



Ecole Doctorale - 104

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

ESTABLISHMENT : University of Lille

Laboratory(ies) of affiliation : 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: HERCKES Pierre, Professor, pierre.herckes@asu.edu

Co-supervisor (non HDR): TAAMALLI Sonia, Research Engineer, sonia.taamalli@univ-lille.fr

Affiliate programme(s): CPER ECRIN/Labex CaPPA-CDP AREA

Planned (co)-funding: thèse labellisée ULille (obtained), région Hauts-de-France (in progress) or Labex CaPPA-CDP AREA (in progress)

Title of the thesis : Assessing the fate of emerging contaminants in the environment

THESIS SUBJECT (ABOUT 1/2 PAGE)

Context

The presence of emerging contaminants results either from direct emission or from diffuse emissions or re-emissions from contaminated soils or waterbodies. This phenomenon concerns a great diversity of molecules, which originate in human uses or activities releasing semi volatile organic compounds such as tire wear additives or perfluorinated compounds (PFAS). On one side, tire wear particles are a new focus as a form of environmental microplastics, with their role in air pollution expected to grow as tailpipe emissions decrease. On the other side, significant research currently focuses on PFAS due to the growing awareness of their toxicity and emerging regulations that often set their allowable concentrations at extremely low levels (a few parts per trillion, ppt). Despite this, many knowledge gaps remain regarding the environmental fate and transport of these compounds, often referred to as "forever chemicals" because of their environmental persistence. Given the limited reactivity of PFAS,



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a critical consideration is their partitioning behavior within environmental media. One particularly important aspect is the interaction between PFAS and microplastics, as these compounds are frequently found together due to their anthropogenic origins.

Goal of the project

The main goal of this PhD thesis is to investigate using computational kinetics the atmospheric degradation processes of emerging contaminants at the molecular level unraveling their most favorable pathways, their atmospheric fate and impact to the environment as well as their ecotoxicity towards aquatic species. The goal is to inform the experiments on recommended products to look for, and vice-versa, to support the kinetics and products already identified.

This project will also perform within the framework of a larger research program (CPER Ecrin; Labex CaPPA, and CDP AREA). This work will be conducted in close collaboration with the experimental works performed in the group led by Pierre Herckes at Arizona State University (USA).

Expected date of recruitment : 26/04/2025

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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 Arizona State University is mandatory. The work will take place at PC2A laboratory of the University of Lille.