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Amaya Santos, Gema; Ali, Agha Zeeshan; Lettieri, Paola

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Sustainable advanced wastewater treatment via photoelectrocatalytic oxidation: insights from life cycle assessment

Gema Amaya Santos[1], Agha Zeeshan Ali[2,3] & Paola Lettieri[1] ✉

This study presents a life cycle assessment (LCA) of a scaled-up photoelectrocatalytic (PEC) oxidation system for wastewater treatment, modelled using computational fluid dynamics (CFD). The system used a $BiVO_4/TiO_2$-GO photoanode for solar-driven degradation of micropollutants. The LCA assesses energy use, resource demand, and emissions to evaluate the system's sustainability in line with EU wastewater regulations. Compared to a full-scale ozonation plant in the Netherlands, the PEC system shows superior environmental performance during operation and end-of-life phases, despite higher construction impacts. Solar energy use and potential material reuse drive these advantages. A comparison with theoretical pilot-scale oxidation technologies from literature adds depth, though the study acknowledges limitations such as micropollutant variability and wastewater complexity. Overall, the findings highlight PEC oxidation's promise as a sustainable and effective approach for micropollutant removal in water treatment.

Water pollution is a major environmental concern exacerbated by factors such as industrial growth, population expansion, and water scarcity[1]. The importance of clean water and sanitation has been recognized by the United Nations, by including them as one of their Sustainable Development Goals[2]. As a primary source of drinking water, the preservation of surface water bodies is paramount[3]. Wastewater generated from domestic, industrial and commercial activities can trigger environmental processes that inflict severe damage upon ecosystems when inadequately treated. This underscores the uppermost importance of research within the field of wastewater treatment which prioritizes ensuring the safety of wastewater treatment plan (WWTP) effluents for aquatic life and human health[4]. This emphasis is particularly critical given the potential for micropollutants, such as pharmaceuticals and industrial chemicals to contaminate water bodies through WWTP effluent. These contaminants can produce harmful effects on aquatic ecosystems and human health, including endocrine disruption, toxicity and bioaccumulation[5,6]. Therefore, the development and implementation of efficient wastewater treatment technologies capable of effectively removing these micropollutants before their release into the environment is imperative[7].

To address the pressing issue of micropollutant contamination in wastewater, advanced oxidation processes (AOPs) have emerged as promising end-of-pipe solutions for WWTP effluents[8,9]. AOPs generate highly reactive oxidative species, such as hydroxyl radicals (OH·) in situ. These radicals can effectively decontaminate water through their potent oxidizing power, which enables them to rapidly react with organic molecules, even those that are difficult to oxidize[10,11]. Various methods can be employed to generate oxidative radicals in AOPs. One approach involves adding chemical substances, such as hydrogen peroxide or ozone, to enhance oxidation. Another method utilizes photo-assistance, where ultraviolet radiation promotes the oxidation of organic molecules. Additionally, oxidative radicals can be generated using radical generation promoter elements. Electrochemical advanced oxidation processes (eAOPs) represent a novel technology for generating oxidative radicals. In eAOPs, radicals are produced through electron transfer rather than the addition of chemical reagents, making them a cleaner alternative[12].

Photoelectrocatalytic (PEC) advanced oxidation processes are emerging as a promising technology for wastewater treatment due to their ability to utilize solar energy to generate reactive species. These processes employ semiconducting anode materials to produce in situ oxidants, primarily hydroxyl (OH·) and superoxide ($O_2^{\bullet-}$) radicals, which effectively oxidize organic pollutants[13]. While metal oxide-based photocatalysts like TiO_2,

[1]Department of Chemical Engineering, University College London, London, UK. [2]Department of Water Management, Faculty of Civil Engineering and Geosciences, Delft University of Technology, GA Delft, the Netherlands. [3]Center of Expertise MNEXT, Avans University of Applied Sciences, Breda, the Netherlands.
✉e-mail: p.lettieri@ucl.ac.uk

WO_3, ZnO, ZrO_2 and Fe_2O_3 have been widely studied, their large band gap energy limits their photon absorption capacity. Bismuth vanadate ($BiVO_4$) offers a more suitable alternative due to its smaller bandgap and ability to absorb visible light. Moreover, its stability and non-toxicity make it an ideal anodic material for PEC-based micropollutant removal[14,15]. The PEC activity of $BiVO_4$ can be significantly enhanced by forming heterojunctions with other photocatalysts, such as bismuth oxyodide (BiOI) or graphene oxide (GO). Previous studies have explored the application of $BiVO_4$/BiOI heterojunction photoanode for simultaneous micropollutant removal[16]. Graphene oxide (GO) is a photoactive semiconductor material that has been explored for its potential in water applications, particularly when combined with TiO_2 in heterojunction configurations[17]. This combination enhances the specific surface area available for pollutant adsorption. Recent research carried out by Ali et al.[18] demonstrated the effectiveness of $BiVO_4$/TiO-GO heterojunction photoanodes for the simultaneous removal of difficult-to-treat micropollutants, including benzotriazole (BTA), carbamazepine (CBZ), caffeine (CAF), and diclofenac (DIC). Using a controlled laboratory setup, the researchers evaluated the performance of the photoanodes by measuring the removal rate coefficients of these pollutants in deionized water. Building upon these findings, they utilized computational fluid dynamics (CFD) modeling to stimulate the performance of a scaled-up reactor. While CFD has been used to assess photocatalytic degradation, its application to the simultaneous removal of multiple, low-concentration micropollutants is limited[19]. The authors[18] used CFD modeling to extrapolate the experimental findings to a scaled-up PEC reactor for a minimum of 80% removal rate of multiple micropollutants from water. This successful CFD extrapolation leveraged the established value of CFD in photocatalytic reactions and addressed the application of such modeling to multi-micropollutant removal at low concentrations.

The European Union provides a robust regulatory and financial framework that incentivizes advanced tertiary and quaternary treatment technologies. Under the Water Framework Directive[20], Member States must monitor and reduce priority substances including many organic micropollutants[21]. More recently, the revised Urban Wastewater Treatment Directive[22] introduced mandatory quaternary treatment for micropollutants in urban effluents, with costs largely borne by pharmaceutical and cosmetics producers under an extended producer responsibility scheme[23]. This combination of polluter pays financing and uniform performance standards will de-risk investment in decentralized, modular treatment units. Furthermore, EU funding programs such as Horizon Europe and Innovation Fund[24], offer dedicated support for pilot-scale and scale-up projects.

Given the increasing stringency of European wastewater treatment regulations[23], which necessitate the exploration of sustainable and efficient alternatives for micropollutant removal, and the promising results of this simulated scaled-up PEC system, it becomes essential to contextualize its environmental performance against existing technologies that are already implemented at full scale. Among these, ozonation stands out as one of the most widely adopted advanced oxidation processes in real-world wastewater treatment plants. Ozonation has demonstrated high efficacy in degrading a broad spectrum of micropollutants, offers operational simplicity, and enjoys regulatory acceptance. These attributes make it a suitable and practical benchmark for evaluating the environmental sustainability of emerging technologies like PEC. Therefore, to enable a meaningful comparative assessment and provide insights into its feasibility, advantages, and limitations in real-world applications, a comprehensive LCA of the scaled-up PEC system was conducted, benchmarking it against ozonation.

Specifically, this research aims to: (1) Evaluate the environmental performance and implementation costs of this CFD-derived, scaled-up PEC system encompassing the entire life cycle stages: construction, operation and maintenance, and end-of-life (EOL) and alternative scenarios to identify potential areas for environmental impact reduction. (2) Benchmark the environmental sustainability of the scaled-up PEC system against the documented performance of a real-world, full-scale operation plant[25]. (3) Contextualize the findings by comparing the performance of this system with other scale-up models found in the literature that have the same purpose, thereby providing a robust assessment of the PEC technology's potential for large-scale application.

