A Guide for JHM authors focusing on Advanced Oxidation and Reduction Processes for Environmental Applications

Shikha Garg, John Atkinson, Sungjun Bae, Baiyang Chen, Yang Deng, Anett Georgi, Zaher Hashisho, Haizhou Liu, Jelena Radjenovic, Danmeng Shuai, Meiping Tong

All are corresponding authors

Over the past decade, JHM has received numerous manuscript submissions on pollutant removal using advanced oxidation and reduction processes, including, but not limited to, Fenton or Fenton-like process, ozone-based technologies, photolysis/photocatalysis, electrochemical processes, single- and double-atom catalysis, and/or piezocatalysis. When editors receive these submissions, there are certain criteria used to decide whether to reject the manuscript or send out the manuscript for peer review. JHM editors have prepared this editorial to provide clarity regarding handling of these types of manuscripts and, more importantly, to highlight aspects making these submissions suitable for publication in JHM.

- "Environmental suitability" of the technology is a key criterion. Experimental conditions used should be environmentally relevant. Performance evaluation performed solely in pure solvents (i.e., unbuffered deionized water, organic solvents, etc.) is not acceptable. Similarly, use of concentrations that are much higher than what is relevant in the environment is also not suitable. While it is agreeable to perform some studies in pure solutions and at magnified concentrations to gain mechanistic insights, authors should also investigate removal in natural/real wastewater matrices and at environmentally relevant pollutant concentrations. Use of surrogate dyes (such as methylene blue, methyl orange, rhodamine B) as a model "pollutant" is discouraged due to their environmental irrelevance. However, authors can use dyes that are used in industry. Many submissions focus on the removal of phenolic compounds (e.g., phenol, bisphenol A, nitrophenol), antibiotics (e.g., tetracycline), and Cr (VI). While these chemicals are good benchmarks for comparing the new material/technology performance with previous studies, their degradation pathways and mechanisms are already well-understood. We encourage authors to study important persistent or emerging contaminants that can attract broad interest in the environmental community.

- Clear description of novelty and environmental relevance of the work in comparison to published research on the topic is required. The novelty of the work should not be limited to synthesis of new material or a new application of the existing material. Authors should highlight the novelty with respect to contaminant-material interaction, material performance in generation of reactive species (RSs), contaminant transformation, and/or the impact of complex environments on contaminant degradation. Research should be generalizable, instead of predominantly focusing on material properties and performance under a narrow set of conditions. Environmental implication that accompanies the manuscript should provide fresh insights on the novelty and relevance of the work to the editors, and not be a reiteration of the abstract.

- For research focussing on developing new materials, a clear delineation of procedures and chemicals used for making new material(s) should be presented to a level that readers can follow and replicate. Authors should avoid presentation of excessive material characterization results at the expense of environmental content. Ideally, crucial material characterizations that explain the performance or structure-activity relationships of the materials should be included in the main manuscript. Other relevant characterizations can be briefly summarized within the manuscript, with detailed information presented as supplementary material. Clear explanation of why the materials work, from a mechanistic perspective, needs to be provided rather than just demonstrating performance improvement for a certain set of conditions. Use of computational tools, such density functional theory (DFT) calculations, to support the role of material properties in the observed effect is encouraged. However, given that idealized material properties and simple matrix properties are used in such model setup, it is essential that the conclusions made based on DFT are also supported by direct experimental evidence. Over-reliance on computational tools to gain mechanistic insights into the process is not acceptable. Similarly, only using computational tools to predict toxicity of degraded contaminants is discouraged.

- The new material/technology should be benchmarked against their rivals in terms of performance, and energy use. It is important to recognize that these comparisons are made under similar operating conditions (pH, contaminant concentration, material dosage, etc.). Similarly, benchmarking cost effectiveness is encouraged, but not required. However, any claims regarding cost competitiveness should be substantiated and the cost analysis should be fair and objective. Authors should explore the limits of new materials rather than showing simple repeatability experiments over a few usage cycles. While it is desirable that authors test performance of the material either for a long period of time or under harsh conditions, such testing can also be part of a future study focussing on stability and robustness of the new material. If long term measurements or testing under harsh conditions is not performed, authors are discouraged from claiming reusability/recyclability, longevity, and robustness of the material. Authors should also consider the environmental impact of the proposed material. Materials with a high potential for leaching of hazardous substances (e.g. heavy metals) should be avoided. If used, their leaching behaviour must be evaluated under realistic conditions of application. Submissions that cannot show stability over even a few usage cycles and/or show significant leaching of hazardous substances (such as heavy metals) will be rejected if material development is the main contribution of the work.

