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# ASSESSING THE EFFECTIVENESS OF A PHOTOCATALYTIC PAINT FOR DEPOLLUTION IN A CONTROLLED INDOOR ENVIRONMENT

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**Abstract**: The current study aims to investigate the effectiveness of a novel photocatalytic paint developed as part of the EU LIFE VISIONS project in reducing air pollutants and enhancing indoor air quality (IAQ). To achieve this goal, numerical Computational Fluid Dynamics (CFD) simulations were performed in various scenarios to assess the concentration levels of indoor environments painted with the new photocatalytic paint compared to conventionally painted indoor spaces under identical conditions. Initially, the methodology was implemented in demonstration houses at the Foundation for Research and Technology – Hellas (FORTH), where controlled mechanical ventilation conditions were applied in order to investigate the impact of natural and artificial light on the photocatalytic $NO_x$ reduction. A second case was examined in a teaching room at the Hellenic Naval Academy (HNA) under real-world conditions, with ambient nitric oxide being transported into the rooms from the outdoor environment. The results revealed a notable decrease in $NO_x$ concentrations in the FORTH room painted with the photocatalytic paint, both in the presence of natural light only and when natural light was supplemented with artificial light. Additionally, a significant decline in nitric oxide levels, particularly in proximity to the photo-painted walls, was observed in the HNA case. Finally, a Life Cycle Assessment (LCA) was conducted in order to describe the overall environmental performance of the photo-paint. The study mainly focused on the footprint of the paint's production stage, as well as on the energy saving benefits of its application.

***Key words:*** *Indoor air quality, photocatalytic paint, Computational Fluid Dynamics, Life Cycle Assessment*

## INTRODUCTION

The exposure of populations to high concentrations of air pollutants can lead to several negative impacts on human health. Over the past two decades, there has been increased scientific interest in indoor air quality (IAQ), as people in cities spend an estimated 80% of their time in indoor environments (Klepeis *et al.*, 2001). In the direction of concentration reduction, innovative technologies for the production of paints incorporating photocatalytic materials have been developed. Previous studies have shown that these paints applied on indoor surfaces can reduce levels of various pollutants such as nitrogen oxides ($NO_x$), volatile organic compounds (VOCs), and toluene.

The primary goal of the EU LIFE VISIONS project (https://lifevisions.gr/) is the production of a photocatalytic paint to improve IAQ by decreasing the concentrations of pollutants such as $NO_x$ and VOCs. Within the LIFE VISIONS framework, a new paint with the addition of $TiO_2$ nanoparticles was tested in real-scale applications to investigate its capability to reduce concentration levels within rooms and buildings. To evaluate the effectiveness of the paint's photocatalytic properties, field trials were carried out in two different cases: Firstly, the photo-paint was used in demonstration houses on the premises of the Foundation for Research and Technology – Hellas (FORTH) in Heraklion, Greece, under controlled conditions and secondly, in a room at the Hellenic Naval Academy (HNA) in Piraeus, Greece, under real-life conditions. In both cases, the concentration levels were compared under the same set of conditions with the levels of a similar room painted with conventional paint.

The current study aims to investigate the efficiency of the paint in depolluting $NO_x$ in these two cases by using Computational Fluid Dynamics (CFD) models. For this purpose, CFD numerical simulations were performed for the indoor space geometries of both FORTH and HNA cases with photocatalytic and conventionally painted rooms.

Moreover, in the context of the project and in order to achieve an integrated assessment of the overall environmental performance of the photo-paint, Life Cycle Assessment (LCA) was conducted, as a suitable tool for environmental management and certified according to ISO 14044 and 14040 (https://www.iso.org/standard/38498.html, https://www.iso.org/standard/37456.html).