Results

Environmental performance of the scaled-up PEC oxidation system

Table 1 shows the results of the life cycle environmental impact assessment of the PEC oxidation system allocated to the functional unit. The highest relative contribution is found in the operation of the plant in all categories, with the exception of freshwater eutrophication (E fw), for which construction phase is the main contributor, primarily attributed to the production of the aluminum trough. Acidification (A), freshwater eutrophication (Efw), and human toxicity-cancer (HT c) in the end-of-life phase display a negative contribution, meaning beneficial outcome for the environmental performance.

To better understand the environmental performance of the PEC oxidation system, the relative contribution to the environmental impact is assessed with a hotspot analysis (Fig. 1). The system is divided into five key operational units, namely: photoanode, cathode, reactor, storage tank and pump. The contribution to environmental impact of each unit was assessed across the construction (CON), operational phase (USE) and end-of-life

Table 1 | Total environmental impact contribution of the PEC oxidation system per functional unit

Impact Category	units	Total	Life Cycle Stage		
			Construction	Operational phase	End of Life
A	Mole of H+ eq.	**2.75E-04**	1.17E-05	**2.66E-04**	**-2.60E-06**
CC	kg CO2 eq.	**4.03E-01**	2.02E-03	**4.01E-01**	**-5.25E-04**
EcoTOX	CTUe	**5.46E-01**	3.57E-02	**5.06E-01**	**4.24E-03**
E fw	kg P eq.	**2.56E-04**	**2.56E-04**	3.30E-07	**7.92E-08**
HT c	CTUh	**1.10E-10**	5.63E-11	**6.29E-11**	**-8.98E-12**
HT non c	CTUh	**1.10E-09**	2.90E-11	**1.06E-09**	**7.99E-12**
RU f	MJ	**1.04E+00**	3.27E-02	**1.01E+00**	**-6.24E-03**
RU m	kg Sb eq.	**4.75E-08**	1.29E-08	**3.43E-08**	**3.78E-10**

Red cells with white font denote the highest impact, while green cells with bold black font represent the lowest contribution.
A acidification, *CC* climate change, *EcoTOX* Ecotoxicity (freshwater), *E* fw-freshwater eutrophication, *HT c* human toxicity, cancer, *HT non c* human toxicity non-cancer, *RU f* fossil resource use, *RU m* mineral resource use.

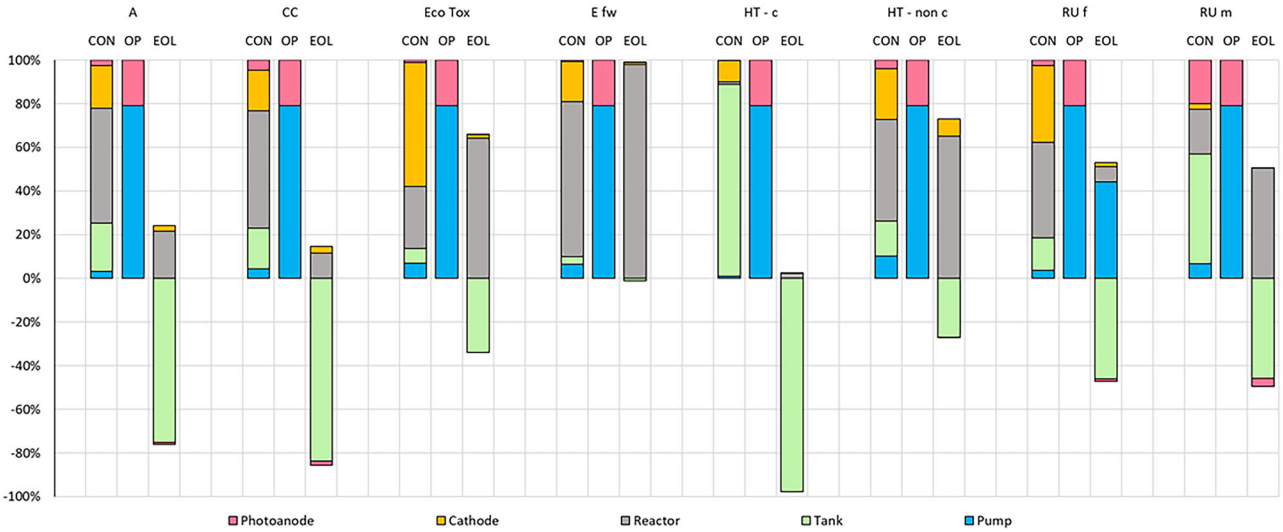


Fig. 1 | Hotspot analysis. Relative contribution of the life cycle stages: construction (CON), operation and maintenance (OP), and end-of-life (EOL) to the environmental impact of the PEC oxidation system per functional unit. The impact categories are displayed on the x-axis. A – acidification, CC – climate change, ECO Tox – ecotoxicity, Efw – eutrophication freshwater, HT-c – human toxicity-cancer, HT-nc – human toxicity-non cancer, RU f – resource use fossil, RU m – resource use mineral.

(EOL) stages. During construction, contribution is attributed to process related to extraction of materials; manufacturing and transport (see Table S1). In the operational phase, the impact mainly stems from resource consumption during operation and maintenance. Ultimately, EOL impact contribution is linked to activities for collection and disposal of the materials constituting the operational units.

The hotspot analysis in Fig. 1 showed the primary contribution of the reactor in CON and EOL phases, and electricity consumption allocated to the pump operation as the main contributor in the operational phase across the impact categories examined. During the construction phase, the reactor appears as the primary impact in five out of eight environmental impact categories: acidification (53%), climate change (54%), freshwater eutrophication (71%), human toxicity non-cancer (47%) and fossil resource use (44%). For the hotspot analysis, the operational unit 'reactor' encompasses both, the reactor itself, built out of borosilicate glass, and the aluminum parabolic trough. The production of the latter is the main driver of these impacts. The primary stages involved in aluminum production are extraction, bauxite conversion to alumina, and processing into aluminum, which are energy intensive processes which translate in a significant environmental burden[26].

In the end-of-life phase, a negative contribution to the impact across all environmental impact categories studied is attributed to the storage tank. At the EOL stage of the PEC oxidation installation, the stainless steel from the tank is recycled with downstream material recovery. This results in energy reduction and significant material recovery, and it is credited as beneficial for the environment because it offsets the extraction of raw material and energy consumption for stainless steel production[27].

During the operational phase, the primary impacts were mainly due to electricity consumption for the catalytic photo-oxidation process. The photoanode required auxiliary energy (0.2 kWh) for the oxidation process, whereas the pump consumed 0.75 kWh. Consequently, the energy consumption of this operational unit was responsible for the impact contribution in all the categories studied. These findings align with existing literature on environmental impact assessments of advanced oxidation technologies. For instance, Notarnicola et al.[28] compared various UV-C based lab-scale technologies for micropollutant removal, identifying the highest contribution in the operational phase, attributed to the electrical consumption of pumps, followed by UV lamps. Similarly, Feijoo et al.[29] conducted a life cycle analysis of a pilot-scale electrochemical oxidation model, and found that energy consumption of peripheral equipment, particularly the recirculation pump, exceeded the impact of oxidizing radical production.