- The mechanistic investigation should be performed in a critical manner. It is also important that authors highlight the operational window within which the mechanism proposed is reasonably applicable. To gain insight into the role of RSs involved in pollutant removal, it is a general trend that authors employ organic scavengers to competitively outcompete the reaction of pollutant with RS and/or employ probe compounds or electron paramagnetic resonance (EPR) to measure RS generation. However, it is important to recognize that these approaches to quantify RSs have limitations, which need to be considered when interpreting results and making conclusions. Some good articles which discuss these limitations are Lee et al, 2020, ES&T,54; Guo et al, 2021, Appl. Catal. B, 280; Lei et al, 2023, ES&T, 57; Chen et al, 2023, ES&T, 57; Garg et al, 2022, ACS ES&T: Engineering, 2, Wang et al, 2022, ES&T, 56, Wang et al, 2021, JHM, 404. [1-7]

- Use of appropriate statistical descriptors (standard deviation, range, error bars etc.) in the data presented is required. Submissions that do not include replication of experimental results will be immediately rejected. Terminology such as "significant change" or "significant increase" should not be used unless relevant statistical testing of significance is shown. The number of significant digits in reported values should be consistent with the estimated error.

- Authors should describe the experimental procedures used for performance evaluation in the main manuscript. It is imperative that authors use appropriate ionic strength and buffers to maintain pH during experiments, given that most of these advanced treatment technologies are strongly influenced by pH and co-existing ions. Most current submissions on this topic employ acid or base to adjust initial pH of contaminant solution prepared in deionized water, however, it is important to recognize that while no buffering capacity was present in this pure contaminant solution, this will not be the case in real wastewater where the presence of buffering ions such as carbonate and/or phosphate ions will resist change in pH. As such, pH changes (and as a result the effect of pH on process performance) in pure solutions will be more severe compared to that will occur during real wastewater treatment. While it is acceptable to avoid use of buffers to gain mechanistic insights if the buffering ions interfere with the treatment process, authors should measure pH changes during experiments and take these pH changes into consideration when interpreting their results. If the pH during experiments is different from initial pH, authors should not conclude that process/catalysts work for that initial pH condition. Unless authors demonstrate good performance of the technology under controlled pH (preferably in the circumneutral pH range), the environmental relevance of the work is not evident.

By adhering to the guidelines outlined here, submissions focussing on advanced oxidation and reduction processes for pollutant degradation will be more likely to align with the journal's scope and engage the wider JHM community.

References

1. Lee, J.; von Gunten, U.; Kim, J.-H., Persulfate-Based Advanced Oxidation: Critical Assessment of Opportunities and Roadblocks. *Environmental Science & Technology* **2020,** *54*, (6), 3064-3081.
2. Guo, Y.; Zhang, Y.; Yu, G.; Wang, Y., Revisiting the role of reactive oxygen species for pollutant abatement during catalytic ozonation: The probe approach versus the scavenger approach. *Applied Catalysis B: Environmental* **2021,** *280*, 119418.
3. Lei, Y.; Yu, Y.; Lei, X.; Liang, X.; Cheng, S.; Ouyang, G.; Yang, X., Assessing the Use of Probes and Quenchers for Understanding the Reactive Species in Advanced Oxidation Processes. *Environmental Science & Technology* **2023,** *57*, (13), 5433-5444.
4. Chen, Y.; Miller, C. J.; Xie, J.; Waite, T. D., Challenges Relating to the Quantification of Ferryl(IV) Ion and Hydroxyl Radical Generation Rates Using Methyl Phenyl Sulfoxide (PMSO), Phthalhydrazide, and Benzoic Acid as Probe Compounds in the Homogeneous Fenton Reaction. *Environmental Science & Technology* **2023,** *57*, (47), 18617-18625.
5. Garg, S.; Yuan, Y.; Mortazavi, M.; Waite, T. D., Caveats in the Use of Tertiary Butyl Alcohol as a Probe for Hydroxyl Radical Involvement in Conventional Ozonation and Catalytic Ozonation Processes. *ACS ES&T Engineering* **2022,** *2*, (9), 1665-1676.
6. Wang, L.; Li, B.; Dionysiou, D. D.; Chen, B.; Yang, J.; Li, J., Overlooked Formation of H2O2 during the Hydroxyl Radical-Scavenging Process When Using Alcohols as Scavengers. *Environmental Science & Technology* **2022,** *56*, (6), 3386-3396.
7. Wang, L.; Chen, Y.; Chen, B.; Yang, J., Generation of hydroxyl radicals during photodegradation of chloroacetic acids by 254 nm ultraviolet: A special degradation process revealed by a holistic radical determination methodology. *Journal of Hazardous Materials* **2021,** *404*, 124040.