**METHODOLOGY**

The methodology relies on the following computational steps: Initially, a CFD simulation of air flow and photocatalytic removal is performed within the room painted with conventional paint. In the second step, a CFD simulation is performed within the photocatalytically-painted room using the same initial and boundary conditions as in the conventionally painted one. To calculate the deposition flux of the pollutant in the walls, a flow term $F_d$ is introduced in the CFD solver based on the following equation (Moussiopoulos *et al.*, 2008):

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

where $U_{dep}$ is the deposition velocity of the paint, determined by laboratory measurements for different wall treatments and radiation scenarios and $C_{wall}$ is the concentration at the walls.

Finally, the concentration levels of the examined pollutant within in the indoor environment of the photocatalytically painted room are compared with the corresponding concentrations in the conventionally painted room to assess the efficacy of depollution facilitated by the photocatalytic paint.

The methodology was initially tested in the FORTH demonstration houses depicted in Figure 1. One house had internal wall surfaces painted with photocatalytic paint, while the other was painted with conventional paint. The interior of both houses was filled with $NO_x$ in each scenario application. Two radiation conditions were studied: one using natural light only, and the other using both natural and artificial light. This research assesses the efficacy of photocatalytic paint in $NO_x$ depollution under mechanical ventilation conditions, which enhance mixing and are facilitated by a small fan.

**Figure 1:** Front and back view of the two demonstration houses in the premises of FORTH

For the CFD simulations, a CAD model was constructed to represent the geometry of the demonstration houses. This model was used to create a computational mesh, comprised of a total of $10^6$ hexahedral cells. The simulations were performed in steady-state using the Reynolds-averaged Navier-Stokes (RANS) approach along with the standard k-ε two-equations turbulence closure. Each simulation started with an initial $NO_x$ concentration of 500 ppb throughout the computational domain. In the room with the photocatalytic paint, deposition velocity values ($U_{dep}$) were set to 0.028 cm $s^{-1}$ for the natural light scenario and 0.034 cm $s^{-1}$ for the natural and artificial light scenario. It's worth noting that no additional external $NO_x$ was introduced into the house from the outdoor environment during the simulations.

The front view of the HNA 3D building model geometry is presented in Figure 2. The investigated rooms with photocatalytic and conventional paint were located on the second floor and share similar geometry and dimensions to facilitate comparison. The pollutant of interest in this case is nitric oxide (NO), as it was the pollutant selected for in-situ ambient measurements. In this case, both measurements and numerical simulations involve real-life conditions where the pollutant enters from the outdoor environment through the windows, and no mechanical ventilation is taken into account.

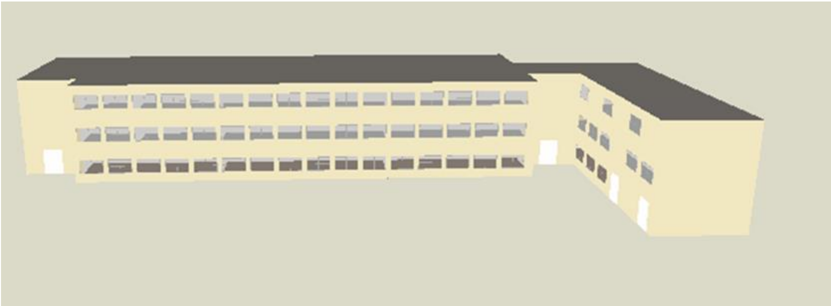

**Figure 2:** Front view (3D) of the HNA building

The generated computational mesh contains 758449 tetrahedral cells. Air and pollutants enter through inlet boundaries, set at the windows, and exit through the outlet boundary, set at the door. Simulations were performed using the RANS model with a k-ε turbulence model. For a typical day with low wind speed, the wind velocity at the inlet boundaries was set to $(u, v, w) = (1, 0, 0)$ m $s^{-1}$. Outdoor NO concentration levels were assumed to be 50 ppb, as in-situ measurements frequently show NO concentrations exceeding this value. In accordance with in-situ measurements, the deposition velocity, $U_{dep}$, was set to 0.05 $cms^{-1}$.

