Chem Catalysis

CellPress

Activity

Key engineering design aspects of photo-assisted electrochemical reactors for water treatment

Ashley Hesterberg Butzlaff[1,*] and Mohamed Ateia[1,2,*]

Ashley Hesterberg Butzlaff (environmental engineer at the US Environmental Protection Agency) and Mohamed Ateia Ibrahim (environmental engineer and group leader at the US Environmental Protection Agency and adjunct assistant professor at Rice University) delve into the pivotal role of reactor design parameters and tools in advancing the performance and scalability of photo-assisted electrochemical systems for water treatment. These insights highlight the necessity of precise reactor design in optimizing efficiency, ensuring scalability, and ultimately transforming water-purification technologies.

Traditional UV reactors ensure robust disinfection for full-scale water treatment, but simple design also limits innovations in photochemical (PC) water treatment. If reactor design is carefully reevaluated, then PC treatment can provide attractive opportunities to integrate additional (i.e., electrochemical [EC]) processes for improved synergetic treatment efficacy. Current literature studies have already leveraged this opportunity by arranging PC and EC unit operations in series. However, the integration of the two fundamental processes into a single unit operation is still lacking. Photo-assisted EC (PEC) systems promise to provide enhanced treatment efficacy by synergistically combining PC and EC processes in the pre-existing treatment footprint. PEC systems cannot meet these high expectations until the individual components (e.g., light source and photoelectrodes) are integrated in well-designed reactors. PEC efforts were first limited to solar water splitting, but an accelerating environmental focus now drives the demand for PEC pollutant degradation. This article outlines the critical design parameters and performance metrics for developing efficient PEC reactors for water treatment.

A.H.B. discusses reactor types and configurations

PEC reactors are commonly studied at the bench scale in batch mode (Figure 1A)—historically for solar water splitting—but flow reactors (Figure 1B) are imperative to satisfy the operational requirements for continuous operation in existing water-treatment systems. For EC and PEC reactors, flow configuration is often defined by the electrode material, shape, and position.[1,2] Thin-film or plate electrodes are most commonly employed, but these materials allow for only the flow-by configuration. Because of their photoactive advantage, flexible and transparent thin-film electrodes could overcome mass-transfer limitations across diverse reactor types. The flow-through configuration, which can significantly decrease mass-transfer limitations, becomes possible with the use of porous and/or three-dimensional electrodes. However, flow across three-dimensional electrodes introduces a pressure drop that will govern operational parameters and overall system performance. Divided reactors require an additional physical component, most commonly an ion-exchange membrane, but conveniently provide control over pH and reaction products without the need for chemical inputs (e.g., buffers).

There are two fundamental physical laws that are integral to PEC reactor design: the Beer-Lambert law and Ohm's law. The Beer-Lambert law guarantees transmittance losses between the working electrode (WE) and the light source, whereas Ohm's law sustains potential losses between the WE and the counter electrode (CE). Therefore, PEC reactor design depends on the distance between and placement of these three key components (the WE, CE, and light source). The reactor must maximize incident light at the electrode surface, where direct electron transfer occurs. Sunlight could be a viable light source with continued innovations in (photo)electrode materials—as accelerated by PEC water splitting—but reactor design must cater to the external radiation. Multiple light sources, adjustable light intensity, or concentrators (reflectors and lenses) could be necessary to compensate for transmittance losses, especially in complex or turbid matrices. The electrode position, within the reactor and with respect to each other, will affect reactor hydrodynamics (flow pattern and uniformity) and current distribution. The placement of these key components affects not only treatment performance (e.g., degradation efficiency) but also capital cost and energy consumption. Reactor considerations, as discussed above, could be increasingly important if photo-processes are to be integrated

[1]Center for Environmental Solutions and Emergency Response, US Environmental Protection Agency, Cincinnati, OH, USA

[2]Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA

*Correspondence:
butzlaff.ashley@epa.gov (A.H.B.),
ibrahim.mohamed@epa.gov (M.A.)