Scenario analysis results

During the operational phase (Fig. 2), replacing grid-supplied electricity by solar energy for the photoanode and photovoltaic-sourced energy for the pump significantly reduced environmental impacts in acidification (−52%), climate change (−93%), ecotoxicity (−75%), freshwater eutrophication (−82%), human toxicity-cancer (−76%) and fossil resource use (−68%). This reduction primarily stems from decreased energy demand from the grid, which is associated with environmental burdens from energy production. However, photovoltaic electricity introduces a notably 97% increase in mineral resourced use due to material extraction and photovoltaic panel manufacturing[30]. A significant finding across several studies is the reduction of environmental impacts when switching to renewable energy sources, rendering a clear advantage over conventional energy sources. Pesqueira et al.[31] performed a LCA on pilot-scale solar advanced oxidation technologies and concluded that solar photolysis had the lowest environmental impact. However, they also observed lower mineralization efficiency and overall process performance. A similar reduction in carbon dioxide emissions (88%) was observed in another study[32] when solar panels powered the electrochemical oxidation of olive mill wastewater. Fernandez-Marchante et al.[33] also observed this trend in their LCA of electrolytic wastewater treatment. They compared three bench-scale plants using conductive-diamond electrochemical oxidation (CDEO) technology, each powered by a different electricity source: the power grid, in-situ photovoltaic power, and wind power. The plants were evaluated for the removal of 0.1 g of 2,4-dichlorophenoxyacetic acid (2,4D)in 1 L of synthetic wastewater. Their findings showed a one-fold reduction (~ 90%) in climate change impact when the system was powered by green energies compared to grid electricity. However, the study also noted that using solar energy led to variations in applied intensity, which influenced the time needed for oxidant production and could promote the accumulation of intermediate compounds.

At the end of the life cycle (Fig. 3), Scenario 1, which involves recycling the aluminum trough, has a greater environmental impact due to the energy-intensive recycling process[34]. Scenario 2, where graphite and the solar trough are reused, exhibits the lowest impact, as it eliminates direct end-of-life burdens in all studied environmental impact categories. In relation to the baseline, this scenario presents the most advantageous outcome.

Toxicity assessment results

Figure 4 presents the toxicity assessment results for the selected scenarios. No significant differences were observed in freshwater Ecotoxicity between the baseline and the alternative scenario that involves the use of photovoltaic

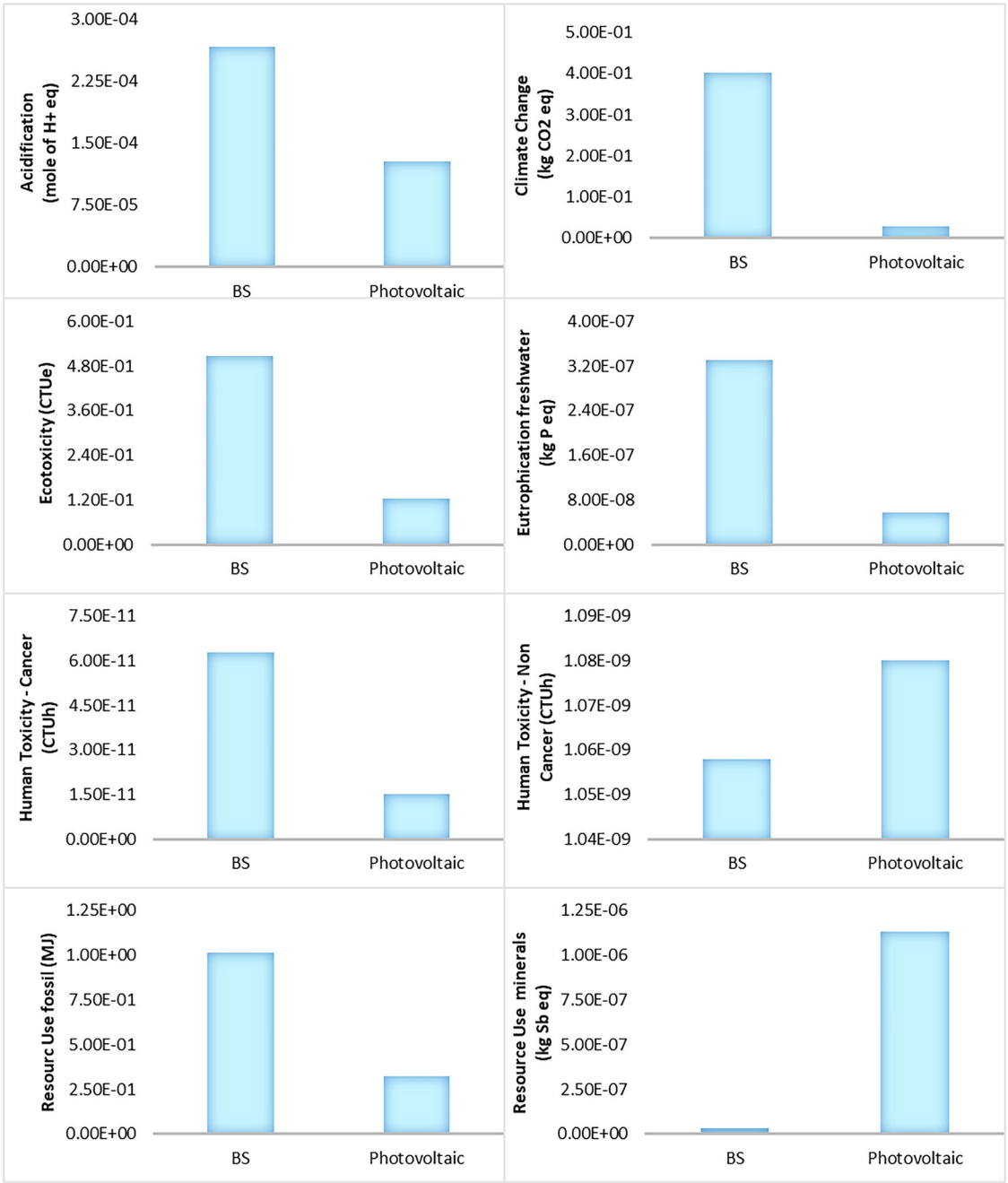


Fig. 2 | Scenario analysis of the operational phase. Scenarios (x-axis): BS (baseline) using average European electricity grid mix; Photovoltaic 100% photovoltaic electricity supply for the pump and 100% natural solar energy for the photoanode. Environmental impact categories displayed in y-axis.

and solar energy supply and the end of life strategies of scenario 2 (PV + SC2), contrary to what observed when studying the overall environmental performance and their contribution to the selected environmental impact categories. This could suggest that selecting a more sustainable strategy for developing and implementing this electrochemical advance oxidation system may not directly correlate with reduced ecotoxicity in freshwater. However, a notable reduction in impact values is observed in both, cancer and non-cancer human toxicity under the alternative scenario (PV + SC2). The baseline scenario exhibited a higher overall impact, primarily attributed to aluminum recycling and energy consumption. In contrast, the alternative scenario's primary contributor was the photovoltaic energy supply, specifically the production of silicon for solar panels. These findings are comparable to those obtained by Fernandez-Marchante et al.[33]. When toxicity reduction was assessed for the removal of 2,4D using the USEtox methodology, the authors found minimal variation when using electricity from the grid vs. solar power (~ 0.04%). Notably, the reduction in human toxicity was more pronounced when solar power was utilized, comparably to the findings of the present study.

Life cycle costing results

The comparative analysis of capital expenditure (CAPEX) and operational expenditure (OPEX) per functional unit is found in Fig. 5. CAPEX contributions involve the cost of material procurement, labor for installation, and associated energy consumption. Conversely, OPEX includes energy, labor for operation and maintenance, and component replacement. Labor for photocatalytic reactor assembly is the most substantial contributor to CAPEX, accounting for 68%. The pump, while the next largest contributor, represents a substantially lower share of total CAPEX at 14%. Regarding OPEX, the pump incurs the highest costs (77%) due to its energy consumption during operation, followed by the photoanode at 21%.

