

Editorial

Advanced Oxidation Processes for Removal of Emerging Contaminants in Water

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Abstract: This Special Issue includes manuscripts on mechanistic understanding, development, and implementation of advanced oxidation processes (AOPs) for the removal of contaminants of emerging concern in water and wastewater treatment. The main goal was successfully achieved under the joint effort of authors, anonymous reviewers, and editorial managers. Totally, one review and 15 research papers are included in the Special Issue. These are mainly focused on catalyst synthesis, reactor design, treatment performance, kinetic modeling, reaction mechanisms, and by-product formation during electrochemical, photocatalytic, plasma, persulfate, chlorine, ozone-based, and Fenton-related AOPs at different scales. This Special Issue received attention from researchers from different parts of the world such as Argentina, Brazil, Canada, China, Germany, India, Mexico, and the USA. The guest editors are happy to see that all papers presented are innovative and meaningful, and hope that this Special Issue can promote mechanistic understanding and engineering applications of AOPs for the removal of contaminants of emerging concern in water.

Keywords: advanced oxidation; concern; contaminant; electrochemical; emerging; hydroxyl radical; oxidation; ozonation; persulfate; photocatalysis; radical; UV; chlorine; UV/chlorine; Fenton; plasma; water



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1. Introduction

Efficient and cost-effective removal of various contaminants in water matrices is a major challenge in water and wastewater treatment [1,2]. In this regard, advanced oxidation processes (AOPs) have been considered a promising option because highly reactive radicals such as hydroxyl and sulfate radicals generated in AOPs can effectively oxidize a broad range of emerging contaminants; other radicals such as reactive chlorine and nitrogen radicals can also play significant roles [1,3–5]. Nevertheless, the practical application of AOPs is challenged by the high energy demand, formation of harmful oxidation byproducts, difficulty in scaling up, etc. [3,6,7]. Therefore, both novel mechanistic understanding and improved engineering designs are needed to overcome these challenges and thus bridge academic research with practical applications.

In this Special Issue, we attempted to focus on the mechanistic understanding, development, and implementation of AOPs for the removal of emerging contaminants in water and wastewater treatment. Ozone-, UV-, H₂O₂-, chlorine-, persulfate-based AOPs, electricity-driven AOPs, and photocatalytic AOPs were among the technologies of interest in this Special Issue. Relevant topics of interest included reaction kinetics, catalyst fabrication, model simulation, theoretical calculations, by-product formation, and degradation mechanisms. Topics on reactor design, economic evaluation, and experiments at different scales (lab- and pilot-scale) were also of interest.

2. Summary of This Special Issue

Two papers were published on the topic of persulfate technology. In Liu et al. [8], the authors investigated the degradation of acyclovir and atenolol by the UV/peroxydisulfate (UV/PDS) process from the perspective of degradation kinetics, model simulations, and reaction pathway. Results show that the UV/PDS process could effectively generate sulfate radicals ($\text{SO}_4^{\bullet-}$) and hydroxyl radicals ($^{\bullet}\text{OH}$) to remove the two micropollutants, with $\text{SO}_4^{\bullet-}$ playing a more significant role in the process. In the other study, Mo et al. [9] focused on the synthesis of a copper-magnesium oxide/carbon nitride composite (CM/g- C_3N_4) to activate peroxymonosulfate (PMS). The CM/g- C_3N_4 presented superior catalytic performance and reusability for PMS activation and Rhodamine B (RhB) degradation, and $\text{SO}_4^{\bullet-}$ and singlet oxygen ($^1\text{O}_2$) were found to be important for RhB removal. Therefore, different oxidant species can be generated by various activation methods during the persulfate oxidation process, which is beneficial for the degradation of micropollutants with varying reactivities.

The electrochemical oxidation process is another effective technology for micropollutant removal. For instance, Yanagida et al. [10] used the boron-doped diamond (BDD) electrode to electrochemically oxidize PFAS in contaminated water and then scaled up the technology for the treatment of 189 L of PFOA and PFOS-contaminated water. LC/MS/MS analysis results show that micrograms per liter (ppb) PFAS could be easily degraded by BDD electrochemical oxidation. Considering the great importance of electrode material, da Silva et al. [11] evaluated the performance of three anodes (Ni/BDD, Ti/Pt, Ti/ RuO_2) to treat groundwater contaminated by petroleum-derived fuel, with the Ti/ RuO_2 anode achieving the highest chemical oxygen demand (COD) degradation efficiency and lowest energy consumption. Besides, a pilot-flow plant was established to further verify the viability of electrochemical treatment at a larger scale.

