Technologies for Pollution Control

Advanced Oxidation Processes

KEYWORDS: Photoreactors / CFD Modelling / FluHelik / NETmix / AOPs / Solar Driven AOPs / Photocatalysis / Photo-Fenton

Design of cost-effective photoreactors, from the development of catalysts/supports to designing computational fluid dynamics models and testing breakthrough reactors for advanced oxidation processes.

Introduction

Advanced oxidation processes (AOPs) are characterized by the production of oxidizing species, such as hydroxyl and sulfate radicals, which are quite reactive and non-selective, able to react with virtually all classes of organic and inorganic compounds in a relatively short time. Additionally, specific AOPs can also generate electrons or reducer species, enabling their use for reduction processes.

Our research has been oriented to: (i) the use of natural solar radiation as ultraviolet (UV)-visible photon source, combined with artificial UV-visible light, to promote the light-induced AOPs, turning these processes even more economically attractive through the use of renewable solar energy; (ii) development of breakthrough designs for the optical system used in sunlight capture based on compound parabolic collectors (CPCs) by non-imaging optics (NIO) techniques and for photoreactors using artificial light by computational fluid dynamics (CFD) tool.

Current Development

Different AOPs were applied for the following niche applications: (i) removal of UV filters from swimming pool water, (ii) degradation of volatile organic compounds from indoor air streams, (iii) tertiary treatment of urban wastewaters, as polishing step to eliminate the so-called contaminants of emerging concern, (iv) treatment of landfill leachates contaminated with high loads of recalcitrant organic compounds, (v) treatment of wastewaters containing inorganic oxyanions (As(III) and Cr(VI)), and (vi) decontamination of other liquid streams. The main AOPs include: UVC/H_2O_2, UVC/persulfate, Fenton, photo-Fenton, solar-photo-Fenton, and heterogeneous and homogeneous photocatalysis using different metal oxide nanomaterials.

New hardware/photoreactors for AOPs have been developed, such as: (i) solar photoreactors with cost-effective collectors optics, using NIO techniques, targeting the capture of UV-visible radiation to promote iron-based catalytic reactions for the oxidation of high-strength wastewaters (Fig 1a); (ii) innovative photoreactor using artificial light, FluHelik photoreactor, designed by CFD, for photochemical and iron-photocatalytic oxidation processes (photo-Fenton); (iii) a mili-photoreactor based on the NETmix technology, using microscale illumination (LEDs), for gas-streams decontamination through heterogeneous titanium dioxide (TiO_2)-P25 photocatalysis, minimizing photon and mass transfer limitations, thereby markedly reducing the reactor size and significantly boosting its efficiency.

Concerning the reflector's optical efficiency of solar collectors (geometry: flat, single double parabola, and traditional double parabola; materials: anodized aluminum with (MS) and without (R85) protective coating, soiled aluminum (R85s) and stainless steel (SS)) it was possible to conclude (Figs 1b,c): (i) the negative impact of 8-years of outdoor exposure of the R85 anodized aluminum (loss of 38.7% of specular reflectance and a decrease of 26% in the optical efficiency); (ii) for flat geometry the difference in the material reflectance has a negligible influence on the optical efficiency; (iii) the inclusion of a simple flat reflective surface, increases the optical efficiency up to 17% when compared to the absence of reflector.

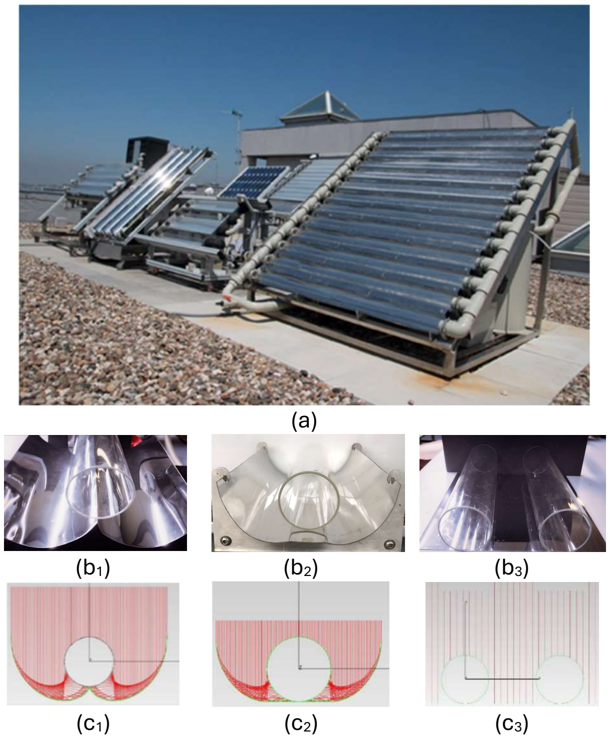


Fig 1. Photograph of solar photoreactors with compound parabolic collectors (a); Photograph of collector optics (b) and 2D ray trace analysis for incident angles of 45º (c), for the traditional (b$_1$, c$_1$) and simple (b$_2$, c$_2$) double parabola geometries and flat reflector (b$_3$, c$_3$).