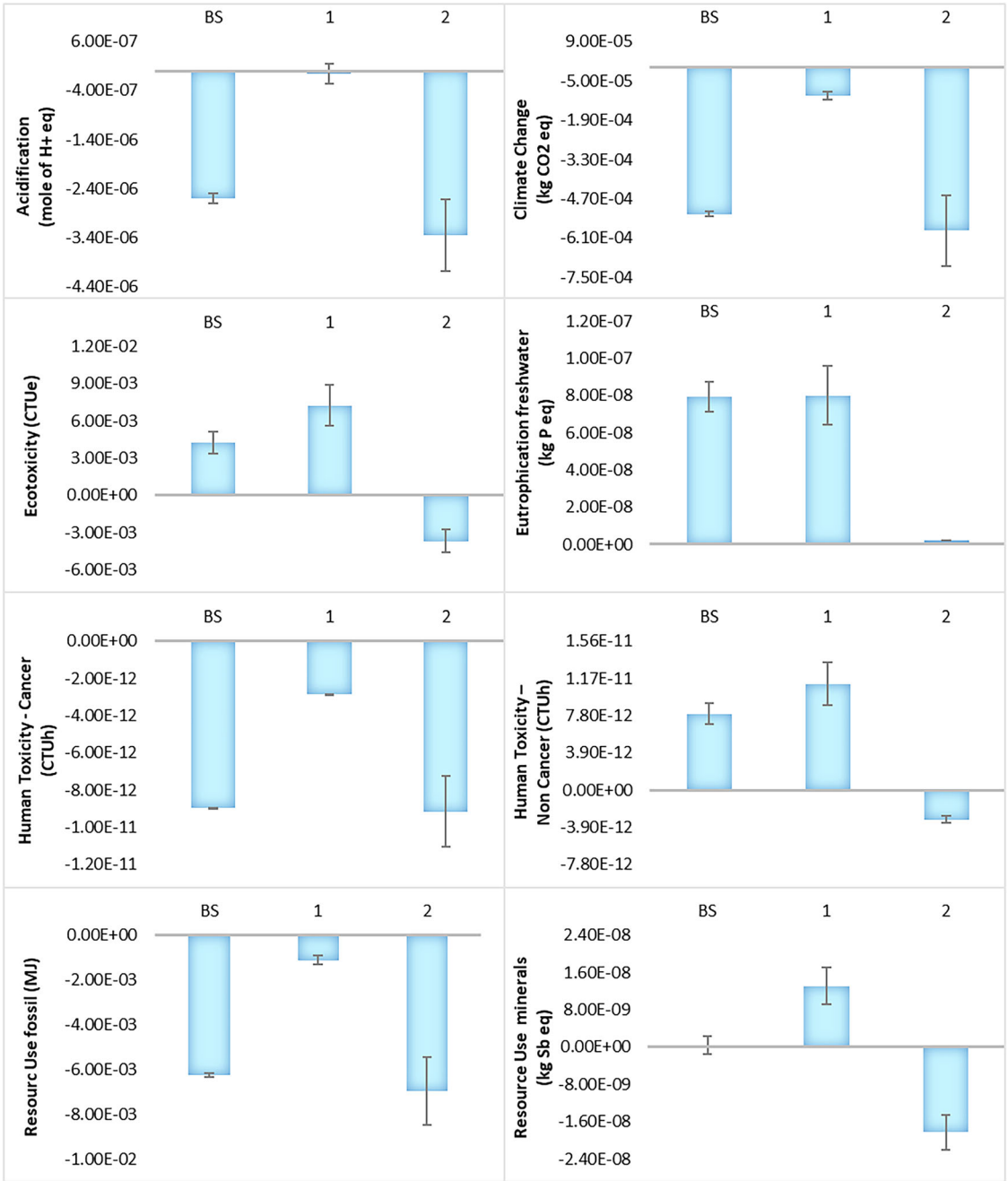


Fig. 3 | Scenario analysis of the end-of-life phase. Scenarios (top x-axis): baseline (BS), scenario 1 (1) and scenario 2 (2). The error bars represent the standard deviation, reflecting the variation of construction material.

Comparison with Full-Scale Ozonation Plant

The comparative life cycle assessment of PEC and ozone treatments for wastewater purification reveals that photocatalytic processes generally exhibit lower environmental impact across most categories, with the exception of eutrophication (Fig. 6). The primary contributor in both technologies is found during the operational phase across all the environmental impact categories studied, and that it is primarily due to energy consumption. In ozonation, energy consumption is mainly attributed to ozone generation, whereas PEC system is primarily due to the operation of the pump.

In acidification, ozonation presents a significantly higher impact during the operational phase, while construction phase impacts are comparable. In this category PEC oxidation offers a slight advantage at the end-of-life due to steel recycling. Similar trends are observed for climate change and fossil resource use. Ozonation has a more pronounced impact on freshwater ecotoxicity than PEC oxidation, primarily due to energy consumption for ozone generation. Conversely, PEC oxidation has a significantly higher end-of-life impact linked to aluminum recycling compared to concrete treatment in ozonation. Eutrophication is the only category where PEC oxidation consistently demonstrates an overall greater impact. The construction and end-of-life phases of the photoelectro catalytic reactor significantly outperforms the ozone plant in terms of environmental performance. The analysis suggests that aluminum, a key component of the PEC reactor, presents a more substantial environmental burden in eutrophication than concrete, particularly at the end of its lifecycle.

The findings presented in this study align with those reported by Tarpani & Azapagic[35], who conducted a comparative life cycle analysis of various large-scale wastewater treatment technologies, including ozonation

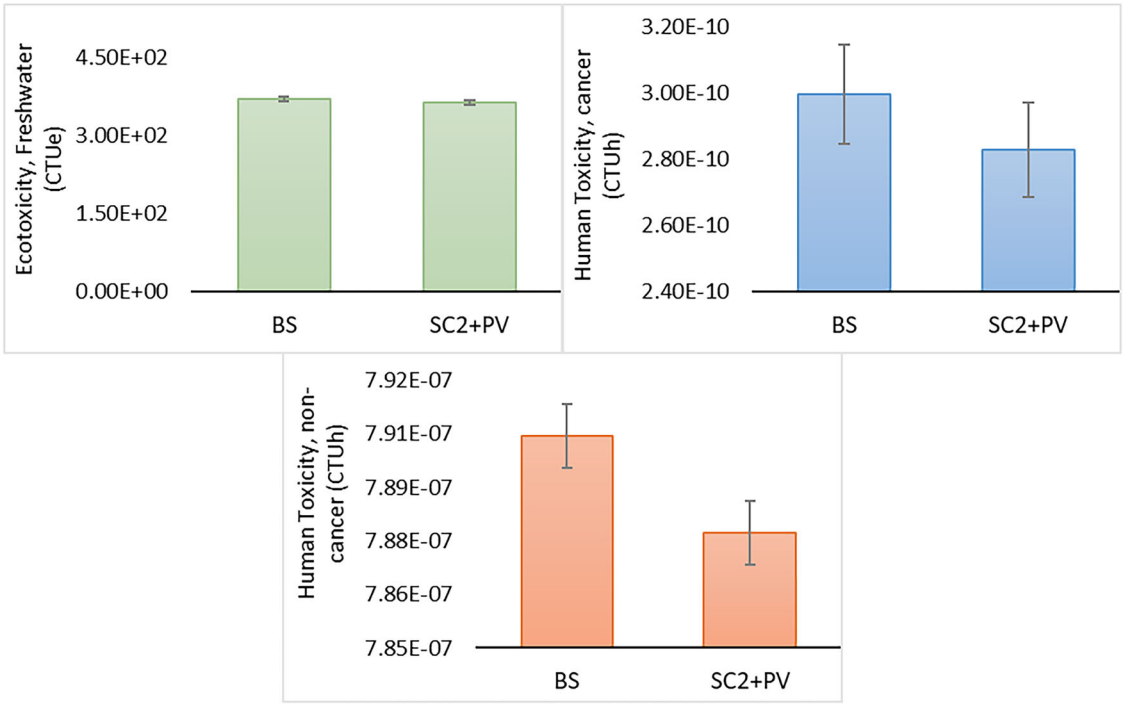
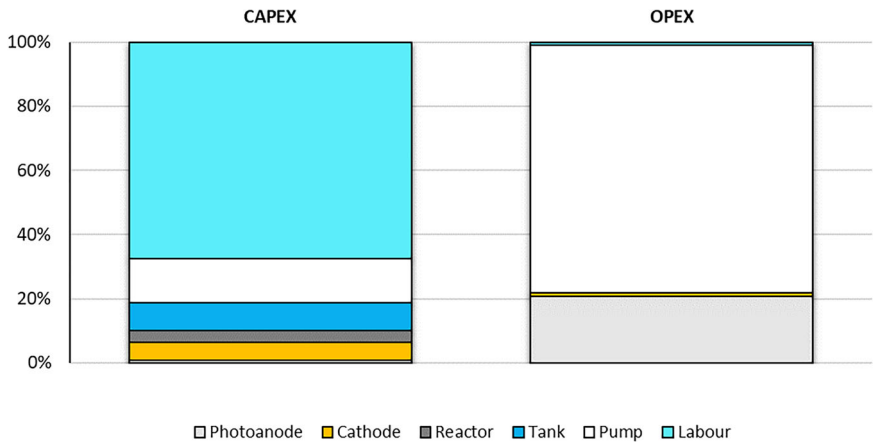


