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LIFEVISIONS
InnoVative photocatalytIc paintS for healthy envirOnment and eNergy Saving

Action B.4
Numerical Modelling and Data Analysis

Life Cycle Assessment and Air Quality Modelling

Aristotle University of Thessaloniki
Faculty of Mechanical Engineering
Energy Sector
Sustainability Engineering Laboratory

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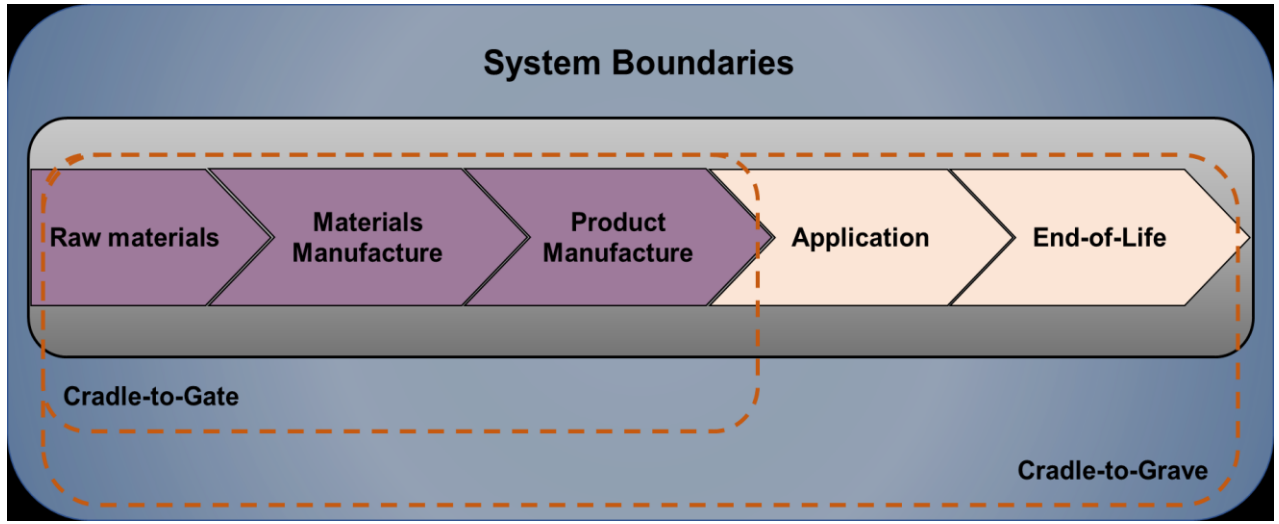
LCA Methodology

Goal & Scope

- Environmental impacts comparison:
  - Conventional vs Photocatalytic paint
- Cradle-to-Gate & Cradle-to-Grave approach



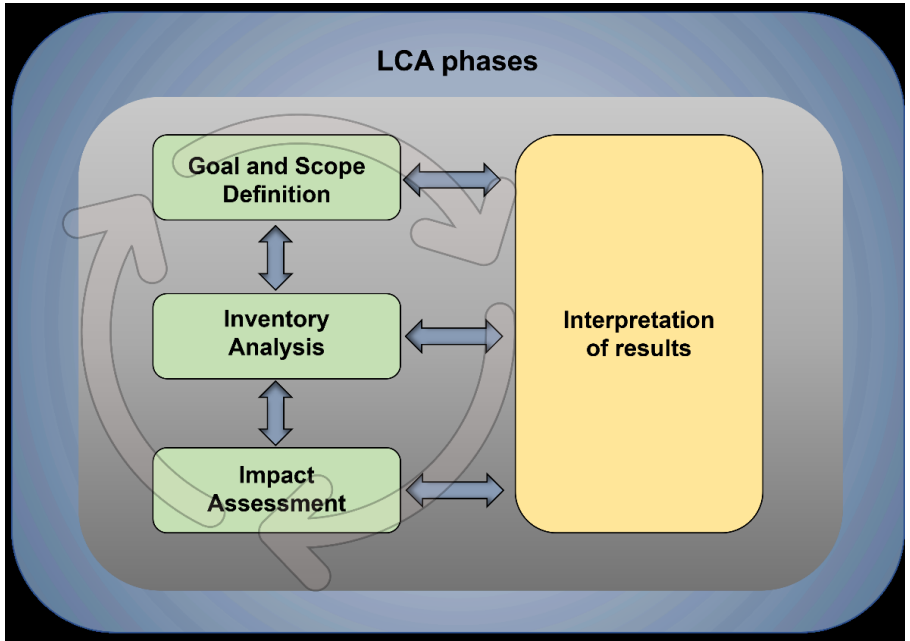
Inventory

- Data were collected from VITEX, FORTH, HNA, PEDL and literature
- Choice of software (openLCA) and database (PEFs)

