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Life Cycle Assessment and Cost Benefit Analysis for the integrated assessment of an innovative Mn-TiO2 nanoparticle photocatalytic paint

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Abstract. Life Cycle Assessment (LCA) and Cost Benefit Analysis (CBA) are applied for an integrated assessment of a new photocatalytic paint-product developed within LIFE VISIONS project. The TiO2-nanoparticle photocatalytic paint has been demonstrated to efficiently remove NOx and VOCs, thus contributing to improved indoor air quality with substantial related human health benefits. LCA was conducted using openLCA software and Product Environmental Footprint (PEF) dataset. Cradle-to-grave approach was followed, considering all life cycle processes related to production, application and disposal, in order to examine the potential environmental benefit compared to conventional paint. Thus, simulations were performed considering different building types and electricity needs, to evaluate the sustainability advantage of the photocatalytic product under different conditions. Computational Fluid Dynamic (CFD) simulations are also deployed to reveal the efficiency of the proposed photocatalytic paint in terms of indoor air quality improvement under different scenarios of application. The results are used to evaluate the health benefits for the CBA, on the basis of a Driver-Pressure-State-Impact-Response (DPSIR) methodology. Indoor pollutant concentration levels from the CFD simulations will be used as input to estimate the dose-response functions for quantifying health impacts. Resulting health impact indicators will be translated into monetary terms during the final stage of CBA.

Keywords: TiO_2 photocatalytic paint, indoor air quality, computational fluid dynamics modelling, life cycle assessment, cost benefit analysis

1. Introduction

1.1. Indoor air quality and photocatalytic TiO_2-based nanomaterials

Indoor air quality is an important issue for human health (URL1), as nowadays people spend most of their time in closed spaces, such as schools, offices, residences, hospitals, etc. Worldwide, various strategies and technologies are currently being under development to promote healthy indoor environments.

Much research is carried out on photocatalytic nanomaterials, often involving titanium dioxide (TiO_2), which is an innovative and promising solution for degrading indoor air pollution (Wang et al., 2022; Binas et al., 2017). Anatase TiO2 nanoparticles can show significant photocatalytic properties, when exposed to ultraviolet (UV) radiation (Geoffrey et al., 2011)., Additionally, attempts have been carried out for manufacturing nanoparticle TiO_2 materials which photocatalize air pollutants also in the visible spectrum of light, when doped in metals, such as manganese, etc. (Binas et al., 2011).

1.2. LIFE VISIONS project

In this context, the LIFE VISIONS project (URL2) targets at developing a nanoparticle TiO_2-based photocatalytic paint, in order to improve air quality of indoor spaces, specifically by degrading the concentrations of NO_x and VOCs, when illuminated by UV and visible light. Based on the improvement of indoor air quality, mechanical ventilation needs are reduced by the application of the photocatalytic product, thus also decreasing the electrical energy consumption of the painted room/building. The project is still ongoing and takes place in Athens, Thessaloniki and Heraklion, of Greece.

2. Methodology

The study refers to an integrated assessment of the photocatalytic paint by combining LCA, CFD and CBA.

2.1. Life Cycle Assessment

The goal and scope of the LCA study is to compare the environmental impacts related to the paint industry sector, between a conventional and the photocatalytic paint, so as to investigate the potential sustainability advantage of the photocatalytic product through its life cycle.

For this reason, two approaches were followed, a cradle-to-factory's exit gate and a cradle-to-grave. Regarding the first, the life cycle of paint production was examined, involving all related secondary stages (raw materials extraction, transportation, materials manufacturing, etc.). In the second approach, a cradle-to-grave approach took place, expanding the system to the point of paint application in rooms/buildings and its End-of-Life (EoL) phase (Figure 1).

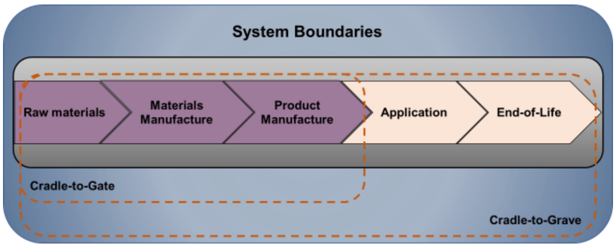

Figure 1. System boundaries

The development of the Life Cycle Inventory (LCI) involved the definition of the processes and the quantification of the relevant inputs and outputs needed (Figure 2). Primary data were provided by the VITEX paint industry (paint producer), as well as by the Foundation for Research and Technology (FORTH) (photocatalytic powder producer).