Fig. 4 | Toxicity assessment results from USEtox analysis. Axis x represents 2 different scenarios: BS – baseline scenario and SC2 + PV – photovoltaic and solar energy supplied to the photocatalytic reactor and end-of-life scenario 2 strategy.

Fig. 5 | Life cycle costing results. Relative contribution to life cycle cost for capital expenditures (CAPEX) and operational expenses (OPEX) for the scaled-up photocatalytic oxidation reactor.



and solar-driven photo Fenton. Both studies consistently indicate that ozonation exerts a predominant influence on environmental impact across the studied categories, primarily driven by energy consumption. However, when comparing the performance of ozonation to photo Fenton in the work of Gallego-Schmid et al.[36], results show that ozone outperforms photo Fenton. This superiority is attributed to the more established nature of ozonation technology, its efficient oxidation performance, a longer installation lifespan and the avoidance of external chemical addition.

The toxicity reduction of the scaled-out photocatalytic oxidation system was compared with that of the full-scale ozonation plant treating the same effluent flow for the baseline scenario. Table S3 presents the results, which incorporate the presence of micropollutants and their 70% removal from the effluent. The results demonstrate a significantly higher toxicity contribution from the ozonation plant. In ozonation, the operational phase, mainly driven by energy consumption, predominates in contributing to toxicity impact. Conversely, in photocatalytic oxidation is the end of life the most substantial contributor. In ecotoxicity, the contribution from the ozonation plant is two orders of magnitude higher than that of the photocatalysis system. After energy consumption in the operational phase, the subsequent most impactful contribution is found in the construction phase. More specifically, in the precious metals like platinum used in the manufacturing of the ozone generator. In contrast, aluminum recycling is the main contributor to the ecotoxicity impact in photocatalytic oxidation. For human toxicity, both cancer and non-cancer categories show a three-order-of-magnitude difference in impact, favoring photocatalytic oxidation. In ozonation, the contribution is found in electricity consumption during the operational phase, followed by the steel production for plant construction in human toxicity cancer. In the non-cancer category, the provision of liquid oxygen contributes significantly to this category. In contrast, the environmental burden associated to aluminum recycling predominates in both, human toxicity cancer and non-cancer categories for photocatalytic oxidation.

To further evaluate toxicity reduction, a comparative analysis was conducted using the findings of Tarpani & Azapagic[35]. In their study, the freshwater ecotoxicity of nine micropollutants present in wastewater effluent was assessed using the USEtox methodology. However, only two

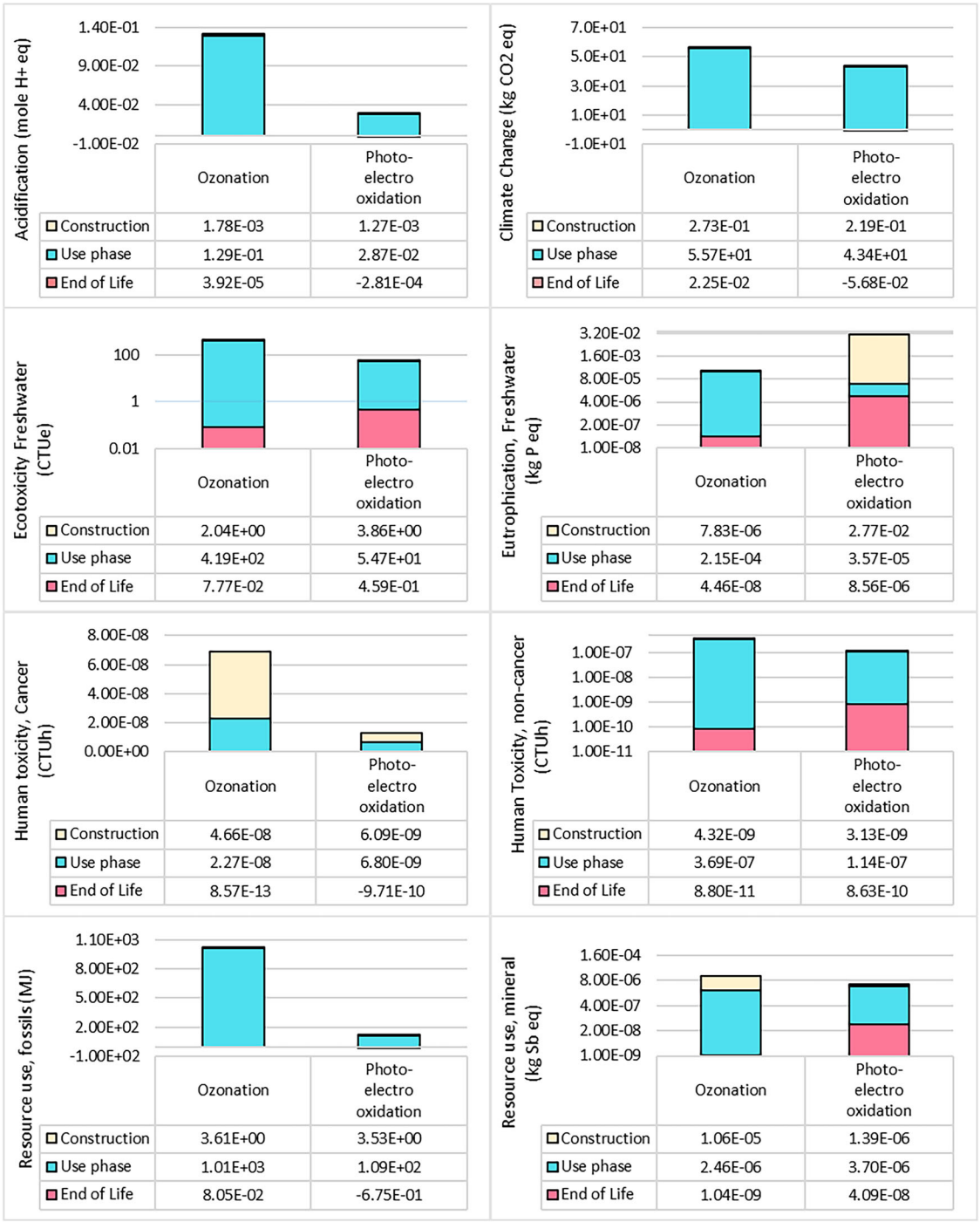


Fig. 6 | Comparative LCA of photocatalytic and ozonation for micropollutant removal in wastewater treatment. The x-axis shows the technologies compared and their respective life cycle contributions to environmental impact. Environmental impact categories are displayed on the y-axis.

of them, diclofenac and carbamazepine, were common to all three studies (ozonation[25,35], and PEC oxidation in the present study). For each treatment, the USEtox methodology was employed to quantify freshwater ecotoxicity, assuming a 70% removal efficiency. Additionally, the freshwater ecotoxicity of the untreated effluent was calculated by multiplying the characterization factor to each compound by its concentration in the water. Detailed results are presented in Table S4, which includes the toxicity impact values for both, the untreated effluent and the effluent with 70% removal of common micropollutants. The findings reveal that, despite the initially elevated micropollutant concentration, PEC oxidation exhibits the lowest freshwater ecotoxicity impact, whereas the impact observed in the ozonation plant evaluated in this study surpasses both technologies by one order of magnitude. Results obtained for the PEC oxidation system are comparable to those reported by the ozonation system of Tarpani & Azapagic[35], with a 22% reduction in contribution.