Impact Assessment

- Choice of LCIA (PEF) to conduct all related calculations and analysis

Results Interpretation



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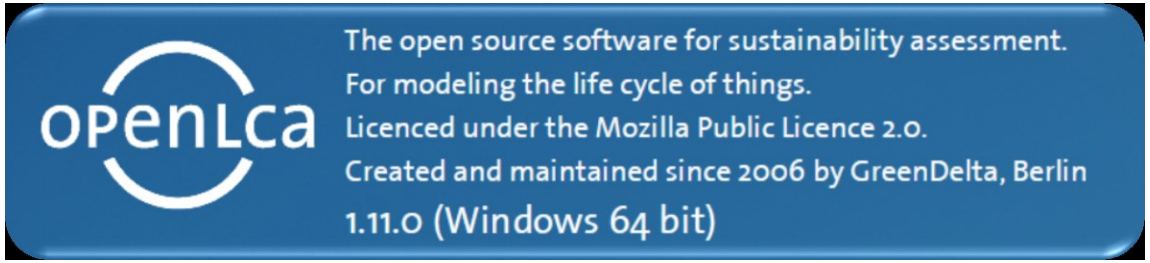
Software and Database

- **OpenLCA software:**
  - A free and professional approach to Life Cycle Assessment
  - Compliant to ISO 14040 and 14044.
  - Completely Open Source
  - Version 1.11.0

- **Features include:**
  - Fast and flexible import and export
  - OpenLCA Nexus – source for 27 databases and more than 40 LCIA methods
  - Own data quality systems can be defined by the user
  - Automatic and graphical creation of product systems
  - Statistical analysis tools



Product Environmental Footprints (v.2.0)

Developed by **GreenDelta** GmbH in the frame of the European Single Market for Green Products initiative

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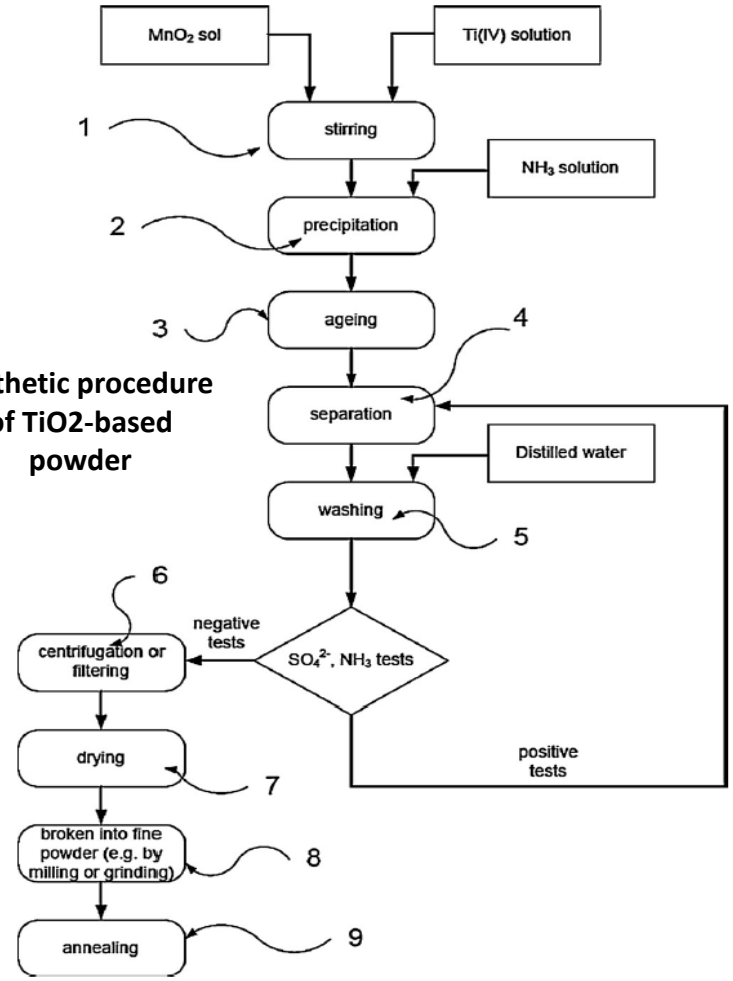
Cradle-to-Gate approach | Production



ynthetic procedure of TiO2-based powder

Raw materials data

Titanium oxysulfate	2.85 kg
NH3 solution (NH4OH)	4.28 kg
Distilled water	37.1 kg
Iron acetate	1.5 g
TCM-1	**1 kg**