Regarding the LCA study, its goal was to assess the environmental performance of the novel photocatalytic paint, while the scope was to compare its life cycle with the respective of a conventional paint, examining the potential sustainability advantage of the photocatalytic product. Two methodological approaches were employed for this purpose: a cradle-to-gate, focusing on the production of the paints, and a cradle-to-grave assessment, extending the system boundaries to the End-of-Life (EoL) stage, while focusing on their application (see Figure 3). Primary data to create the inventory were provided by VITEX paints, FORTH, the HNA, the Process Equipment Design Laboratory (PEDL) of Aristotle University of Thessaloniki (AUTh) and literature. Secondary data were based on the Product Environmental Footprints (PEF) database, while the software used was openLCA. Impact analysis was also based on the PEF's impact method.

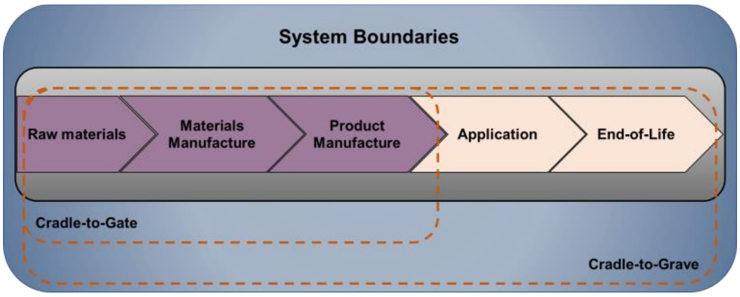


**Figure 3.** System boundaries

**RESULTS**

In Table 1, numerical simulation results for the FORTH application under two different radiation scenarios with mechanical ventilation for the mixing process are presented. The results are referenced to a point near the walls, corresponding to the sampling point of the measurement campaign. They show a significant reduction in $NO_x$ percentage in both scenarios: natural light only and natural light combined with artificial light. Specifically, under natural light conditions, a 70% reduction is observed, while a higher decrease of 85% in concentration levels is achieved by enhancing photocatalytic processes with the addition of artificial light.

**Table 1.** Concentration reduction percentage for two radiation scenarios (FORTH case)

| **Radiation scenario** | **Concentration reduction (%)** |
|---|---|
| Natural light | 70 |
| Natural + artificial light | 85 |

Figure 4 illustrates concentrations on three section surfaces aligned with the x–y plane in the room with photocatalytic paint (HNA case). These sections are positioned below (*z*=0.5 m), above (*z*=3.3 m), and at the same level (*z*=1.9 m) as the windows from where pollutants are transported from the outdoor environment into the room. The NO concentration distribution shows a significant reduction near the walls, indicating the activation of the deposition removal mechanism across all three horizontal sections heights.

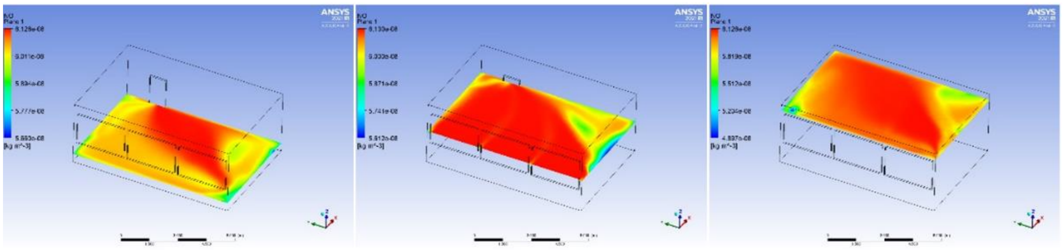

**Figure 4:** NO concentrations on a *x*–*y* section for *z*=0.5 m, *z*=1.9 m, and *z*=3.3 m (HNA case)

Table 2 presents the highest percentage reduction at a distance of 10 cm from the surfaces for both the entire room and the three layers. The point that observed the lowest NO concentration within the whole room indicates a reduction of 31.5% compared to the conventionally painted room. Regarding the three horizontal levels, the point with the highest NO de-pollution (20.1% decrease) is observed in the layer for *z*=3.3 m. In the section for *z*=0.5 m, the highest percentage reduction is 7.7%, while at *z*=1.9 m, it is 8.5%.

