Multi - criteria optimization approach applied to photocatalytic nano-structured systems for waste water remediation

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Background, Motivation and Objective

Assuring the availability and sustainable management of water and sanitation converted in 2015 into one of the 17 Sustainable Development Goals (SDGs). The goal set by the world leaders to create a better world by 2030[1]. This work is inspired by this vision and it takes advantage of nanotechnologies to provide effective responses to the increasing water challenges. Photocatalysis is being explored as an Advanced Oxidation Processes (AOPs) in wastewater treatment, against persistent organic pollutants and emerging contaminants. In this work five nanomaterials (NMs) were assessed as alternative options to obtain a Safe and Sustainable by Design (SSbD) AOPs. The same incorporation process was used for all NMs and the same testing conditions were applied by using a water purification lab scale unit. Experimental models and in-silico tools were used to identify the best design options, which simultaneously maximise oxidation functionality, economic and environmental performances. This allowed to identify the best material candidate and the optimal operating conditions in terms of irradiation time.

Statement of Contribution/Methods

1. *The reactivity of four different nano photocatalysts was evaluated. We applied a Multi Criteria Optimization (MCO) algorithm to combine three main response functions correlating synthesis parameters to corresponding performance attributes: the functionality was evaluated in terms of photocatalytic efficiency; the environmental sustainability in term of CO_2 emission and the cost in terms of energy consumption. The objective of the MCO analysis was to maximize the functionality and minimize the environmental impact and cost, identifying the most sustainable solutions in the design space.*
2. *The photocatalysts were immobilised as coatings on fabric substrates by dip-pad curing process and integrated in a semi-pilot plant (6L) in order to extend the design investigation also to plant prototypes for waste water treatment.*
3. *The ROS (Reactive Oxygen Species) mediated reactivity of the tested photocatalysts was assessed, through different experimental models, in order to predict their functionality and provide acellular descriptors for the evaluation of oxidative stress in cells.*
4. *A predictive machine learning tool (linear estimator) revealed the input parameters that significantly influenced the outcome: amounts of probes molecules consumed by ROS mediated reactivity.*

Results/Discussion

As example of the achieved results, we report in Fig. 1 the MOC analysis, revealing that based on cost criteria, the use of composite photocatalysts is not recommended, however, if we consider environmental sustainability as the predominant factor, TiO_2:SiO_2 performed optimally.

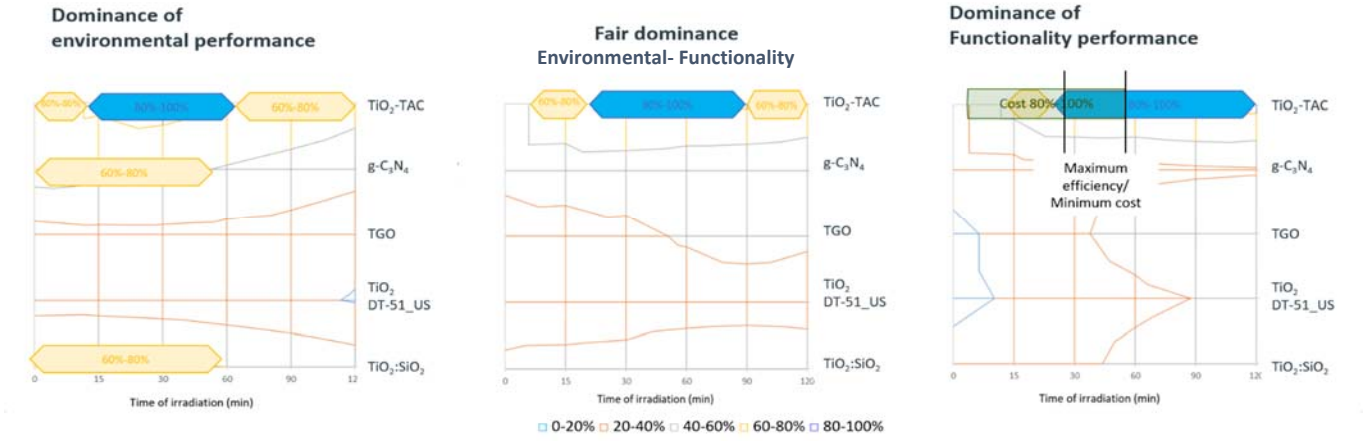

Figure 1. Decision – making space and partition of the optimization domain as a function of the multicriteria performance responses.

The predictive machine learning tool (R^2: 0.96) applied to reactivity data obtained with different experimental models (Cys, GSH, RNO) provided information about the experimental parameters (assay, conditions of light and incubation time) and pchem properties (i.e., zeta potential) that tune the photocatalytic process relevant to both the degradation of organic pollutants and to the assessment of their pro-oxidative hazard for human health and for the environment.

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[1] United Nations; Transforming our world: the 2030 Agenda for Sustainable Development. *Resolution adopted by the General Assembly on 25 September* A/70/L.1