Kinetic modelling of the combustion of toxic chemicals

Job title: Researcher in chemical kinetics

General information:
Postdoctoral researcher at Laboratoire Réactions et Génie des Procédés in Nancy.

Date of publication of the offer: November 8, 2022
Start date: February 1st 2023
Contract duration: 24 months
Remuneration: 2850 € (gross)
Level of study: PhD

Mission:
Mechanisms of the degradation mechanisms of toxic chemical agents, of the model molecules used to study them (simulants) and of industrial toxics remain poorly known. These quantities are nevertheless essential to evaluate the impact of an atmospheric emission of these products, to size stock disposal processes or to predict their evolution if they are subjected to a rise in temperature or pressure as during an accidental fire or explosion.
In collaboration with the Centre d'Etudes du Bouchet of the Délégation Générale pour l'Armement (DGA), this project aims to develop detailed kinetic models predictive of the combustion of a number of toxic chemical agents such as organophosphorus and halogenated derivatives. The work revolves around the study of reaction pathways, rate constants and thermodynamic data of chemical species. The lack of data in the literature and the experimental difficulties related to the nature of the molecules require the use of the tools of theoretical chemistry (*ab initio* calculations). The objective of the study is to develop predictive kinetic models of the decomposition of new compounds and to improve the reaction bases of decomposition products, based on experimental results.

Activities:
A first part will be dedicated to the development of a detailed kinetic model predictive of the thermal decomposition and combustion of several specific chemical agents. The models will be built in a systematic way taking into account molecular and radical reactions. Theoretical calculations will be used for the analysis of reaction pathways and the evaluation of thermodynamic and kinetic quantities.
A second part will consist of the re-evaluation and improvement of the bases of gas phase reactions of small phosphorus products produced by the decomposition of agents. These common bases for the decomposition mechanisms of the different products studied will be validated thanks to data from the literature and new experimental measurements obtained with light phosphorus species. These bases are also important for simulating the combustion inhibition effects of organophosphates used as flame retardants in many materials.

Expected skills:
The candidate, who holds a PhD, will have research experience in physical chemistry, chemical kinetics and reactive systems modeling. Skills in the field of *ab initio* calculation will be appreciated.

Work context:
Based in Lorraine, the Laboratory of Reactions and Process Engineering (LRGP) is a Joint Research Unit of the CNRS and the University of Lorraine. It is located in Nancy in the Meurthe-et-Moselle department. It is mainly located in the city centre, on the premises of the École Nationale des Industries Chimiques de Nancy (ENSIC). The Radical Kinetics Group is part of the laboratory and has recognized expertise in chemical kinetics.

Supplementary information:

Deadline for receipt of applications: December 22, 2022
Required documents: CV, including list of publications, cover letter and two references (people likely to be contacted)

Application : https://emploi.cnrs.fr/Offres/CDD/UMR7274-PIEGLA-002/Default.aspx

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