In addition to electrochemical oxidation, a heterogeneous electro-Fenton (HEF) process using MnFe_2O_4 -GO catalyst was employed to remove Rhodamine B from aqueous solution [12]. This study focused on the efficiency of electrodes and catalyst, as well as their application in real textile wastewater treatment. Significant color reduction and obvious biodegradability enhancement were observed after treatment. Two other Fenton-related studies were also reported in this Special Issue. In the study of Olea-Mejia et al. [13], a $\text{Cu}_2\text{O}/\text{Al}_2\text{O}_3$ catalyst was synthesized to improve Bisphenol A (BPA) oxidation and mineralization during the photo-Fenton process driven by UV radiation and visible light. Besides, Lin et al. [14] applied the Fenton process to treat acrylic manufacturing wastewater. The results show that total organic carbon and nitrogen can be effectively removed to meet related discharge standards, providing a successful example of industrial wastewater treatment by the Fenton technology.

Three papers on the photocatalytic process were included in this Special Issue. In Juárez-Cortazar et al. [15], TiO_2 was doped with metal waste (door key) to improve its photocatalytic efficiency, and a synergistic effect of the dopants and TiO_2 was achieved for diclofenac mineralization. Meanwhile, Mehling et al. [16] investigated the energetic efficiency of TiO_2 photocatalysis from a different perspective, i.e., reactor design. Three reactor systems were evaluated, with catalyst arrangement and irradiation power identified as the major influencing parameters on energy consumption performance. Other than TiO_2 doping and reactor design, Manassero et al. [17] focused more on radiation modeling and kinetics in different photocatalytic reactors. In their study, a strategy was proposed to obtain intrinsic kinetic parameters independent of reactor geometry, reactor size, and irradiation conditions. The results indicate that the radiation model can be employed for photocatalytic reactor design, optimization, and scaling-up, thus bridging the gap between laboratory experiments and real applications.

Ozone-based AOP, as a promising research and development option, was investigated from two different perspectives in this Special Issue. In the study of Luo et al. [18], ozonation was combined with electro-coagulation (i.e., the electro-hybrid ozonation-coagulation process) to remove surfactant and microplastics from laundry wastewater. In addition,

Zhang et al. [19] prepared a mesoporous CeO₂ by the nano-casting method and applied the catalyst for the catalytic ozonation of atrazine. The well-ordered mesoporous structure, high surface area, and redox Ce³⁺/Ce⁴⁺ cycling contributed to the superior activity of the synthetic CeO₂. Both studies present the effectiveness and important role of ozone-based AOPs in the removal of emerging contaminants in water.

Plasma technology was also reviewed and studied in this Special Issue. In the research paper of Liu et al. [20], a novel reactor was designed for simulated dye wastewater treatment by plasma in the presence of various catalysts, and the results show that the plasma/PS/Fe²⁺ system achieved the best synergy and highest removal rate. In the review paper of He et al. [21], they summarized recent research progress on non-thermal plasma technique for remediation of water and soil contaminated by emerging organic pollutants in terms of pollutant degradation mechanism, the synergy of non-thermal plasma with other techniques, bottlenecks, and suggestions to promote plasma technology toward practical applications.

Besides, one paper investigated the removal of emerging contaminants by novel material adsorption [22]. Specifically, a carbon material was derived from the nitrogen-rich bio-based metal-organic framework (MOF) and was evaluated as an adsorbent for pharmaceutical elimination from the water environment. The high surface area and abundant mesoporous structure of the obtained MOF contributed greatly to hydrophobic pharmaceutical removal.

In addition to contaminant removal, the study of Li et al. [23] paid attention to disinfection by-product (DBP) formation during medium-pressure UV/chlorine AOP. Results show that DBP formation is highly dependent on the precursor activity, solution pH, and the presence of Br⁻. The authors suggest that the UV/chlorine-induced change in total chlorine demand might be taken as an indicator to predict the change in DBP formation potential.

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