https://doi.org/10.1016/j.checat.2024.101031

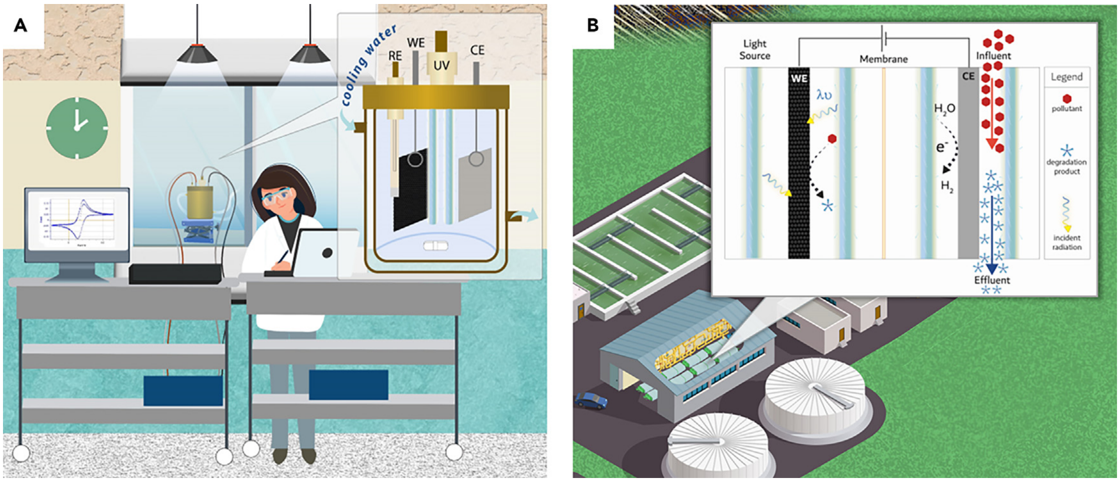

Figure 1. Schematic illustrating photoelectrochemical systems
(A) Commonly tested batch-mode systems at the bench scale.
(B) Representative flow system for full-scale treatment applications.

into microbial electrolysis cells (MECs) for high performance.[3]

Reactor scale-up

PEC treatment feasibility, efficiency, and energy consumption cannot be determined from the existing body of knowledge because previous studies were often conducted at the lab scale.[1] Increased efforts must be devoted to PEC reactor scaling so that realistic performance evaluations can be made across treatment technologies. For instance, full-scale PEC reactors should provide the same volumetric capacity as comparable single-unit operations for existing treatment technologies (e.g., reverse osmosis). Moreover, full-scale reactors need extensive testing in various arrangements (in series and in parallel). There is also a need to evaluate reactor performance in real matrices with diverse water-quality parameters (organic content and salinity). In particular, residual waste streams that are concentrated prior to PEC treatment provide increasingly favorable economics as a result of decreased treatment volumes and energy consumption relative to dilute concentration conditions.[4] The complex nature of this design challenge requires diverse multi-disciplinary teams—consisting of chemical, electrochemical, and environmental engineers—to develop high-performing PEC reactors at scale. Because of the many interrelated parameters for reactor design, the performance of each electrode-reactor-influent combination must not be widely prescribed to similar combinations with different materials, configurations, or influent characteristics.

Reactor design tools

It is critical to identify the trade-offs between design parameters, overall performance, and functionality; these trade-offs can be more easily identified and elucidated with the help of multiphysics simulation. Current multiphysics software (e.g., COMSOL) have been used to identify optimal operational parameters for the design of electrochemical systems,[5] which encourages modeling of PEC systems. The complicated environment of the PEC reactor provides a rich opportunity to examine the intimate relationships between mass transfer, charge transfer, fluid dynamics, and optics. Experimental tracer studies can complement modeling by providing full characterization of hydrodynamics and mass transport. Real-time monitoring can estimate operational parameters and elucidate mechanisms for refining PEC performance. Lastly, additive manufacturing provides an opportunity to easily customize and quickly produce reactors and associated components. The collective use of these effective tools will create interdisciplinary collaboration and accelerate reactor design.

M.A. responds: Innovative reactor design motivated by modeling tools

I appreciate the comprehensive discussion on engineering design considerations for PEC water-treatment systems. This response aims to provide additional thoughts on (1) combining modeling with experiments for enhanced design insights, (2) exploring alternative reactor designs for decentralized treatment, and (3) leveraging photocatalytic membranes for water treatment.