- **Paint → VITEX**
- **Powder → FORTH**

Raw materials / Water / Energy / Fuel

Photocatalytic paint	%
TiO2 – 100% solids (proxy)	1.95
Photocatalytic TiO2	20
Tap water (proxy)	39.6166
Copolymer dispersion Vinyl Acetate (VAM) and Vinyl Versatate (VEOVA) – 50% in water	3.01
Calcium carbonate grounded – 100% solids (proxy)	33.41
Dispersing agent – 100% solids	0.15
Defoamer – 100% solids	0.17
CIT/MIT	0.0014
Benzisothiazolinone (BIT) – 100% solids	0.042
Monoethylene glycol	0.89
Amino methyl propanol, 95% in water	0.01
Cellulose thickener	0.73
Paints additive - 100% solids (generic proxy)	0.02

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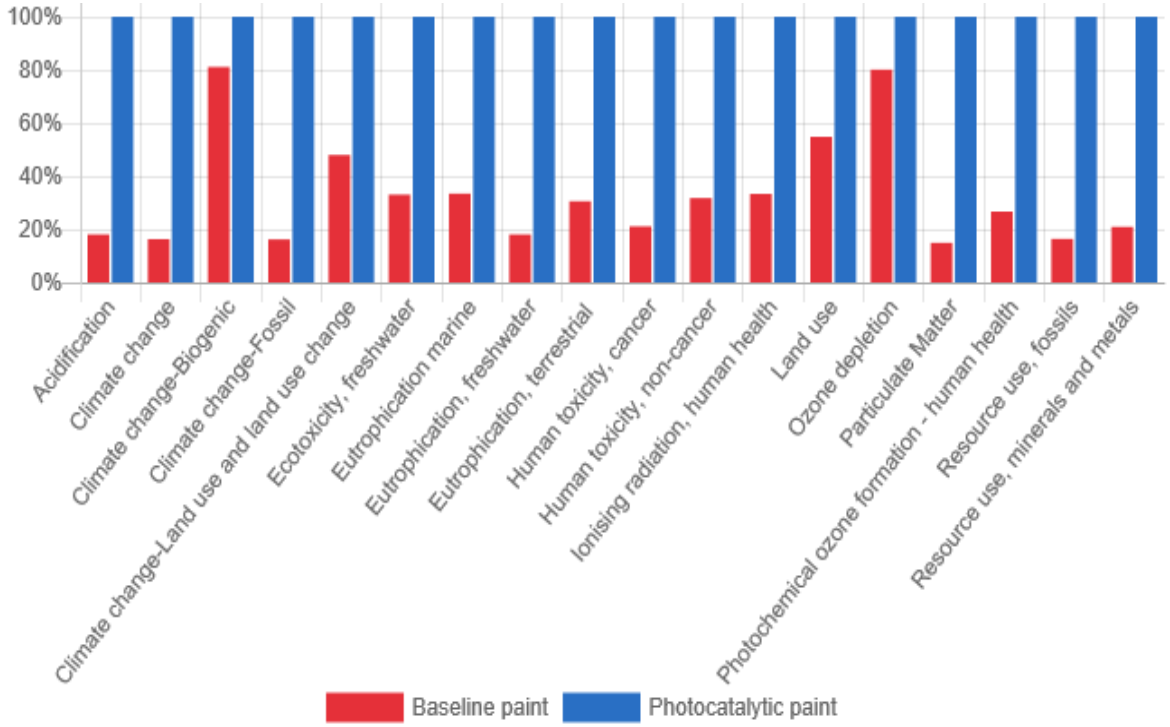
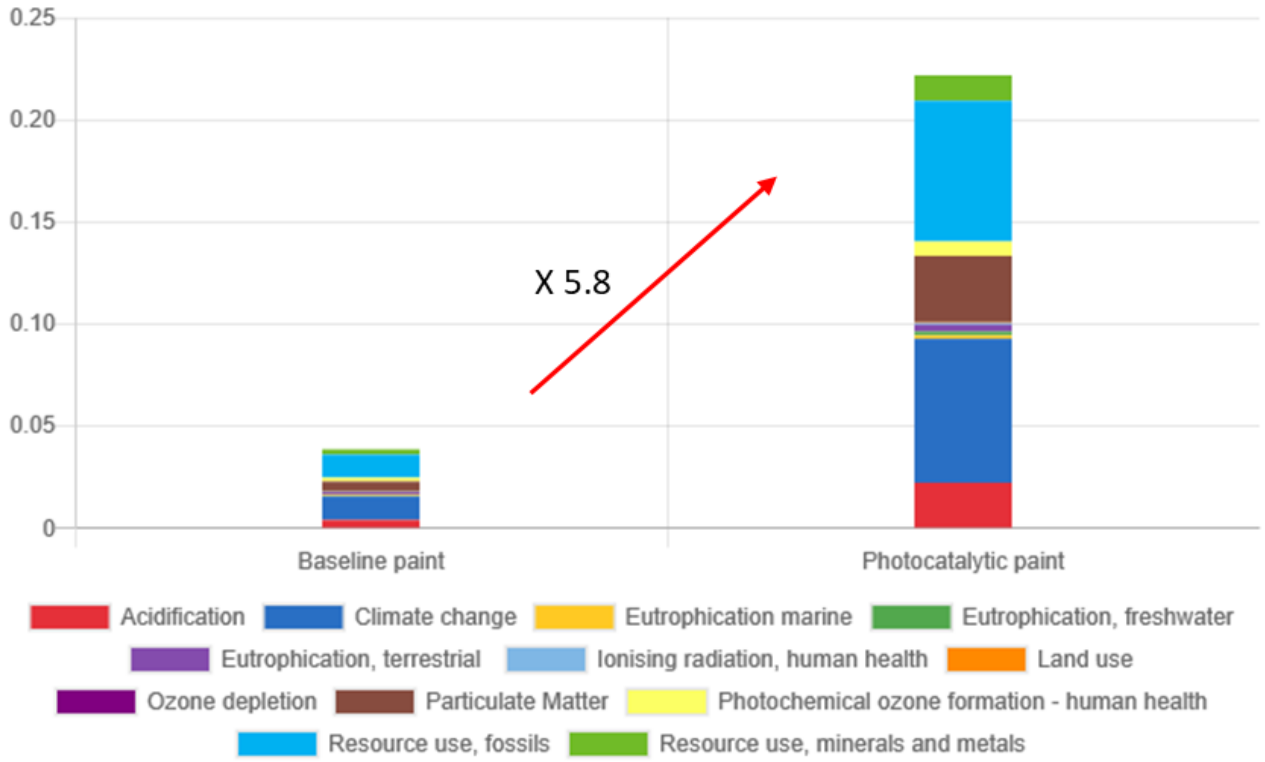
Cradle-to-Gate approach | Production



