1. Research project objectives

The scientific aim is to obtain a wide knowledge on reduction reactions driven by novel types of reductive radical species (RRS) and hydrated electrons with organic compounds in aqueous phase. These studies should provide several scientific findings with high usefulness for development of advanced chemical treatment processes for degradation of organic pollutants in water and wastewater.

Highly reactive species causing reduction reactions are able to provide great effectiveness for degradation of organic compounds that are persistent for oxidation, thus developed processes will be an alternative to widely studied Advanced Oxidation Processes (AOPs).

RRSs will be generated from several precursors (chemicals). Selected precursors and formed RRSs were - till now - not studied for ARPs. Possibility of formation of RRSs will be studied for activation methods such as photolysis, catalysis, photocatalysis and cavitation.

As formed RRSs will be used directly to degrade organic pollutants as well as to form secondary RRSs with other chemicals, enhancing overall effectiveness as well as providing different degradation mechanism and selectivity.

2. Research project methodology

Planned studies will be done for several groups of compounds – emerging pollutants present in water as well as industrial effluents. Target pollutants will be partially or fully halogenated, some will contain nitrogroups and/or unsaturated bonds. Types of degraded chemical compounds containing such atoms/functional groups will belong to PFAS, pharmaceuticals, pesticides, and will include different types of organic compounds. Several reaction systems will be used in this project based on UV and visible light aided processes, hydrodynamic cavitation (HC) and sonocavitation (SC). Degradation of target pollutants will be controlled by modern analytical techniques, including chromatographic techniques (GC, UHPLC, IC with various detectors, including MS technique); COD, TOC and BOD; biotoxicity evaluation; RRSs analysis by EPR and scavenging tests. Other techniques (DFT calculations, Quantum Chemistry/Molecular Mechanics (QC/MC) and Ab Initio Molecular Dynamics (AIMD), ICP-OES, elementary analysis) are planned to be used for deep evaluation of important aspects of the process (mechanism, leaching of metals from catalysts, changes in overall effluents composition etc.). Studied systems will be compared in terms of degradation effectiveness, radical yield, selectivity, degradation mechanisms, kinetics, matrix effects (cations, anions and natural organic matter effects), type of formed by-products and their toxicity. For each developed process, optimal conditions will be determined along with evaluation of its energetic and chemical efficiency.

3. Expected impact of the research project on the development of science

Precursors of RRSs, that will be used for this project are of natural origin and biodegradable, thus developed solutions will be a green alternative to currently used technologies. This project assume also application of novel types of catalysts and photocatalysts, that can significantly improve process efficiency. Combined systems, including proposed methods of process intensification, can allow to develop entirely new strategy for reductive degradation processes for water and wastewater treatment. Research done under the framework of currently submitted project should results in publications in best journals in the discipline. The published outcomes of this project are expected to make a significant impact on the discipline, providing a strong foundation for future investigations. The research will reveal key mechanisms underlying the activation of novel reducing agents, introduce novel types of reductive radical species, and support the optimization of process parameters to maximize treatment efficiency. It will also enable the identification of compound classes that undergo effective transformation under the studied conditions. This fundamental knowledge paves the way for extended research, particularly in developing water and wastewater treatment applications. Future directions may include the design of tailored catalysts (belonging to the types studied in this project) to enhance ARPs, exploration of novel external reductant systems, and application-focused studies targeting specific pollutant groups, especially within industrial wastewater contexts in the broader scope of environmental science.