Environmental Catalysis and Technologies

Life Cycle Assessment and Sustainability

KEYWORDS: Life Cycle Assessment (LCA) / Wastewater treatment / Catalysis / Environment / Sustainable technologies / Packaging

The Life Cycle Assessment (LCA) methodology was employed in the comparative analysis of advanced wastewater treatment processes, identifying areas for improvement and assessing the environmental impacts associated with various oxidants used in decontamination procedures. The results underline the fundamental role of LCA as a versatile tool, crucial for improving wastewater treatment processes, obtaining essential knowledge for sustainable alternatives, and bridging gaps in global life cycle assessments. Moreover, the work has been extended to assess the environmental performance of other technologies and products, such as packaging.

Introduction

Comprehensive studies evaluating the environmental impacts of advanced treatments in urban wastewater treatment plants (UWWTPs), particularly concerning the removal of priority substances (PSs) and contaminants of emerging concern (CECs), along with associated toxicological benefits, are notably scarce. Optimal solutions should strike a balance between environmental sustainability, cost-effectiveness, resource availability, social impacts, and other relevant variables. LCA stands out as a standardized, robust, and widely accepted decision-making tool, offering insights into the environmental impacts of products and processes throughout their entire life cycle — from resource extraction to production, use, recycling, and final disposal.

Within this context, the present research topic aims to assess the potential environmental impacts of various advanced wastewater treatment options, with a particular focus on catalytic processes for the removal of micropollutants via LCA.

This tool consists of four iterative stages: (i) definition of goal/scope, (ii) inventory assessment, (iii) impact assessment, and (iv) interpretation. SimaPro is the most widely used software nowadays for applying the LCA methodology, and it was used for a proficient comparison of different scenarios. The overall aim is to support the development of more environmentally sustainable technologies with a basis for preserving ecosystems, water bodies, and human health. Collaboration with industry and companies from various sectors is also underway.

Current Development

Thus far, the following case studies were developed within the assessment of advanced wastewater treatments: *i)* the comparative LCA of solar photocatalysis using TiO_2-P25 with or without H_2O_2 or circumneutral photo-Fenton; *ii)* comparison of H_2O_2 with sulphate-based oxidizing agents (peroxymonosulfate, persulfate) in UVC photolysis; *iii)* and comparison of solar photocatalysis using TiO_2-P25 with a carbon-based composite (GO-TiO_2) synthesized via liquid phase deposition. This latter case study (*iii*) included the determination of first-proxy CFs for several contaminants of emerging concern and priority substances. The selection of these case studies was preceded by a literature review on the application of the LCA tool on this topic, from which it was concluded that mainly Fenton-based processes had been explored until that point [1].

The use of TiO_2-P25 in solar photocatalysis appears to be a more compelling choice than alternative processes like circumneutral photo-Fenton, irrespective of whether dissolved iron is partially or completely removed after the photo-Fenton treatment. Additionally, it was concluded that ensuring iron removal from the treated effluent is crucial, as a partial removal could yield a final effluent with a higher freshwater ecotoxicity potential than that caused by the micropollutants targeted for removal. The slight acidification step of urban wastewater to pH 5.5, necessary to prevent iron precipitation occurring at neutral pH, was found to be the bottleneck in the solar circumneutral photo-Fenton process. As for introducing H_2O_2 into the solar/TiO_2 treatment, it did not prove to be advisable under the investigated conditions, as the enhanced abatement of micropollutants may not offset the higher potential environmental impacts resulting from the additional oxidant production [2].

To evaluate alternative oxidants, hydrogen peroxide (H_2O_2) was compared to two sulphate-based oxidizing agents (peroxymonosulfate and persulfate) under UVC radiation. In this case, UV radiation was chosen, as solar light may not be viable in some geographical regions or during specific seasons. Among the oxidizing agents examined, H_2O_2 demonstrated superior performance in overall micropollutant removal and exhibited lower potential environmental impacts than peroxymonosulfate and persulfate, even if the latter were used at lower concentrations. In the UVC processes utilizing the assessed sulphate-based oxidizing agents, the production of the oxidants emerged as the primary contributor to potential environmental impacts (Fig. 1), with peroxymonosulfate showing a higher contribution than persulfate.

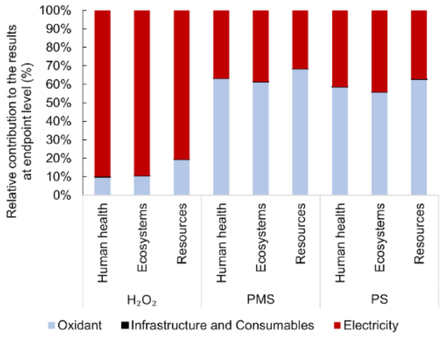

Fig 1. Relative contribution of the oxidant, infrastructure and consumables and electricity use to the results at endpoint level (ReCiPe) for the different 18 s of UVC solutions using 0.50 mM of oxidant [3].

2%).

In a study comparing heterogeneous photocatalysts, the graphene oxide-TiO_2 composite (GO-TiO_2) was chosen for comparison with the typically used, commercially available TiO_2-P25, due to its more recent prominence in the field of photocatalysis. Under the investigated conditions of solar photocatalysis, it was observed that the treatment process employing GO-TiO_2 exhibited higher potential environmental impacts compared to the use of TiO_2-P25, mainly due to the use of ammonium hexafluorotitanate and boric acid to obtain TiO_2 in the composite via the liquid deposition method. If another synthesis method is applied, GO-TiO_2

could become a more environmentally viable alternative in advanced treatment processes. Such was verified for GO-TiO_2 synthesis via mechanical mixing. However, a more comprehensive investigation is essential, as the composites may exhibit a different photocatalytic activity depending on the synthesis method [1].

