

Master 1 Physics of the XXth Century – Option Atmospheric Sciences: Research Training 2021-2022

Laboratory: PC2A

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Better insights into the atmospheric degradation of iodinated oxygenated compounds using molecular simulations

After Fukushima accident, significant differences have been observed between the atmospheric measured and modeled iodine concentrations. It may be attributed to the reactivity of iodine-containing species not considered by the IRSN simulations. To improve the model, the chemical mechanism was recently developed in our laboratory showing that there is a need to understand the reactivity of iodinated oxygenated compounds with the major photooxidant present in the atmosphere (OH radicals). Molecular simulations will be performed to determine the thermochemical properties ($\Delta_f H^\circ_{298K}$, S°_{298K} , $C_p = f(T)$) as well as the kinetic parameters of a set of reactions.

This project will also aim to contribute to a larger research program devoted to the study of atmospheric processes (Labex CaPPA). This work will be conducted in collaboration with the Comenius University in Bratislava (Slovakia). The work will take place at PC2A laboratory, Lille University.

Key words: Atmosphere, reactivity, iodine, molecular simulations