Discussion. To date, the absence of comprehensive life cycle assessment for scaled-up photoelectrocatalytic wastewater treatment systems specifically targeting micropollutant removal precludes direct comparisons with the results of this study. Given the relatively nascent nature of this technology, a comprehensive literature search was conducted to identify existing LCAs of scaled-up advanced oxidation technologies applied to micropollutant removal in wastewater treatment. Building upon the

work of Pesqueira et al.[37], which provided a comprehensive list of such studies, an updated search was conducted in the scientific literature databases Scopus and Web of Science. Three more pilot-scale projects with potentially comparable LCA results were found. Table S5 presents a summary of these studies. The literature review reveals that the Fenton method, including the solar and photo Fenton variations, is the most frequently scaled advanced oxidation technology and has been the subject of numerous environmental studies.

To ensure a homogeneous comparison, results from large-scale studies were normalized to impact per cubic meter. However, studies by Feijoo et al.[29] and Conde et al.[38] were excluded from this normalization due to their functional unit being smaller than 1 m^3, to avoid misinterpretation of the results. Most studies used the ReCiPe 2016 methodology[39] for impact assessment, with the exception of Zou et al.[40], which used CML 2001[41] and the present study, that used EF 3.0. To maintain consistency, impact units were homogenized to those for EF 3.0 impact assessment methodology. Specifically, the molar equivalence of H^+ for acidification category was recalculated[42], and a conversion factor for freshwater ecotoxicity was applied[43]. For the resource use fossil category, the MJ equivalent to 1 kg oil was calculated[44].

The comparative analysis demonstrates that the environmental performance of PEC oxidation technology assessed in the present study outperforms other scaled-up advanced oxidation technologies evaluated in the scientific literature. These promising results suggest the potential for large-scale implementation. Conversely, Tarpani & Azapagic[35] and Gallego-Schmid[36] reported inferior environmental performance than the present work. This discrepancy can be attributed to the necessity of chemical additives, which is not a requirement for our proposed approach. Pesqueira et al.[31] results aligns with the present study to some extent, since the authors only take into account the impact of the operational phase. They evaluated TiO_2-based photocatalysis, which was the scenario chosen for the present comparison. One of the advantages of TiO_2 as a catalyst relies in their reusability benefits, which may have contributed to their favorable environmental performance outcomes. However, the authors did not consider the environmental impact of peripheral equipment, such as pump, which can significantly contribute to energy consumption. Conde et al.[38] highlighted the environmental performance of electro and photoelectro Fenton scaled-up configurations, noting that acidic operation conditions can improve degradation but at the expense of environmental performance. The circumneutral photoelectro Fenton scenario was chosen for the comparative analysis, and the results were the least favorable when compared to the rest of the technologies, particularly when considering the smaller functional unit. Zou et al.[40] evaluated the large-scale implementation of advanced oxidation for pharmaceutical refractory wastewater pre-treatment. Their study identified eutrophication and ecotoxicity as the primary areas of environmental impact, attributed to hydrogen peroxide and iron sludge incineration.

Feijoo et al.[29] observed that the complexity of the wastewater matrix, including the number of micropollutants present, has an influence in the efficiency of the treatment technologies. Increased matrix complexity can lead to a proliferation of competing reactions, hindering degradation kinetics and potentially increasing energy consumption. This may compromise the effectiveness of toxicity reduction. In the present study, the environmental performance of treating distilled water containing a mixture of four pollutants was evaluated. To comprehensively assess the impact of micropollutant loads on process performance, incorporating a sensitivity analysis into the model is recommended. This would involve varying the concentrations of micropollutants to evaluate their influence on the environmental footprint of the process.

When observing the life cycle impacts of these technologies, the operational phase consistently emerges as the primary contributor to environmental impact. However, the main driver of environmental burden is constituted by chemical addition, rather than electricity consumption. The energy consumption per m^3 in the operation phase of ozonation (0.29 kWh/m^3) is comparable to the operation of the PEC oxidation system (0.25 kWh/m^3). This consumption is lower than the reported in the large-scale solar photo-Fenton study of Gallego-Schmid et al.[36] (0.35 kWh/m^3), and the ozonation electricity consumption in the study of Tarpani & Azapagic[35] (~ 0.9 kWh/m^3). However, the latter study compares ozonation to solar photo Fenton, for which 0 kWh/m^3 is reported. Arzate et al.[45] reported lower operational electricity consumption per m^3 in their comparative analysis for ozonation (0.17 kWh/m^3) and for photo Fenton (0.13 and 0.1 kWh/m^3).Energy consumption was identified as a secondary contributor during the operational phase, with the impact of chemical agents predominating[36,40,45]. Conversely, lab-scale LCA studies on photocatalytic treatment of wastewater frequently point out energy consumption as the main impact carrier[37]. These findings are particularly noteworthy, because they suggest a more nuance perspective on the limiting factors for large-scale implementation of advanced oxidation technologies, challenging previous assumptions pointing at energy consumption as the primary contributor[46,47].

The interconnectedness of wastewater treatment and energy is a critical aspect of sustainable development. The wastewater treatment landscape is evolving towards a more sustainable approach prioritizing net-zero emission[48]. Advanced solar-based oxidation techniques such as PEC oxidation, offer a promising approach as an additional post-treatment step for municipal wastewater effluent purification, due to their minimal energy consumption. The environmental performance of this technology outperforms not just a consolidated technology such as ozonation, but also other scaled-up solar-based processes, as demonstrated across multiple impact categories including acidification, freshwater ecotoxicity, eutrophication and resource use. Beyond these quantified environmental benefits, a comprehensive sustainability assessment necessitates an explicit consideration of the water-energy nexus. Effective wastewater treatment is inherently energy-intensive, requiring significant power for pumping, aeration, and advanced purification processes. By utilizing an in-situ solar-driven radical generation mechanisms, the PEC process minimizes the external energy input per unit of water treated, offering a more energy-efficient pathway for micropollutants removal. This could potentially contribute to the overall resource efficiency of the urban water cycle, promoting a more resilient and sustainable water infrastructure. In addition to our work, other cost-effective options based on AOP also exist for polishing wastewater effluents. Metal-free g-C_3N_4 photocatalysts work under solar light but benefit from heterojunctions for charge carrier separation[49]. Sulfate-radical AOPs (PMS/PDS) can be activated by biochar and Fe/Mn-doped carbons, enabling radical and non-radical pathways at near-neutral pH[50]. Catalytic ozonation with Fe/Mn oxides or doped biochar upgrades ozone efficiency and allows easy catalyst recovery[51]. Electro-Fenton with carbon felts and soluble/heterogeneous Fe is modular and energy-competitive for OMP mixtures[52]. Non-thermal plasma is emerging for simultaneous OMP and pathogen control, though energy and by-products must be benchmarked[53].

