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HIGH-ENERGY ELECTRON BEAM DEGRADATION OF PFAS AND PERSISTENT ORGANIC POLLUTANTS IN WATER: EXPERIMENTAL AND MODELING INSIGHTS

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Persistent organic pollutants (POPs) are a group of organic compounds that have toxic properties, persist in the environment, accumulate in food chains and present a risk to human health and the environment. Most of them are of anthropogenic origin, associated with industrial processes, product use and applications, waste disposal, leaks and spills, fuel combustion and waste incineration. Among alternative techniques to incineration, high energy electron beam (e-beam) accelerators has been used for water treatment to degrade a wide range of recalcitrant POP. The interaction between primary e-beam and water generates water radiolysis which produces secondary electrons called hydrated electrons as well as free radicals. These hydrated electrons play a determining role in the degradation of the POP, and the free radicals from water radiolysis induce oxidative and reductive degradation of organic pollutant. Although the mechanism of water radiolysis is well known, there is no multi-purpose general experimental and simulation framework for predicting the destruction rate of the POP as a function of primary e-beam characteristics.

This invited lecture aims to review the current state of literature regarding the experimental method and modelling of POP destruction. Our objective is to introduce a pioneering multidisciplinary and multiscale methodology, encompassing the integration of dedicated experimental device together with a multi-scale modelling used to understand the process and predict the best recipe for POPs destruction. As a Proof of Concept (POC), we will apply our methodology to the case of PFAS. Per- and polyfluoroalkyl substances (PFAS) are a group of synthetic chemicals used since the 1950s in a wide variety of applications due to their water-repellent, grease-repellent, and dirt-repellent properties. PFAS compounds contain at least one fully fluorinated carbon (CF3- or -CF2-) and usually a functional (terminal) group that differs between PFAS groups and subgroups. Due to the strength of their carbon-fluorine bonds, they are called "Forever Chemicals" because they are very difficult to degrade in the environment. Currently, there are no effective technologies for treating PFAS on an industrial scale, other than expensive thermal or chemical treatments that have known environmental impacts.

Experimental results are provided for various samples with different matrices and starting concentrations, irradiated at doses ranging from 250 kGy to 2 MGy using an accelerator TT300 Rhodotron® 10 MeV e-beam accelerator. Water samples underwent analysis through Solid Phase Extraction (SPE) and LC-MS/MS using an Aquity Iclass LC and Orbitrap Q Exactive MS/MS. In addition to experimental analysis, a radio-kinetic model based on ordinary differential equations was employed to monitor the transformation of PFAS parent and descendant compounds. This approach specifically assessed the degradation of PFOA or PFOS through interactions with aqueous electrons and OH• radicals. Moreover, this modeling approach—when integrated with physics-informed AI—can forecast the irradiation dose necessary to achieve a tenfold reduction in PFAS concentrations.

Other results related to new PFAS and halogenated compounds will also be presented.