To enhance PEC reactor design, the integration of computational fluid dynamics (CFD) modeling with experimental flow visualizations and tracer analysis can provide valuable insights into reactor hydrodynamics.[6] Extending CFD models to simulate PEC reactions, multiphysics interactions, and radiative transfer could enable predictive virtual prototyping. Additionally, incorporating computational optimization algorithms and machine-learning techniques can accelerate the optimized development of PEC reactors.[7]

For resource-limited environments, alternative reactor designs such as rotating bed PEC reactors offer simplicity by eliminating the need for pumps. Rotating fluidized bed PEC reactors with catalyst-coated particles have demonstrated the potential for contaminant degradation. Floating PEC reactors that extract water from below and discharge treated water on the surface represent another innovative option for *in situ* treatment. Exploring alternative reactor designs further can satisfy decentralized treatment needs.[8]

Photoelectrocatalytic membrane (PEM) reactors that combine membrane filtration with PEC technology present opportunities for producing high-purity water while oxidizing recalcitrant organics.[9] Submerged PEC-membrane bioreactors suggest a promising reactor configuration based on the robust performance of EC-membrane bioreactors for both inorganic and organic removal.[10] Investigating photocatalytic electrodialysis and flow-through PEC membrane reactors can lead to more compact and efficient systems.

In summary, by combining modeling and experiments, exploring alternative reactor designs, and leveraging photocatalytic membranes, we can advance the design and optimization of PEC water-treatment systems. These approaches contribute to the development of sustainable and effective solutions for water purification and contaminant removal.

ACKNOWLEDGMENTS

This document has been subjected to the US Environmental Protection Agency's review and has been approved for publication. The views expressed in this article are solely those of the authors and do not necessarily represent the views or policies of the agency. Any mention of trade names, products, or services does not imply an endorsement by the agency. The agency does not endorse any commercial products, services, or enterprises.

DECLARATION OF INTERESTS

The authors declare no competing interests.

REFERENCES

1. Zhang, X., Yu, W., Guo, Y., Li, S., Chen, Y., Wang, H., and Bian, Z. (2023). Recent advances in photoelectrocatalytic advanced oxidation processes: From mechanism understanding to catalyst design and actual applications. Chem. Eng. J. *455*, 140801.
2. Walsh, F.C., and Ponce de León, C. (2018). Progress in electrochemical flow reactors for laboratory and pilot scale processing. Electrochim. Acta *280*, 121–148.
3. Wang, L., Du, H., Elsyed, A.F.N., Yun, N., Wang, X., and Rossi, R. (2024). Impact of reactor architecture and design parameters on the performance of microbial electrolysis cells revealed by the electrode potential slope analysis. Electrochim. Acta *485*, 144072.
4. Urtiaga, A. (2021). Electrochemical technologies combined with membrane filtration. Curr. Opin. Electrochem. *27*, 100691.
5. Castro, J.A., López-Maldonado, J., Cárdenas, J., Orozco, G., Bustos, E., and Rivera, F.F. (2022). Design of an electrochemical flow reactor prototype to the electro-oxidation of amoxicillin in aqueous media using modified electrodes with transition metal oxides. J. Environ. Chem. Eng. *10*, 107165.
6. Rodríguez, A., Rivera, F.F., Orozco, G., Carreño, G., and Castañeda, F. (2018). Analysis of inlet and gap effect in hydrodynamics and mass transport performance of a multipurpose electrochemical reactor: CFD simulation and experimental validation. Electrochim. Acta *282*, 520–532.
7. Luo, J., Canuso, V., Jang, J.B., Wu, Z., Morales-Guio, C.G., and Christofides, P.D. (2022). Machine learning-based operational modeling of an electrochemical reactor: Handling data variability and improving empirical models. Ind. Eng. Chem. Res. *61*, 8399–8410.
8. Udomkittayachai, N., Xue, W., Xiao, K., Visvanathan, C., and Tabucanon, A.S. (2021). Electroconductive moving bed membrane bioreactor (EcMB-MBR) for single-step decentralized wastewater treatment: Performance, mechanisms, and cost. Water Res. *188*, 116547.
9. Wang, X., Wang, G., Chen, S., Fan, X., Quan, X., and Yu, H. (2017). Integration of membrane filtration and photoelectrocatalysis on g-C_3N_4/CNTs/Al_2O_3 membrane with visible-light response for enhanced water treatment. J. Membr. Sci. *541*, 153–161.
10. Asif, M.B., Maqbool, T., and Zhang, Z. (2020). Electrochemical membrane bioreactors: State-of-the-art and future prospects. Sci. Total Environ. *741*, 140233.