PhD thesis offer at INRS-LRGP

Study of reactions between VOCs present in work atmospheres and ozone

Context

The COVID crisis has led to the marketing of a large number of air purifiers combining different treatment processes such as filtration, adsorption, cold plasmas ... either for their bactericidal effect or to remove VOCs. The INRS has found that the use of these purifiers sometimes leads to the formation of ozone (O_3) in high concentrations, between 100 and 1000 ppbv. The presence of volatile organic compounds (VOCs) in work environments combined with O_3 leads to a rapid production of organic molecules and nano-sized aerosols that are potentially harmful to human health.

The reactivity of ozone (O_3) at room temperature with unsaturated molecules, including terpenes such as alpha-pinene, has been known for decades as one of the major sources of aerosols in the atmosphere. The reaction of O_3 with a VOC initiates an oxidation process leading rapidly to the formation of poly-oxygenated, low volatility molecules that upon condensation are particle precursors[1-3]. However, their molecular structure and concentration are not known, even in the case of a characteristic molecule such as α pinene[4]. The review by Bianchi et al.[5] provides an overview of the literature on poly-oxygenated molecules in atmospheric chemistry.

Objectives of the thesis

The aim of the INRS-LRGP thesis is to study the specific chemistry of O_3 with VOCs representative of work environments using ideal reactors (perfectly stirred or piston) to identify and quantify the products in the gas phase, especially those toxic to the health of workers. Ultimately, these data will lead to recommendations on improving the air quality of working environments.

1) The first part of the thesis will consist of a thorough bibliographical study from Web of Sciences type databases, on laboratory experiments and modeling on the reactivity of the main VOCs observed in the tertiary sector with O_3 and the formation of secondary organic aerosols (SOA) associated. Particular attention will be paid to unsaturated VOCs.

2) The thesis work will then include an important part of laboratory experiments using gas flow reactors. The coupling to analytical tools such as time-of-flight mass spectrometer and gas phase micro-chromatograph will allow the identification and quantification of the largest number of products/pollutants. The characterization and speciation of potentially produced AOS will be an important issue in this work. This aspect of the study will rely on the skills and metrology available in the Process Engineering Department of INRS.

3) Based on the experimental data obtained, the third part of the thesis will focus on the development of chemical kinetic models for a quantitative prediction of stable products, such as aldehydes and if possible AOS for which a significant production is expected. The modeling of the formation of polyoxygenated molecules will also be addressed via lumping techniques of species and reactions in the models thanks to the experience of the LRGP in modeling the oxidation chemistry of fuel components.

<u>Requirements</u>

We are looking for a candidate with an engineering degree or a master's degree in process engineering with, if possible, knowledge in chemical kinetics. The candidate must be able to integrate the risk prevention aspects of the INRS partner. Fluent English and ability to work in a team are required.

References :

[1]Ehn+ (2014). *Nature*, *506*(7489), 476-479.
[2]Schobesberger+ (2013). *Proceedings of the National Academy of Sciences*, *110*(43), 17223-17228.
[3]Riccobono+ (2014). *Science*, *344*(6185), 717-721.
[4]Iyer+ (2021). *Nature communications*, *12*(1), 1-6.
[5]Bianchi+ (2019) *Chemical Reviews*, *119*(6), 3472-3509

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Remuneration: 2547 € gross monthly

Duration and start date of the thesis: 3 years with a start in 2023 after recruitment

Practical information: the thesis will take place mainly at the LRGP of Nancy but will include large-scale tests at the INRS of Vandoeuvre-lès-Nancy.