Relative bar chart:
Midpoint impacts of producing 1tn of paint



Single score analysis

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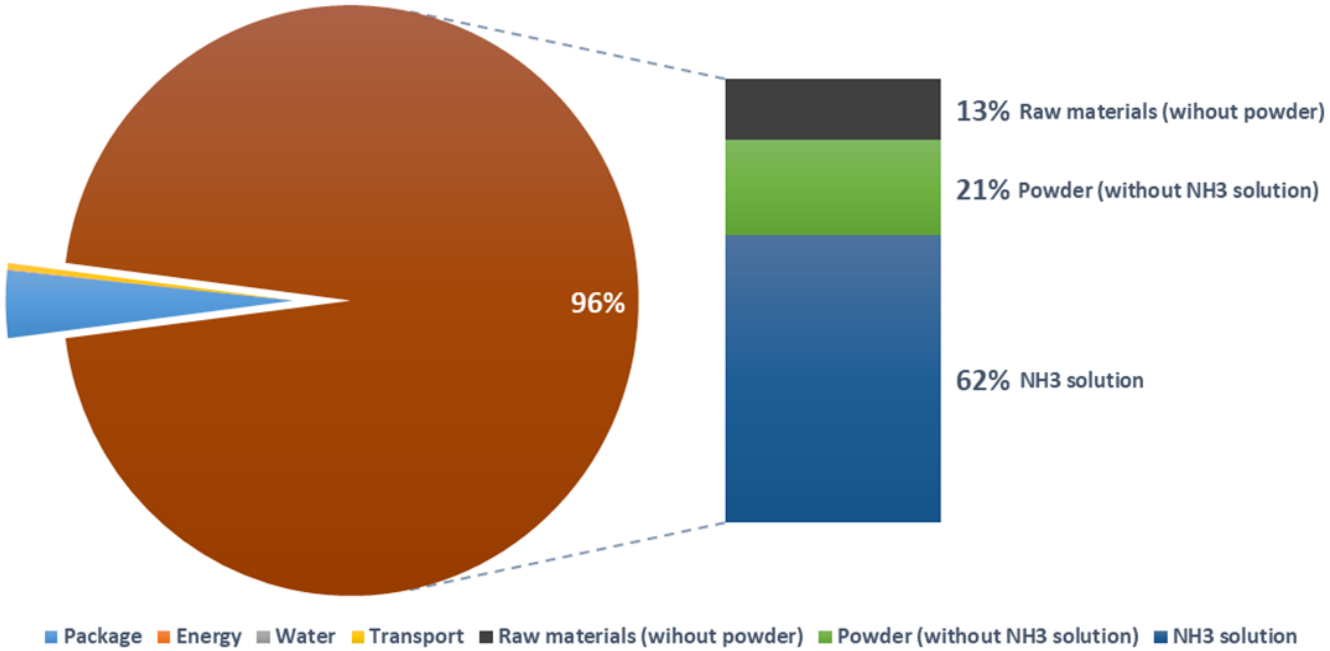
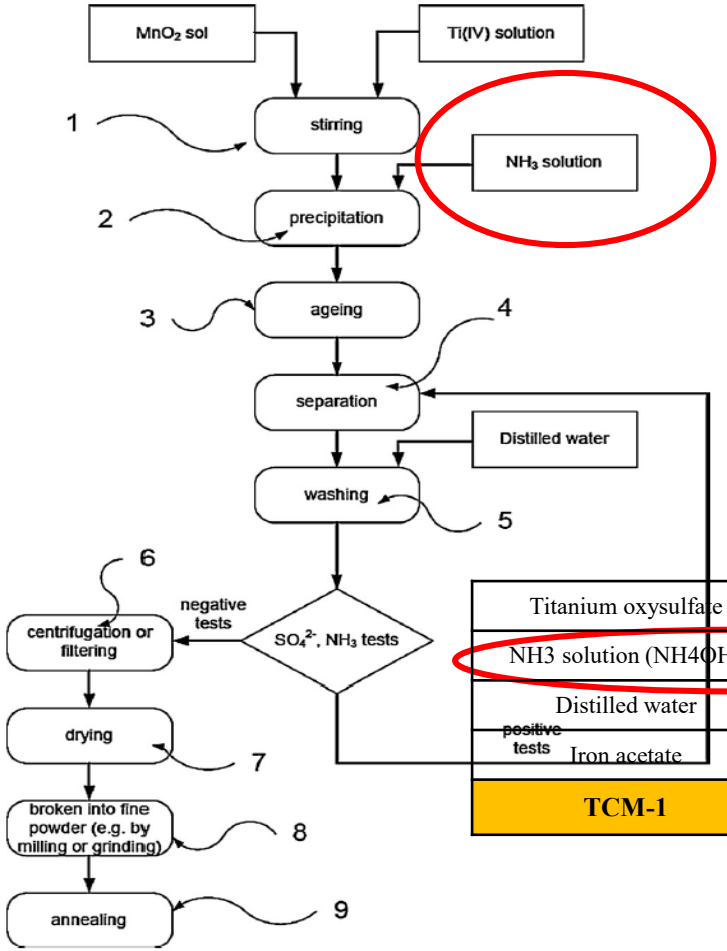
Cradle-to-Gate approach | Production



Process contribution in photocatalytic paint's production life cycle



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Cradle-to-Grave approach | Application

Hellenic Naval Academy case study – Teaching rooms

HNA data

- Comparing two teaching rooms
- First → Painted with the conventional paint
- Second → Painted with the photocatalytic paint

PEDL data

- Energy saving rate was based on simulations, correlating ventilation rate and photocatalysis:
  - 3–4.7% → Average value of 3.85% was used

Literature

- Assumption via a 2014 strategy report of the Greek Ministry of Environment, Energy and Climate Change:
  - Electricity consumption data of different building types and climatic zones