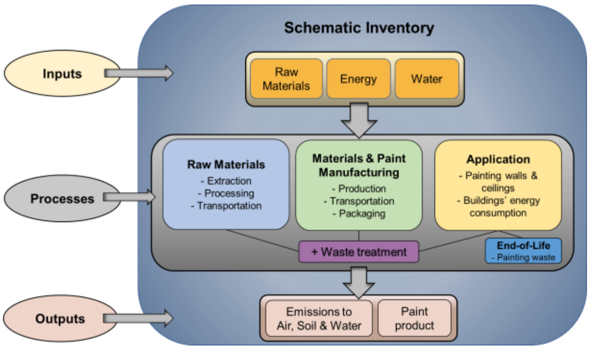

Figure 2. Schematic inventory

For this purpose, PEF dataset (v2.0) and the respective PEF Life Cycle Impact Assessment (LCIA) method were used in the openLCA software (v1.11.0) for all the required calculations and analysis of the study.

2.2. *CFD simulations and Cost Benefit Analysis*

CFD simulations are undertaken for calculating air pollution concentrations to examine the efficiency of the photocatalytic paint in reducing NO_x and VOCs indoor levels. Preliminary model simulations for model evaluation were performed initially in a field trial using two demonstration houses, one coated with a baseline paint and one with the photocatalytic paint (the inner walls of each house were painted). Two radiation scenarios were examined, the first one with natural light only and the second one with both natural and artificial light. Measurements in both houses were conducted simultaneously for NO_x and toluene and measurement results were compared to model output. Regarding model simulations, the commercial CFD code ANSYS CFX was applied in RANS mode. The standard k-ε two-equations turbulence closure model was used, in conjunction with the standard wall functions for the near wall treatment (Launder and Sharma, 1974). NO_x removal at the walls coated with the photocatalytic paint is estimated via a deposition flux F_d. F_d is directly proportional to the deposition velocity U_{dep} of the paint measured at lab scale and to the calculated concentration at the walls (Equation 1) (Moussiopoulos et. al., 2008).

$$F_d = U_{dep} \times C_{wall} \quad (1)$$

U_{dep} values were obtained by measurements for the different wall treatments under the two radiation scenarios. The mass reduction due to the deposition of pollutants is implemented into the momentum equation as a momentum sink. The above CFD modelling methodology will be applied also in the real-life case study of the Hellenic Navy Academy (HNA).

Concentration levels of the HNA will then be used for exposure calculations as part of the Impact-Pathway methodology (ExternE, 2005), for the purposes of the CBA (Figure 3). The Impact-Pathway methodology for deriving impacts in monetary terms is based on the DPSIR approach.

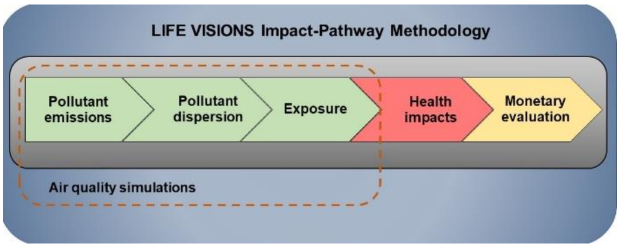

Figure 3. Impact-pathway methodology

The most suitable dose-response functions from epidemiological literature will be identified, so that relevant health endpoints can be correlated to the reduction in NO_x and VOCs concentrations, resulting from the photocatalytic paint application in different scenario studies.

3. Results and discussion

The results are presented in two parts, regarding LCA and CFD simulations seperately.

3.1. *Life Cycle Assessment*

A comparative analysis between the produced photocatalytic and a conventional paint is presented. The PEF dataset does not include endpoint indicators, so the results refer only to midpoint impacts and single score analysis.

3.1.1. Cradle-to-Gate approach (Paints production)

The cradle-to-gate analysis (functional unit: production of 1tn of each paint) reveal that for each midpoint indicator, higher values are calculated for the photocatalytic paint. Moreover, the impacts with the largest differences between the two paints are “Particulate Matter”, “Climate change-Fossil”, “Resource use, fossils”, “Eutrophication, freshwater” and “Acidification”.

