The Challenge of

Micropollutants

in Aquatic Systems

Background: The Challenge of Micropollutants in Aquatic Systems.

About one-fifth of the world's population does not have access to safe water, and two-fifths suffer the consequences of unacceptable sanitary conditions. Pathogens in water cause more than 2 million deaths annually; most are children under the age of 5. The increasing chemical pollution of surface and groundwaters, with largely unknown long-term effects on aquatic life and on human health, could easily lead to a problem of similar or even greater magnitude. More than one-third of the Earth's accessible renewable freshwater is used for agricultural, industrial, and domestic purposes, and most of these activities lead to water contamination with numerous synthetic and geogenic compounds. It therefore comes as no surprise that chemical pollution of natural waters has already become a major public concern in almost all parts of the world. To date, an effective and sustainable global strategy against this insidious and mostly unseen contamination of aquatic environments barely exists. Current challenges are to predict ecosystem responses, to optimize treatment technologies, and to develop integrated policies at the scale of river basins.

Research Area: Advanced Oxidation Processes (AOPs) for

Pollutant Removal

Advanced oxidation processes (AOPs) have become a mainstream technology for the removal of emerging contaminants from wastewater (Ashina et al. 2025). The strong oxidative nature of chemicals used in these processes leads to the mineralization of even non-biodegradable compounds (Brillas 2025). Oxygen species such as ozone (O_3), hydroxyl radicals (•OH), and sulfate radicals (SO_4•-) have been widely utilized in AOPs due to their potent oxidizing capabilities(Gao et al. 2023, Wang and Wang 2021). The degradation efficiency of emerging contaminants through AOPs is typically expressed in terms of oxidation rates, with compounds exhibiting higher oxidation rates being more easily removed by these processes (Liu et al. 2022).

Research gaps：The Applicability Evaluation of AOPs for Pollutant Removal

However, evaluating the applicability of AOPs in removing a particular class of emerging contaminants solely based on the oxidation rate presents certain limitations. The risk posed by emerging contaminants stems from both the difficulty of their removal and their toxicity. There are significant variations in the toxicity of different emerging contaminants, and using the oxidation rate alone to represent their potential risk is incomplete. For example, acetaminophen has a relatively low oxidation rate, yet it is considered a low-toxicity and safe drug (Eskandarian et al. 2016, Qin et al. 2020). Therefore, focusing solely on the oxidation rate while overlooking the toxicity of the compound makes it challenging to accurately assess the potential health risks to humans after AOP treatment. This underscores the urgent need for a risk assessment system that simultaneously considers both the toxicity and oxidation rate of emerging contaminants.

Machine learning-based quantitative structure-activity relationship (QSAR) models integrate mathematical statistics with the chemical structure of substances, offering an effective approach to predict the oxidation rate and toxicity of compounds (Lin et al. 2024, Yin et al. 2025). The oxidation rate of a compound is closely related to its molecular structure. Sulfate radicals ($SO_4^{\bullet-}$) tend to disrupt aromatic rings and amine groups through single-electron transfer, hydroxyl radicals (•OH) prefer to attack sulfonyl structures and unsaturated carbon atoms via radical addition, while ozone (O_3) degrades hydroxyl and unsaturated carbon atoms through hydrogen abstraction and the Crisegee mechanism (Rizzo et al. 2019, Xie et al. 2022). At the same time, the toxicity of a compound may vary based on its structural characteristics. For instance, compounds containing halogens often exhibit more severe toxic effects, including carcinogenicity, growth abnormalities, reproductive dysfunction, and immune-toxic instability (Andrzejczyk et al. 2020, Ding et al. 2024). Nevertheless, current studies have yet to integrate structure-property relationships that account for both oxidation rate and toxicity, leaving a gap in understanding their interplay.

Research Goals：Machine Learning-Based Risk Assessment in AOP Systems

This study aims to explore the synergistic relationship between the oxidation rates and toxicities of emerging contaminants using an interpretable soft-parameter sharing-based multitask deep learning (MTDL) model. By constructing QSAR models that link a compound's molecular structure with its oxidation rates and toxicities, this study identifies key functional groups affecting the applicability of AOPs in removing emerging contaminants. Our findings will offer more precise and comprehensive guidance for the risk assessment of emerging contaminants in the context of AOP treatment.