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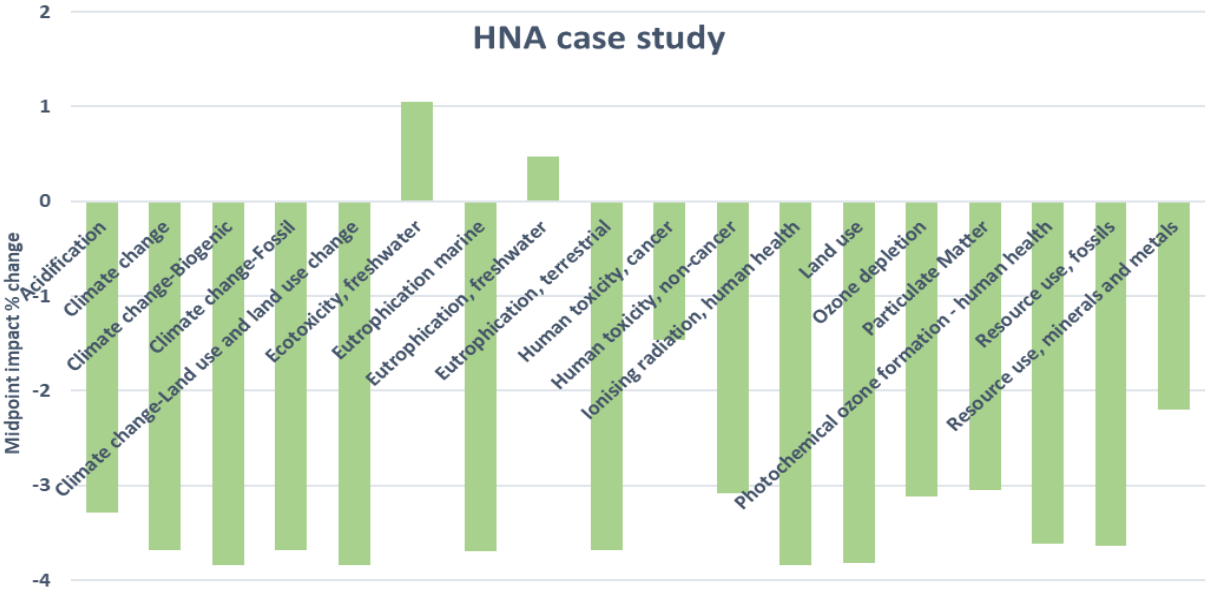
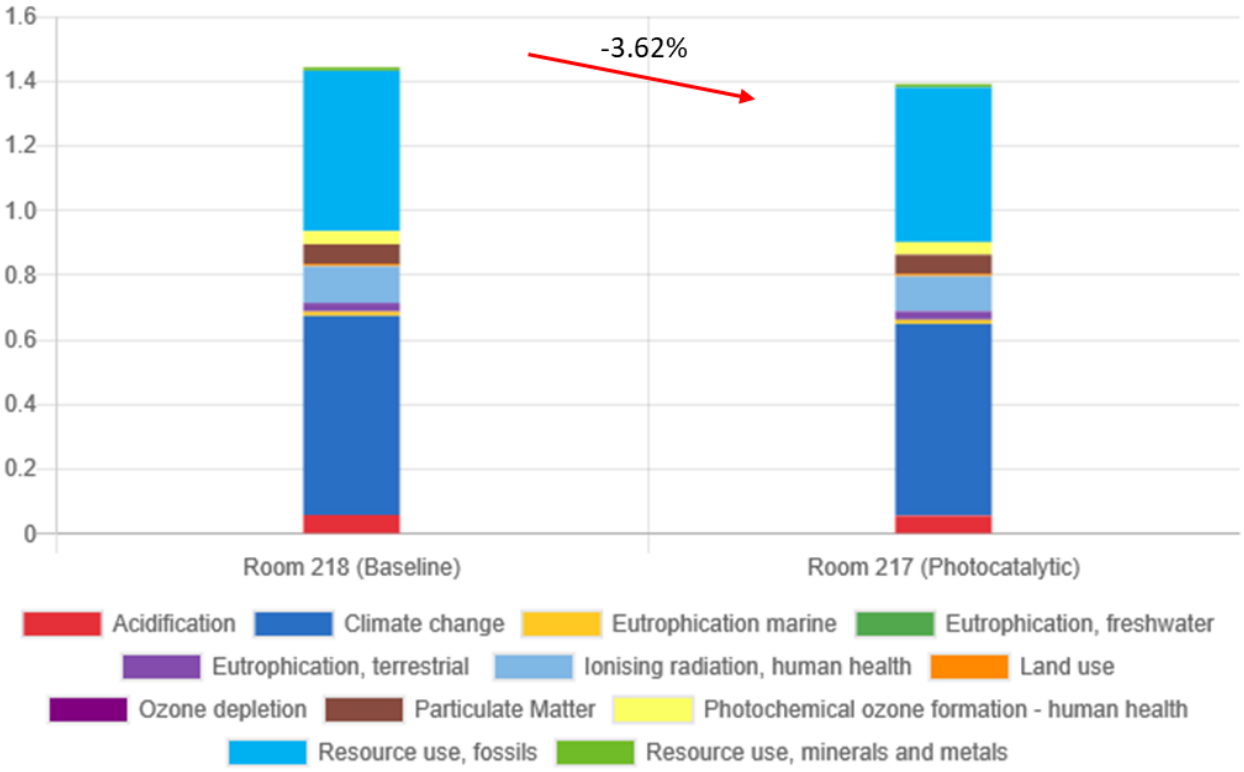
Cradle-to-Grave approach | Application