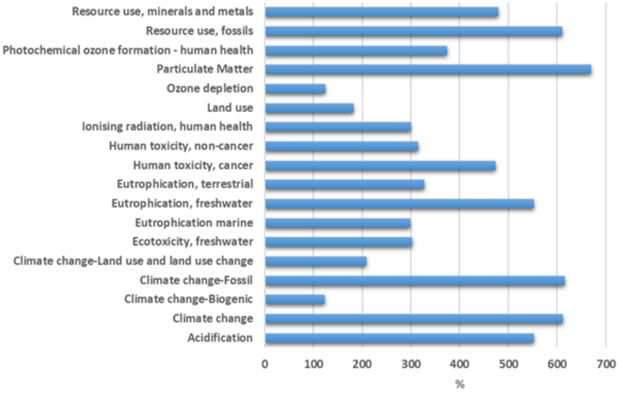

Figure 4. Midpoint impacts % increase of producing 1tn of photocatalytic in relation to the baseline paint

In the next phase, single scores were calculated by normalizing and weighting the above-mentioned values with the provided set, in order to build and compare the total environmental profile of each paint product. It should be noted, that not all midpoint indicators are involved in the single score calculations, as the PEF dataset does not include normalization and weighting factors for all of them. It is concluded, that the photocatalytic paint’s production life cycle has a higher environmental score than the baseline’s, specifically by a factor of 5.8.

By further analyzing the results (Figure 5), it becomes obvious that the photocatalytic paint’s higher environmental load is due to the TiO_2-based powder production and mainly to the NH_3 solution involved. Liquid NH_3 production is the dominant contributor in the total single score, accounting for 62%.

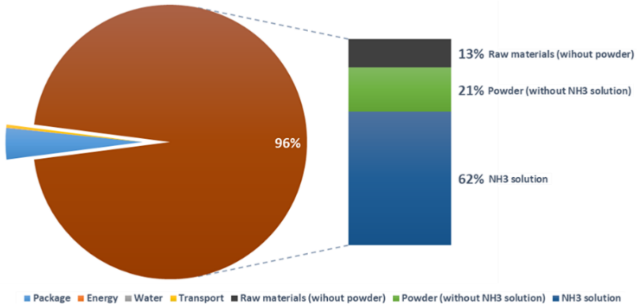

Figure 5. Process contribution in photocatalytic paint’s production life cycle

3.1.2. Cradle-to-Grave approach (Hellenic Navy Academy case study)

The cradle-to-grave approach (functional unit: m^2 of room/building) was implemented for the case study of HNA in Piraeus (Athens), Greece, in which the photocatalytic paint was applied. The comparative analysis was based on conventional and photocatalytic paint application in two different teaching rooms of the academy, i.e. rooms 217 and 218.

As the photocatalytic paint aims also at reducing the energy consumed by ventilation systems, energy was considered as input in the LCI. In the HNA facilities no such system exists, so an assumption was made and respective data were imported from a strategy report of the Greek Ministry of Environment, Energy and Climate Change, published in 2014 (URL3). Consequently, the energy saving % was based on simulations, as a correlation between ventilation rates and photocatalysis was found to exist and calculated to range between 3–4.7%. Thus, the average value was imported (3.85%) in the LCI. Also, the paints’ lifetime was considered to be 5 years.

The results strongly point toward an environmentally better total profile for the photocatalytic paint, when the whole life cycle is taken into account. Compared to the baseline, it presents reductions in almost all impacts within a range of 1.5-3.8%, while the respective single score calculations (Figure 6) suggest a 3.62% reduction.