**Table 2.** Highest NO concentration percentage drop points in the room and the three different horizontal sections (HNA case)

| **Reference Volume or Area** | **Concentration reduction (%)** |
|---|---|
| Whole room | 31.5 |
| (*x-y* slice) *z*=0.5 m | 7.7 |
| (*x-y* slice) *z*=1.9 m | 8.5 |
| (*x-y* slice) *z*=3.3 m | 20.1 |

Assesing the LCA results, the cradle-to-gate approach indicates that all midpoint impacts are bigger for the photocatalytic paint, as well as its calculated single score (by a factor of 5.8), proving that its production is less environmentally friendly than the conventional paint. On the other hand, the cradle-to-grave approach reveals that if energy is saved (with a threshold value of 0.22% reduction) in the building that the photocatalytic paint is applied due to less mechanical ventilation needs for air purification, then it becomes more environmentally beneficial than the conventional in its whole life cycle. Indicatively, single score analysis implemented for the HNA case study shows a benefit of 3.62% in weighted points when a 3.85% energy saving rate is achieved (see Figure 5).

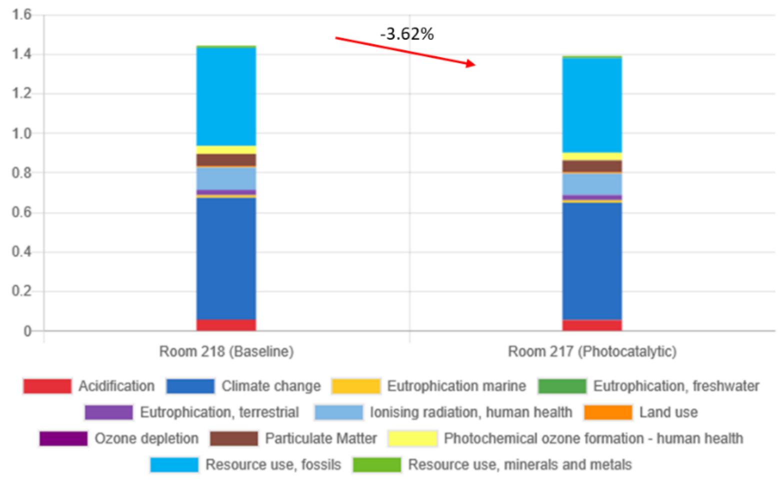


**Figure 5.** Cradle-to-grave single score analysis (HNA case study)

Finally, in the context of the project, LCA results were parameterized and incorporated in the form of generated equations in a developed Decision Support System (DSS) aimed to stakeholders. Multiple simulations were conducted where different energy consumption/saving rates were considered based on various building types and climatic zones, in order to parameterize the sustainability advantage of the photo-paint under different application conditions. Based on this process, two equations (2) and (3) were produced correlating the percentage reduction for the calculated single scores *y*, with a range of a) simulated energy saving rates (3-22%) (*x'* in equation 2, for which $R^2$=1), as well as b) different magnitudes of energy consumption needs (344-2729 kWh $m^{-2}$ per 5 years) (x in equation 3, for which $R^2$=0.95), assuming an energy saving rating of 3.85%.

$$y = 0.9976 \cdot x + 0.1653 \tag{2}$$

$$y = -0.08 \cdot \ln{(x')} - 3.2272 \tag{3}$$

## CONCLUSIONS

Results from CFD simulations illustrate the effect of the photocatalytic paint developed in the LIFE VISIONS project on reducing $NO_x$ and NO concentration levels. A significant reduction in $NO_x$ concentration in the FORTH demonstration houses was found, especially when artificial light supplemented natural light. During the real-world applications in HNA rooms, simulations indicated a noticeable decrease in NO levels, particularly near the painted walls. Finally, LCA results show that although the production of the photo-paint has a high environmental footprint, when at least 0.22% energy saving rate is achieved due to its application, its environmental performance proves to be better compared to conventional paints.

## ACKNOWLEDGEMENTS

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