Midpoint impacts % relative change



Single score analysis

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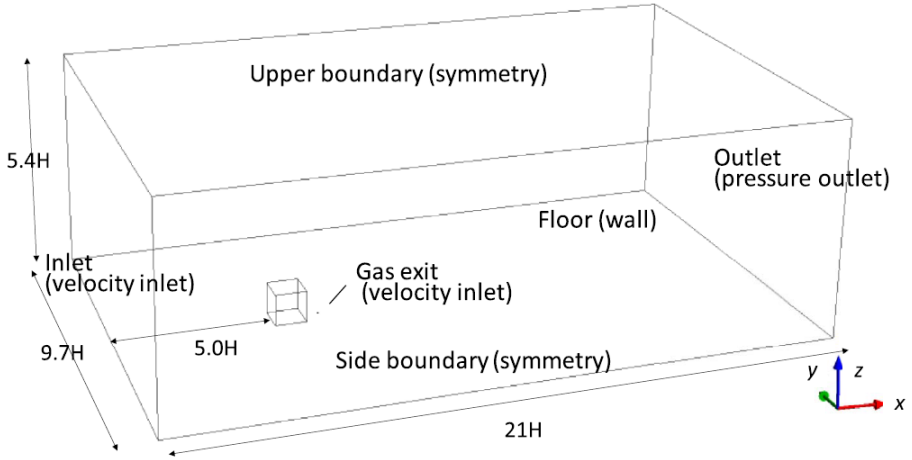
Depollution modelling

- Generally, the CFD methodology includes specific steps.
- In the frame of the Life Visions project the methodology for CFD modelling in indoor environments that will be followed includes 12 steps.
- The steps that will be followed are:
  - ✓Initially the flow and the dispersion problem is formulated.
  - ✓The geometry and the flow domain is modelled.



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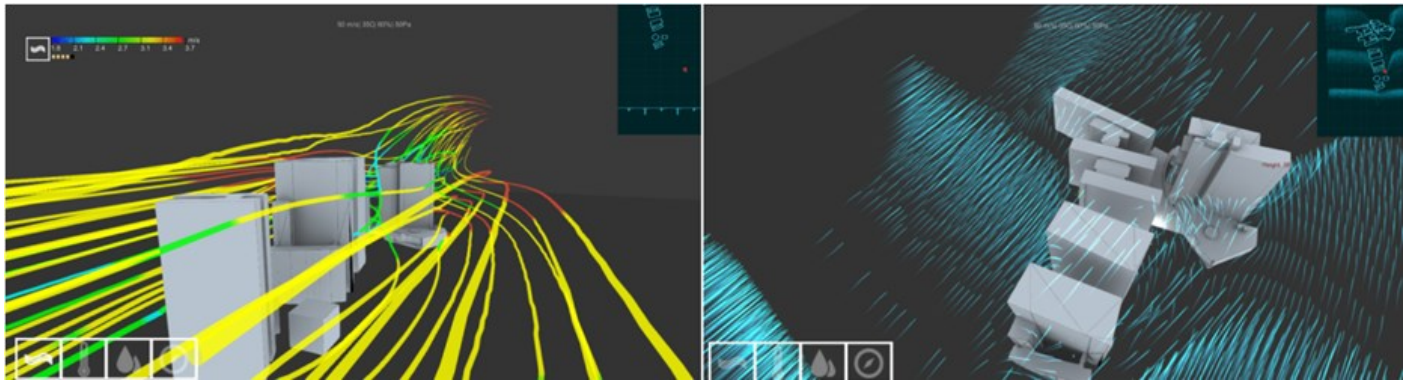
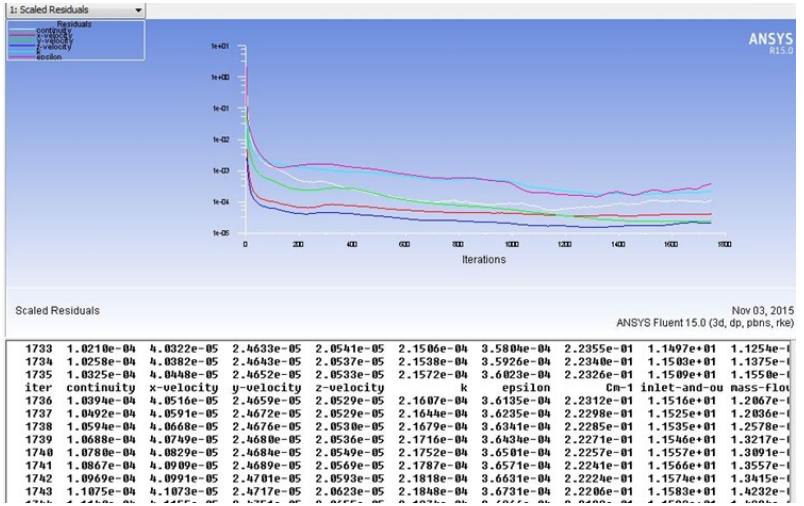
Depollution modelling