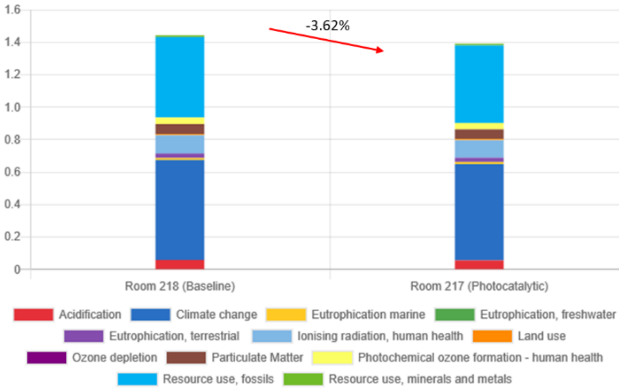

Figure 6. Cradle-to-grave single score analysis (HNA case study)

Therefore, it becomes obvious that although producing the photocatalytic paint is less environmental friendly compared to the production of the conventional product, if the first contributes to lower electricity consumption (at least at a rate of 0.22% for the specific case study), then it proves to have a sustainability advantage over the conventional paint.

3.1.3. Best and worst case scenario

A best and worst case scenario were also examined, considering two important factors that influence the environmental footprint of the paints, the amount of electricity consumed and its % reduction in the facility that are applied. Firstly, as the relation between the amount of electricity consumption and % reduction in the single score is described by the following calculated logarithmic equation: $y = -0.08\ln(x) - 3.23, \mathit{with}\ R^2 = 0.95$, it is understood that the advantage of the photocatalytic paint is more pronounced in facilities with greater ventilation needs, such as hospitals.

So, the worst case application scenario is when the paint is applied in department buildings, which show the less electricity needs (URL3), and simultaneously when the lowest simulated energy saving (3%) is achieved. On the other hand, the best scenario is described by the case of applying the photocatalytic paint in hospitals, which have the highest electricity needs (URL3), and by accomplishing the highest possible energy saving rate of 4.7%.

3.2. CFD simulation results

Numerical modelling results show a good agreement with measurement data in terms of the estimated NO$_x$ degradation due to the photocatalytic coating. Both measurements and modelling results indicate a very high removal of NO$_x$, between 60 % - 85%, depending on the radiation scenario studied (Table 1).

Table 1. Measured vs modelled NOx removal results based on two radiation scenarios

Pollutant	**Radiation scenario**	**Removal (%)**		U_{dep} **(cm s^{-1})**
		Measured	**Model**	
NO$_x$	Natural light	61.7	70	0.028
	Natural+ artificial light	70.1	85	0.034

For both radiation scenarios modelling results seem to overestimate removal rates by 10% (for natural light) to 15% (for natural+artificial light) compared to the measurements. The very high rate of removal can be explained by the operation of the fan, causing a very intense mixing inside the demonstration houses and forcing the air masses towards the treated walls. Considering the fact that the demonstration houses are completely sealed during the measuring period (1hr), the most part of NO$_x$ will inevitably come into contact with the treated walls and will be degraded. Modelled NO$_x$ concentrations are higher in areas near the treated walls compared to the centre of the houses. This is due to the above-mentioned accumulation effect near the volume boundaries, despite the fact that NO$_x$ removal is also enhanced in the same areas. In addition to the pointwise results, which facilitate the comparison with the corresponding measurements, a volume-averaged concentration reduction will be calculated with the CFD model in the HNA case study to provide the indoor concentration distribution for exposure calculation.

4. Conclusions

In the context of LIFE VISIONS project, the study presents an integrated sustainability analysis of the nanomaterial TiO$_2$-based photocatalytic paint. The LCA study indicates that the total environmental impact of the production's life cycle proved to be higher in relation to the baseline, mainly due to the NH$_3$ solution involved in the powder production. On the other hand, when the whole life cycle is considered and if a small % of electric energy is saved, the results signify an environmental advantage of the photocatalytic over the baseline paint. Additionally, worst and best-case scenarios results showed under which conditions the minimum and maximum environmental benefit from applying the photocatalytic paint would be achieved.

The preliminary CFD modelling results from the demonstration houses show good agreement with measurements, exhibiting an overestimation in the order of 10% to 15%. Both measurements and modelling results indicate a very high reduction of NO$_x$ concentrations. However, this is directly related with the operation of the fan which intensifies the mixing and forces pollutants to come into contact with the treated walls. Therefore, such high rates of removal may not be achieved in real life applications. First measurements from the real-life case study of the HNA are very encouraging as they demonstrate a reduction in the order of 20%, depending on the prevailing conditions and the behavior patterns of the building users. The case study estimated concentrations will be used for exposure calculations in the CBA.

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URL2: https://lifevisions.gr/

URL3: https://rb.gy/eh9vau

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