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Editorial

Oxidative Water Treatment: The Track Ahead

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In 2018, *Environmental Science & Technology* (*ES&T*) published a perspective titled, "Oxidation Processes in Water Treatment: Are We on Track?"[1] Five years later, to commemorate the receipt of the 2022 ACS Award for Creative Advances in Environmental Science and Technology by the author of that paper, Prof. Urs von Gunten, the journal commissioned this special issue. Contributions from leaders in the field of oxidative water treatment illustrate the progress that has been made in this important research area while emphasizing the gaps in research that must be addressed to continue our journey toward wider dissemination of technologies that are integral to the provision of safe and affordable water.

Chemical oxidation has been applied in municipal water treatment for more than a century, initially for disinfection. In the early decades, chlorine disinfection was adopted in the fight against waterborne disease. However, the oxidative properties of chlorine had an unintended side effect, generation of potentially toxic disinfection byproducts (DBPs). To mitigate this issue, alternative disinfectants such as chlorine dioxide, chloramine, and ozone were employed, but they posed a different set of hazards.[2] Eventually, it was recognized that operators of drinking water treatment plants had to strike a balance between disinfection and DBP formation. Today, a multidisciplinary approach that combines tools from analytical chemistry, engineering, toxicology, and epidemiology is being employed to navigate the disinfection/DBP trade-off.[3]

Chemical oxidation also has been applied for many decades to control chemical contaminants, initially for improvement of the aesthetic qualities of water. By the late 1970s, oxidants also were being used to treat synthetic organic compounds, termed micropollutants or trace organic contaminants. Chemical oxidation was employed first for abatement of nonpolar contaminants (chlorinated solvents, pesticides, and fuel additives). As analytical methods improved and water utilities pursued enhanced wastewater treatment and potable water reuse, treatment was extended to polar micropollutants, including pharmaceuticals, personal care products, endocrine disruptors, and industrial chemicals.[4]

As the variety of chemicals requiring treatment expanded, a second trade-off became evident. Selective oxidants, such as permanganate, chlorine dioxide, and chlorine, are advantageous for treatment of waters containing mainly one compound class (e.g., phenolic compounds) because such contaminants can be treated with a high oxidant use efficiency. Advanced oxidation processes (AOPs) that employ a combination of oxidants (e.g., O_3 with H_2O_2) or use ultraviolet light (e.g., UV with H_2O_2 or UV with chlorine) generate hydroxyl radical ($^{\bullet}OH$) and other short-lived oxidants. These reactive species oxidize a wider range of chemicals and are thus attractive for the treatment of water that contains multiple contaminants of concern. Broad reactivity usually is accompanied by low oxidant use efficiency because a substantial fraction of the oxidant reacts with nontarget solutes, like dissolved organic matter. Ozone is a special case because it can achieve high selectivity for some compounds through direct reactions while simultaneously producing enough $^{\bullet}OH$ to abate compounds that lack functional groups that are susceptible to direct oxidation. Thus, the users of oxidative treatment technologies must navigate the trade-off between selectivity and efficiency.

The disappearance of target compounds during oxidation is often accompanied by a decrease in their biological effects. However, ensuring that none of the transformation products produced during oxidative treatment exhibit toxicity is extremely challenging. Mineralization of target compounds, the simplest way of ensuring the loss of toxicity, is cost-prohibitive for typical treatment conditions and is often accompanied by the production of high concentrations of DBPs. Thus, oxidative treatment has a third trade-off, the need to balance the benefits of abatement of micropollutants against undesired side effects, like the formation of toxic transformation products and DBPs. These risks can be minimized through a rigorous assessment approach that considers reaction kinetics, the formation of transformation products, and toxicological assessment.

Oxidative treatment of micropollutants has reached a point at which full-scale systems are being designed, optimized, and operated effectively for homogeneous phase processes, such as O_3, O_3 with H_2O_2, and UV with H_2O_2. Approaches that are better suited for specialized applications, like abatement of contaminants that are difficult to treat, including photolytic, (photo)catalytic, and electrochemical methods, have not reached the same level of maturity.[5] In addition to expanding the range of compounds that can be treated, electricity-based methods, such as those involving electrochemical production and/or activation of oxidants, have great potential for application in decentralized systems because they do not require the transport and remote management of chemicals.[6] Further development of robust electrode materials as well as

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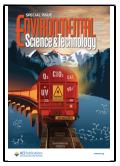

refinement of kinetics-based predictive tools, especially for processes taking place at the solid−water interface, is necessary for these emerging technologies to be adopted more widely.

Given the vast number of micropollutants and transformation products formed during oxidative water treatment, it is impractical to identify and experimentally evaluate their biological effects and potential for producing toxic byproducts. Here, *in silico* approaches for predicting degradation pathways and toxicology/biodegradability are needed to screen for compounds that deserve further analysis. Computer-based tools capable of predicting degradation pathways are available for ozone and $^{\bullet}OH$,[7,8] but further refinement is needed to improve their performance and to extend them to other oxidants. Quantum chemical computation and possibly application of statistical tools like machine learning have great potential to be applied in combination with experimental studies to advance our ability to predict reaction kinetics and product formation.[9] In addition, advanced chemical analysis and toxicological methods [e.g., high-resolution mass spectrometry for (non)target analysis or high-throughput toxicological assays] can contribute new information about transformation products and their toxicity.

Given the complex nature and variability of water sources and the trade-offs inherent in the use of chemical oxidants, it is clear that no single oxidant can be employed for all treatment purposes. Therefore, to stay on track, researchers need to build upon knowledge that has already been generated about chemical oxidants and to employ them in combination with other treatment processes in multiple-barrier systems that create resilience and exploit synergies (e.g., employing biofiltration after chemical oxidation to degrade DBPs). The emergence of highly oxidation-resistant contaminants, such as per- and polyfluoroalkyl substances, reminds us that chemical oxidation is no panacea; rather, it should be considered as one of the many useful tools on *the track ahead* to safe and affordable water.

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