complementarity of the approaches used (numerical simulations and artificial intelligence) in order to provide essential data to adjust the risk assessment and risk management models of pesticide exposure by atmospheric particles.

In parallel with the experimental results obtained at the University of Sherbrooke, numerical simulations at the molecular scale combining methods of electronic structure (quantum) and dynamics (classical) will not only allow a better understanding of the experimental facts observed but also predict the reaction mechanisms involved in the atmospheric reactions of pesticides initiated by major photo-oxidants (hydroxyl radicals, ozone, etc.) whether or not aerosol particles are present. In addition, their ecotoxicity to aquatic species will be estimated by modelling. The data obtained will be compared with those estimated by a machine learning algorithm in order to develop the predictive aspect of artificial intelligence for a large number of organic contaminants.

Expected date of recruitment : april 30th 2026

Contact (e-mail address) : florent.louis@univ-lille.fr

Additional remarks/comments: Candidate profile: Master's degree or engineering degree in environmental chemistry or physical chemistry. Experience in the field of atmospheric chemistry, molecular simulations (quantum chemistry, molecular dynamics) and chemical kinetics will be appreciated. A good level of English (written/spoken) will be essential (at least B2). A mobility between the University of Lille and the University of Sherbrooke is mandatory. The work will take place at PC2A laboratory of the University of Lille.