In this latter study, given that the initial literature review has shown that there was a lack of characterization factors for evaluating the freshwater ecotoxicity and human toxicity of numerous micropollutants, the scientific-consensus characterization model USEtox and existing literature were assessed to discern the availability of freshwater ecotoxicity characterization factors for PSs and CECs. The emphasis was placed on freshwater ecotoxicity, the available literature indicating that it might hold greater relevance than human toxicity, particularly in scenarios involving direct discharges into freshwater, such as those from UWWTPs.

Consequently, in this study, thirty-three first-proxy characterization factors that were previously absent for PSs and CECs in USEtox were estimated.These can be used as an initial approximation in future research. Additionally, since to tackle the existing data gaps, ongoing investigations are delving into *in vitro* experiments and the utilization of Quantitative Structure-Activity Relationship models (QSAR), the newly derived first-proxy characterization factors were also estimated using QSAR models to estimate ecotoxicological data, allowing for comparative analysis. The variation observed between the new first-proxy characterization factors using experimental versus estimated ecotoxicological data fell within the basic uncertainty of the model, indicating a promising avenue for further exploration in future research initiatives.

These case studies, through the identification of the environmental hotspots for the different treatment processes, offer another dimension for their optimization. The LCA results are also useful for providing guidance in the development of other alternatives, implementation of monitoring projects, and help in filling gaps in life cycle assessments.

Within collaboration with industry and corporation, a master dissertation has been developed with a Portuguese paint and varnish corporation (CIN) on their organizational gate-to-gate environmental footprint, which serves as a first step for their future Corporate Sustainability Reporting. Moreover, development of more environmentally-friendly technologies for packaging started to be developed in the framework of the “Embalagem do Futuro” (Packaging of the Future) project, with PRR funding and the participation of several companies. The LCA methodology has also been implemented to study the environmental performance of other products and technologies. Some examples are:

(i) comparative LCA of wood, metal, plastic and composite pallets. This study reviews pallet production, its mechanical properties related to material options (according to European standards and industrial applications) and management systems. A Multicriteria analysis was performed to select the best option considering the environmental impact, cost, service life and load capacity.

(ii) comparative LCA of organic solvent recovery. This study aimed to identify hotspots in the solvent recovery process that could be targeted for action to improve its overall performance.

(iii) attributional LCA of ready meal, based on “stone soup”, to explore the impact of the packaging. Ready meals can have several environmental benefits when compared with homemade food. The ability to carry out in an industrial plant the process of preparing large amounts of meals with optimized proportions of food, water and energy may be more environmentally and energetically efficient when compared with the resources used in the preparation of the same number of meals made at home in regular kitchen facilities. Nonetheless, the need for dedicated packaging to deliver ready meals to consumers is an additional feature that is not required when preparing homemade meals. Particularly, considering that the pre-cooked meal packages are usually based on single-use plastic containers, it is of key importance to understand the influence of such packaging on the total life cycle of ready meals. Thus, a dedicated LCA was conducted to infer the impact of the packaging process on a well-established ready-made meal process.

Future Work

To tackle the complexities of environmental assessments, challenges persist in estimating inventory data for chemical production processes due to the need for more background information, introducing uncertainties in the LCA results. As the exploration of treatment processes and advanced catalysts continues, a key focus on recovery and reuse potential emerges. Future efforts will extend to developing characterization factors for a broader spectrum of substances, microplastics, and biological contaminants, strengthening the data for the LCA. In addition, the LCA will be extended to include the development of more sustainable analytical methods for monitoring PSs and CECs (work to be carried out as part of an individual competition to stimulate scientific employment recently awarded by FCT to a junior researcher in our team). Within future perspectives regarding general collaboration with industry and corporations for LCA use in the development of more environmentally-friendly technologies, the “Embalagem do Futuro” (Packaging of the Future) project, with PRR funding, must be highlighted. In this project, the LCA of different packaging types is under development, allowing for the optimization of packaging production systems.

Related Sustainable Development Goals

Outputs

PhD Theses

Joana Pesqueira, Catalytic Water Treatment Life Cycle Assessment, PDEA, FEUP, 2023

Master Dissertations

Alejandro Jose Bermudez Pulgar, Eco Efficiency production and environmental impact of pallets based on different materials, Master Design Product Engineering, ESTG-IPLeiria, 2023

Catarina Isabel da Silva Monteiro, Reporte Corporativo de Sustentabilidade, MIEQ, FEUP, 2023

Cristiano da Silva Paiva, Análise da ecoeficiência de processos numa indústria do setor alimentar, Master in Energy and Environmental Engineering, ESTG-IPLeiria, 2023

Susana Patrícia Marques Pires, Análise do Ciclo de Vida do Sistema de Recuperação de Solventes, Master in Energy and Environmental Engineering, ESTG-IPLeiria, 2023

Selected Publications

[1] Pesqueira, J. F. J. R., Pereira, M. F. R., Silva, A. M. T., J. Cleaner Prod. 261, 121078 (2020)

[2] Pesqueira, J. F. J. R., Pereira, M. F. R., Silva, A. M. T., Sci. Total Environ. 761, 143258 (2021)

[3] Pesqueira, J. F. J. R., Marugán, J., Pereira, M. F. R., Silva, A. M. T., Sci. Total Environ. 808, 152050 (2021)

Team

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