However, it is essential to acknowledge the limitations associated with large-scale implementation. Theoretical scaling provides insight into potential performance, but experimental validation is crucial. In this study, experiments were conducted with demineralized water spiked with micropollutants to isolate the intrinsic performance of the heterojunction photoanode, and to investigate scale-up feasibility via CFD. However, real effluent treatment with wastewater matrices containing natural organic matter, inorganic constituents, and variable pH may alter photo-electrocatalytic kinetics and anode stability, potentially affecting system efficiency and increasing consumption of energy, compromising the environmental performance, as stated above[29]. Consequently, it is necessary to perform subsequent studies in which a CFD-optimized, modular reactor is tested, utilizing real municipal and/or industrial wastewater samples. These investigations will (i) assess matrix impacts on photocurrent generation and OMP removal kinetics, (ii) evaluate long-term anode durability under realistic water-quality conditions, and (iii) establish necessary pre-treatment or conditioning steps to ensure robust performance in full-scale applications.

The effectiveness of solar energy in driving micropollutant degradation also requires experimental verification. While solar energy utilization leads to a significant reduction of the impacts of the operation, it may have a negative effect in the degradation efficiency, influencing toxicity levels and impacting the process competitiveness[33]. Beyond these operational

considerations, the long-term stability of the reactor components is also a crucial factor for practical application. Although the electrode stability and degradation phenomena such as $BiVO_4$ photocorrosion and GO layer detachment are critical for long-term performance, quantification of these failure mechanisms needs to be addressed in future stages of deployment. The experimental PEC oxidation work[18], demonstrated the efficacy for micropollutant removal by the heterojunction, and validated the scale-up reactor via CFD. In follow-up studies, extended duration experiments will be performed on the CFD optimized reactor design under variable hydraulic regimes to measure photocorrosion rates of the $BiVO_4/TiO_2$-GO anode, characterize GO delamination kinetics and develop and test remedial strategies to improve anode durability whilst maintain high removal efficiencies over prolonged operation.

Regional factors, including specific solar irradiance profiles, the carbon intensity of local electricity grids and varying economic conditions (e.g., labor costs, energy prices), can significantly influence real-word performance and costs. While these considerations were beyond the scope of this initial analysis, they are undeniably critical for detailed project planning and successful plant implementation at later stages of technology deployment. Therefore, further research is necessary to address these limitations and ensure the successful integration of PEC oxidation into large-scale wastewater treatment systems.

The prospective wastewater treatment required proposed by the implementation of the new Wastewater Treatment Directive[23] underscores the necessity of innovative technologies to address micropollutant removal. Successful large-scale implementation of such technologies requires a comprehensive evaluation of technical, economic and environmental factors. Ideally, the environmental and economic aspects should be studied as part of the scaling process, so that the best decisions have been made when the technology is already consolidated. This would prevent the waste of resources and would boost the competitiveness of the technology[54]. The present study conducted a thorough evaluation of a theoretical pilot-scale photoelectro catalytic oxidation system for wastewater treatment, in order to identify the hotspots of the system and thus be able to obtain information of its optimization in its future projection.

In conclusion, LCA revealed that the environmental performance of the PEC oxidation system is predominantly influenced by its operational phase, primarily driven by the electricity consumption of recirculation pumps. The main impacts of the construction phase were linked to the reactor's materials, particularly the aluminum trough. However, a significant reduction in most environmental impact (e.g., 93% climate change impact) was observed when using solar energy, although this introduced a trade-off with a 97 T increase in mineral resource use from photovoltaic panel production. Cost analysis revealed that CAPEX was dominated by the installation costs while OPEX was mainly attributed to pump operation and photoanode maintenance. When comparing to full-scale ozonation, PEC demonstrated a superior environmental profile with lower toxicity and greater end-of-life benefits from steel recycling. Furthermore, PEC consistently outperformed other solar-based advanced oxidation technologies, highlighting its strong potential for scale-up. It is crucial, however, to validate these theoretical findings with experimental data to ensure the model's accuracy and address any limitations in the scaling process.

Methods

A CFD model was developed to simulate a full-scale photoelectrocatalytic water treatment reactor, based on a lab-scale reactor. The reactor design aimed to remove BTA, CBZ, CAF, and DIC from water with at least 80% efficiency. The conceptually designed $BiVO_4/TiO_2$-GO based PEC reactor has been conceived as a tertiary or quaternary treatment step for organic micropollutants in water-reclamation and advanced wastewater-treatment trains. Its integrated light-driven and electrochemical mechanism will enable direct utilization of solar energy particularly advantageous in regions exceeding 5 kWh m^{-2} day^{-1} solar irradiance thus reducing reliance on grid electricity and chemical oxidants. The reactor is designed as a modular unit, allowing flexible scaling by deploying multiple units in parallel or series to match influent flows. Such a decentralized system could be well-suited for small utilities, industrial sites, or remote communities, where conventional advanced oxidation processes may be cost or infrastructure prohibitive. In tertiary/quaternary configurations, installed downstream of secondary clarifiers, membranes, or biological polishing stages, the CFD modeled design could achieve ≥80% removal of representative organic micropollutants (BTA, CBZ, CAF, DIC) within a 25 min hydraulic residence time, potentially fulfilling typical discharge and reuse standards for trace pollutants.

The details of the CFD and the experimental setup are fully explained elsewhere[18]. Briefly, water from a 140 L storage tank is pumped into the cylindrical reactor with a flow of 3.72 m^3/h, where photoelectrocatalytic oxidation occurs near the photoanode surface. The reactor is constructed of borosilicate glass to allow for solar light penetration. The photoanode, also cylindrical, is fabricated from $BiVO_4/TiO_2$-GO to minimize recombination and enhance photoelectrocatalytic removal. A graphite cathode and an aluminum solar trough are used to concentrate solar light onto the photoanode. A recirculation loop ensures sufficient reaction time while maintaining high velocity for better mixing and diffusion-controlled reactions[55]. Water is recirculated until an 80% removal efficiency for each micropollutant is achieved. The CFD model calculated removal efficiency after the first recirculation, assuming a perfect mixing and first-order reactions. A current density of 2.82 A m^{-2} was applied to enhance reaction kinetics and minimize recombination. This value corresponds to the current density at 1 V (vs. Ag/AgCl) in laboratory experiments.

Life cycle assessment methodology

A Life Cycle Assessment was conducted following the standardized procedures outlined in ISO 14040 and ISO 14044. These guidelines establish the methodological framework for assessing the environmental impacts of products or processes[56,57]. In accordance with these standards, the LCA encompassed four phases: goal and scope definition, life cycle inventory (LCI), life cycle impact assessment (LCIA), and interpretation of results. This case study systematically applied these four stages, which are detailed below.

The goal of this study is the performance of a comprehensive LCA of the CFD modeled scale-up PEC for micropollutants removal from wastewater to identify the main impact contributors and potentials areas for improvement. The study involves the whole life cycle of the process, from the material acquisition for reactor assembly, the operation and maintenance and the end-of-life of the advanced oxidation set-up whose continuous operation is predicted to have a life span of 10 years. The functional unit is the treatment of 140 L of water with PEC, for the removal of 80% of the micropollutant concentration initially present in the water stream.

The system boundaries for the scaled-up PEC set-up are shown in Fig. 7. In the background system, the resources that have been extracted from the environment to be provided to the foreground system, such as energy, materials and chemicals are found. The foreground system represents the processes and flows that are modeled within the scope of the study. Secondary data from published databases are used to model the background system, and primary data from the experimental setup and the actual CFD model is collected for the processes in the foreground system[58]. The environmental impact quantification of the scaled-up PEC included both, direct and indirect burdens. The former are associated with operational units and elementary flows, whereas the latter are allocated to external resource supply. Additionally, avoided burdens related to material recovery and energy generation at the end-of-life were also considered[59].