The photo-Fenton applied to urban leachate showed that the process efficiency over time was mostly coherent with the optical efficiency of the different reflective surfaces.

The cost analysis performed for the solar collectors showed that the flat reflector would be the best option, presenting the highest volumetric treatment factor. For the same investment cost that would be required to build 100 m^2 of a collector using the double parabola reflector made of R85, it is possible to construct 126 m^2 of a collector using a flat reflector made of stainless steel, increasing 1.6 times the number of absorber tubes per square meter, corresponding to a treatment rate increment of 51%. Considering that higher illuminated surface-to-volume ratios reduce the reactor dimensions and capital and operating costs, the flat geometry reflectors using a resistant material, such as stainless steel, may be a cost-saving and effective solution in the treatment of wastewater with low transmissibility and presenting UV inner-filter effects, such as leachates, by the photo-Fenton process.

The FluHelik photoreactor (Fig 2) generates a helical fluid motion around a UVC-radiation source, inducing unique dynamics and irradiation properties. Due to its unique configuration, the FluHelik provides a more homogeneous UV radiation distribution, being able to overcome matrix effects (inner UV filter effects) in wastewaters with low to moderate transmissibility. Another advantage of this reactor technology is its easy scalability through its very simple and compact arrangement in series, strongly promoting its use in industrial applications.

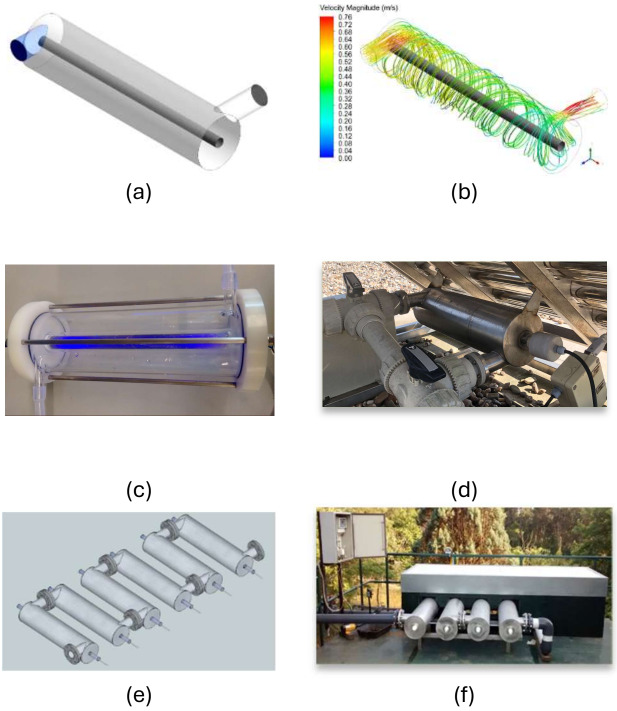


Fig 2. Photographs of lab (c), pilot (d), and pre-industrial (f) scale FluHelik photoreactor; Sketch of the FluHelik photoreactor (a), Sketch of FluHelik reactors mounted in series (e); Streamlines obtained from CFD simulation (b).

The intensification of heterogeneous photocatalytic processes was achieved for air decontamination with the NETmix mili-photoreactor (Fig 3). It consists of a back stainless steel slab imprinted with a network of cylindrical mixing chambers (diameter: 6.5 mm, depth: 3 mm) interconnected by prismatic transport channels (length: 2 mm, width: 1 mm, depth: 3 mm) and sealed with a frontal borosilicate glass slab (reactor window). The illumination system, located above the reactor window, consists of an LED plate.

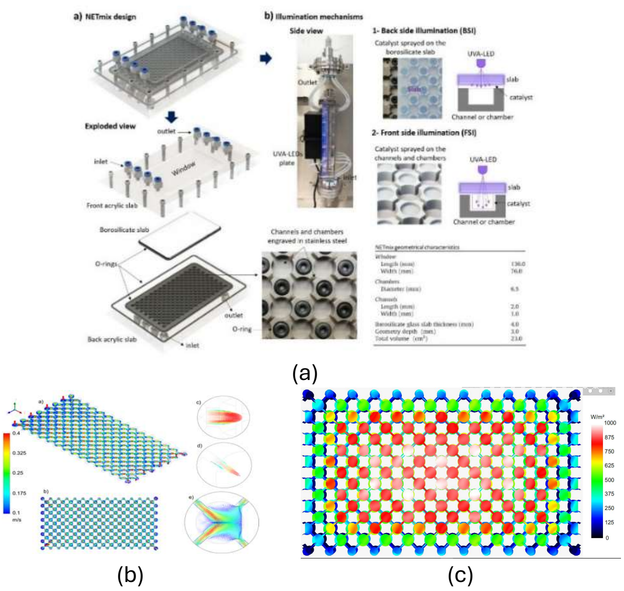


Fig 3. NETmix mili-photoreactor schematic representation and illumination mechanisms (a); Streamlines (b) and radiation profile (c) obtained by CFD simulation.

A thin TiO_2-P25 catalyst film was immobilized in the NETmix network or the reactor window, allowing for two illumination mechanisms: front-side (FSI) and back-side illumination (BSI).

The radiation field in the meso-scale NETmix photoreactor for gaseous stream purification was evaluated employing a Monte Carlo-based algorithm through the use of the software Ansys Speos. The illumination system consists of 18 high-power UV LEDs placed over the reactor window. The distance between each LED and the distance between LEDs plate to the reactor window were varied to determine the impact of LEDs geometrical arrangement in the registered irradiance as well as in the radiation homogeneity over the catalyst surface. 27 illumination schemes were proposed and simulated for each BSI and FSI. The results show that the absorption efficiency increases with the proximity of LEDs to each other and to the reactor window. However, in the same conditions, the homogeneity of the illuminance intensity decreases. The absorption efficiencies range from 29.2% to 42.8% for the BSI and from 31.3% to 40.5% for the FSI. The results also show that the distinct locations of the catalyst films have significant importance. The FSI cases present similar absorption efficiency to the BSI, even though the FSI configuration has almost 4 times more superficial area than the BSI. Also, the FSI cases present higher values of variation coefficient, meaning that the area is less homogeneously illuminated.

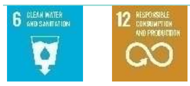
The combination of ray tracing and CFD simulations also allowed the identification of an ideal illumination system composed of 15 inline LEDs with an LEDs-to-reactor distance equivalent to 12 mm.

Future Perspectives

FluHelik at pre-industrial scale: tertiary treatment of urban wastewaters targeting disinfection and contaminants of emerging concern removal, to be carried out at Ave WWTP.

NETmix: impact of NETmix depth and illumination system composed of LEDs with distinct view angles in the photocatalytic oxidation of volatile organic compounds in airstreams.

Related Sustainable Development Goals



Outputs

PhD Theses

[1] Batuira Martins da Costa Filho, Intensification of heterogeneous photocatalytic processes using the NETmix mili-photoreactor for VOCs oxidation at gas phase, FEUP, 2019

[2] Tatiana Matiazzo, Reactive flow and photon fate in a mesoscale reactor applied to the photocatalytic abatement of pollutants in gas phase: a theoretical investigation, UFSC/FEUP, 2022

[3] Sandra Mendes Miranda, Intensification of heterogeneous photocatalytic processes using an innovative static mixer micro-meso-structured photoreactor towards indoor air treatment, FEUP, on-going, 2017-2024

Master Dissertations

[1] Isabel Sofia Oliveira Barbosa, Modelação do foto-reator FluHelik usando ferramentas de CFD, MIEQ, FEUP, 2018

[2] Joana Pinto Monteiro, Intensificação do processo de fotocatálise heterogénea utilizando o mili-fotoreator NETmix para descontaminação de correntes gasosas, MIEA, FEUP, 2019

Selected Publications

[1] A.I. Gomes et al., J. Clean. Prod. 199, 369 (2018)
[2] B.M.C. Filho et al., Chem. Eng. J. 366, 358 (2019)
[3] S.G.S. Santos et al., Chem. Eng. J. 405, 126612 (2021)
[4] J.C. Espíndola et al., J. Environ. Chem. Eng. 9, 105060 (2021)
[5] T. Matiazzo et al., Chem. Eng. J. 444, 136577 (2022)

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Funding

NOR-WATER, 0725_NOR_WATER_1_P, 2019-2022
LSRE-LCM Base Funding, UIDB/50020/2020, 2020-2023
LSRE-LCM Programmatic Funding, UIDP/50020/2020, 2020-2023
LA LSRE-LCM Funding, UID/EQU/50020/2019, 2019
LA LSRE-LCM Funding, POCI-01-0145-FEDER-006984,2013-2018
FCT Grants: CEECIND/01386/2017, CEECIND/02196/2017, CEECIND/01317/2017
FCT Scholarships: CNPq: 202086/2014-3, SFRH/BD/119915/2016, CNPq: 141088/2018-4