Table S1 shows the key inventory flows referred to the functional unit, encompassing materials, chemicals and electricity consumption during construction and operation phases. Additionally, it details the EOL fate of the various materials constituting the operational units. The inventory was compiled using primary data from the CFD model, covering all flows in the foreground related to construction, operation and EOL. Secondary data was used to represent background processes such as electricity grid, waste management and transportation. These secondary data were sourced from LCA databases like Ecoinvent[60] and Sphera dataset aggregated processes[61].

The inventory of the construction stage includes the materials and chemicals used to manufacture and assemble the reactor (Fig. 7), as well as

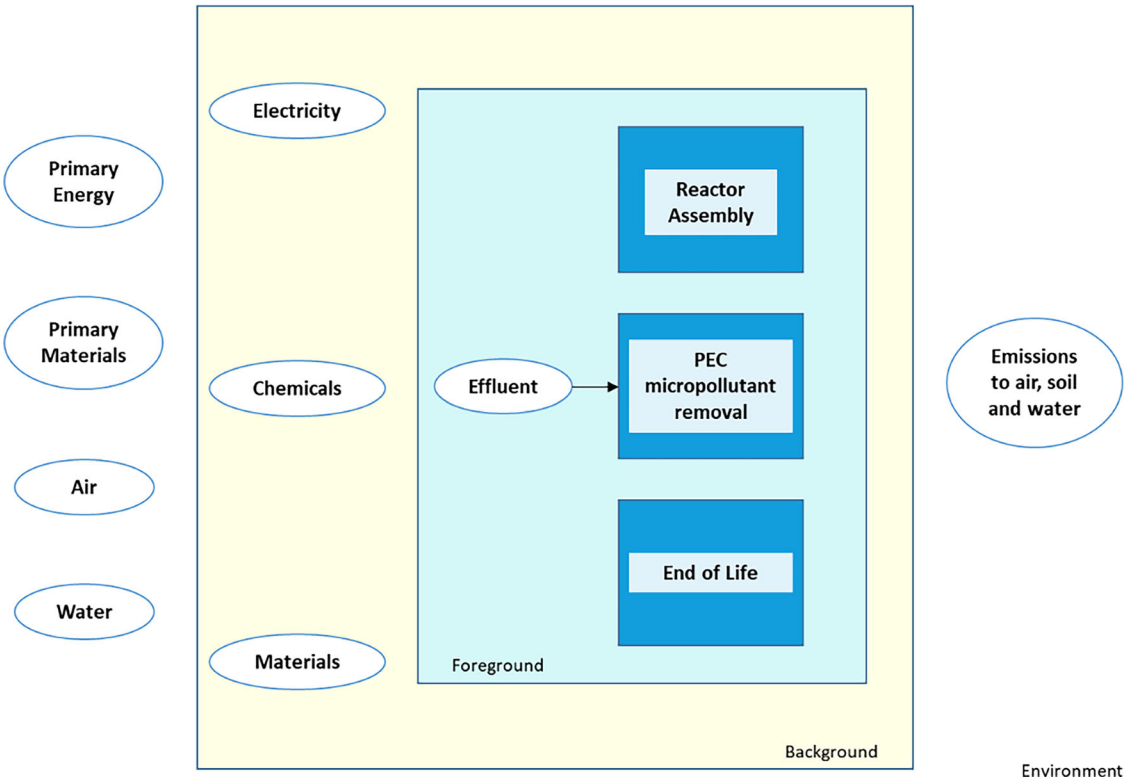


Fig. 7 | System boundaries of the LCA study. The system is divided into environment (source of raw materials and emissions), background (supporting processes like electricity and chemical production) and foreground (primary data-based processes: reactor assembly, micropollutant removal and end of life). The bubbles represent the material and energy flows between systems.

their transport to the plant. Packaging is not included. Materials and chemicals were estimated based on a 10-year operational lifespan, accounting for components replacements. The inventory during the use stage includes all the flows relevant during the operation of the PEC oxidation. At the end of its life span, the PEC system is assumed to be dissembled and the components of each operational units would undergo the pertinent end-of-life (EOL) treatment described in Table S1.

The methodology Environmental Footprint 3.0 (EF 3.0)[62] was used to translate the flows into impacts in different environmental impact categories. The calculations were performed using GaBi 10.6.2.9 software[61]. The interpretation of the Life Cycle Impact Assessment (LCIA) provides an understanding of the overall environmental performance of the scaled-up PEC oxidation setup and identifying the primary contributors to environmental impact. The results of LCIA show the results for the contribution to a selection of environmental impact categories given their relevance in LCA of wastewater treatment studies[4,37], namely: acidification (A), climate change (CC), ecotoxicity (Eco Tox), freshwater eutrophication (E fw) and mineral and fossil resources depletion (RU m and RU f, respectively). Additionally, human toxicity cancer (HT c) and non-cancer (HT n-c) are also included. Subsequently, a scenario analysis is included to assess the effect of photovoltaic powered electricity in the operation of PEC.

Scenario analysis

To evaluate the optimization potential for the photocatalytic oxidation setup, a scenario analysis is carried out by proposing renewable energy consumption during the operational phase and alternative end-of-life strategies for some operational units at the end of the life span of the installation. Table S2 summarizes the scenarios considered.

Toxicity assessment

To assess toxicity, a separate analysis as part of the LCIA was conducted utilizing the single-use method USEtox 2.12 methodology for 2 different scenarios, namely the baseline, and a combined scenario incorporating solar energy and photovoltaic during the operational phase, and end-of-life scenario 2, for its potential for reduced contribution to environmental impacts. The toxicity calculation included the micropollutants BTA, CAF, CBZ, and DIC removal from the wastewater. Their characterization factors were multiplied by their final concentrations post-treatment, and the results were aggregated to determine a single toxicity value. This value was then integrated into the overall toxicity assessment of the photocatalytic oxidation system.

Life cycle costing

The life cycle cost (LCC) was evaluated by performing a comprehensive breakdown of the costs associated with the PEC oxidation system. LCC includes construction, materials, chemicals, activities and services of both, operational expenses (OPEX) and capital expenses (CAPEX). This assessment aimed to provide a conceptual, comparative understanding of the overall economic performance rather than a site-specific financial feasibility study. To ensure relevance within the targeted regulatory context, cost assumptions for OPEX were contextualized to the European Union market, whereas CAPEX costs were more specifically allocated based on the geographic origin of materials and components.

Comparison to full-scale ozonation plant

This study compares the environmental performance of the CFD PEC system with the results obtained from a previous study of a full-scale ozone treatment plant[25]. The authors reported a wastewater flow rate of 400m^3/h, whereas the experimental PEC reactor operated at 3.72 m^3/h. To enable a direct comparison with the environmental performance of the real-life AOP plant, this study extrapolated the PEC system's performance to match the flow rates. Consequently, the functional unit for the comparative analysis was established as the wastewater flow rate. The PEC

reactor was scaled-out by a factor of 108, and its impact was recalculated for comparison with ozonation, to facilitate a consistent comparison for the treatment of 400 m^3/h.

Data availability

Data supporting the findings of this study are available upon request.

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Author contributions

Gema Amaya Santos: Idea, conceptualization, investigation, literature review, visualization, analysis, data curation, writing the original draft, writing-review and editing.Agha Zeeshan Ali: Investigation, conceptualization, data curation, review.Paola Lettieri: Idea, conceptualization, writing-review & editing, funding acquisition.

Competing interests

The authors declare no competing interests.

Additional information

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Correspondence and requests for materials should be addressed to Paola Lettieri.