- ✓ A series of simulations are performed for scenario assessment purposes
- ✓ Post-processing of the simulation is performed to get the results





iter	continuity	x-velocity	y-velocity	z-velocity	k	epsilon	Cm-1	inlet-and-ou	mass-flo
1733	1.0210e-04	4.0322e-05	2.4633e-05	2.0541e-05	2.1506e-04	3.5804e-04	2.2355e-01	1.1497e+01	1.1254e-
1734	1.0258e-04	4.0382e-05	2.4643e-05	2.0537e-05	2.1538e-04	3.5926e-04	2.2340e-01	1.1503e+01	1.1375e-
1735	1.0325e-04	4.0448e-05	2.4652e-05	2.0533e-05	2.1572e-04	3.6023e-04	2.2326e-01	1.1509e+01	1.1550e-
1736	1.0394e-04	4.0516e-05	2.4659e-05	2.0529e-05	2.1607e-04	3.6135e-04	2.2312e-01	1.1516e+01	1.2067e-
1737	1.0492e-04	4.0591e-05	2.4672e-05	2.0529e-05	2.1644e-04	3.6235e-04	2.2298e-01	1.1525e+01	1.2036e-
1738	1.0594e-04	4.0668e-05	2.4676e-05	2.0530e-05	2.1679e-04	3.6341e-04	2.2285e-01	1.1535e+01	1.2578e-
1739	1.0688e-04	4.0749e-05	2.4680e-05	2.0536e-05	2.1716e-04	3.6434e-04	2.2271e-01	1.1546e+01	1.3217e-
1740	1.0780e-04	4.0829e-05	2.4684e-05	2.0549e-05	2.1752e-04	3.6501e-04	2.2257e-01	1.1557e+01	1.3891e-
1741	1.0867e-04	4.0909e-05	2.4689e-05	2.0569e-05	2.1787e-04	3.6571e-04	2.2241e-01	1.1566e+01	1.3557e-
1742	1.0969e-04	4.0991e-05	2.4701e-05	2.0593e-05	2.1818e-04	3.6631e-04	2.2224e-01	1.1574e+01	1.3415e-
1743	1.1075e-04	4.1073e-05	2.4717e-05	2.0623e-05	2.1848e-04	3.6731e-04	2.2206e-01	1.1583e+01	1.4232e-

- ✓ Comparisons of numerical and experimental results are performed for *V&V* purposes
- ✓ If needed, repetition of the process is performed to examine sensitivities
- ✓ Documentation of the findings is finally performed

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Depollution modelling

- Examine the efficiency of the paint
- Preliminary model simulations for model evaluation were performed initially in two demonstration houses:

  One coated with a baseline paint and one with the photocatalytic paint
- Two radiation scenarios:
  - natural light only
  - both natural and artificial light
- Measurements in both houses were conducted and measurement results were compared to model output

- CFD modelling methodology will be applied in the real-life case study of the Hellenic Naval Academy (HNA)

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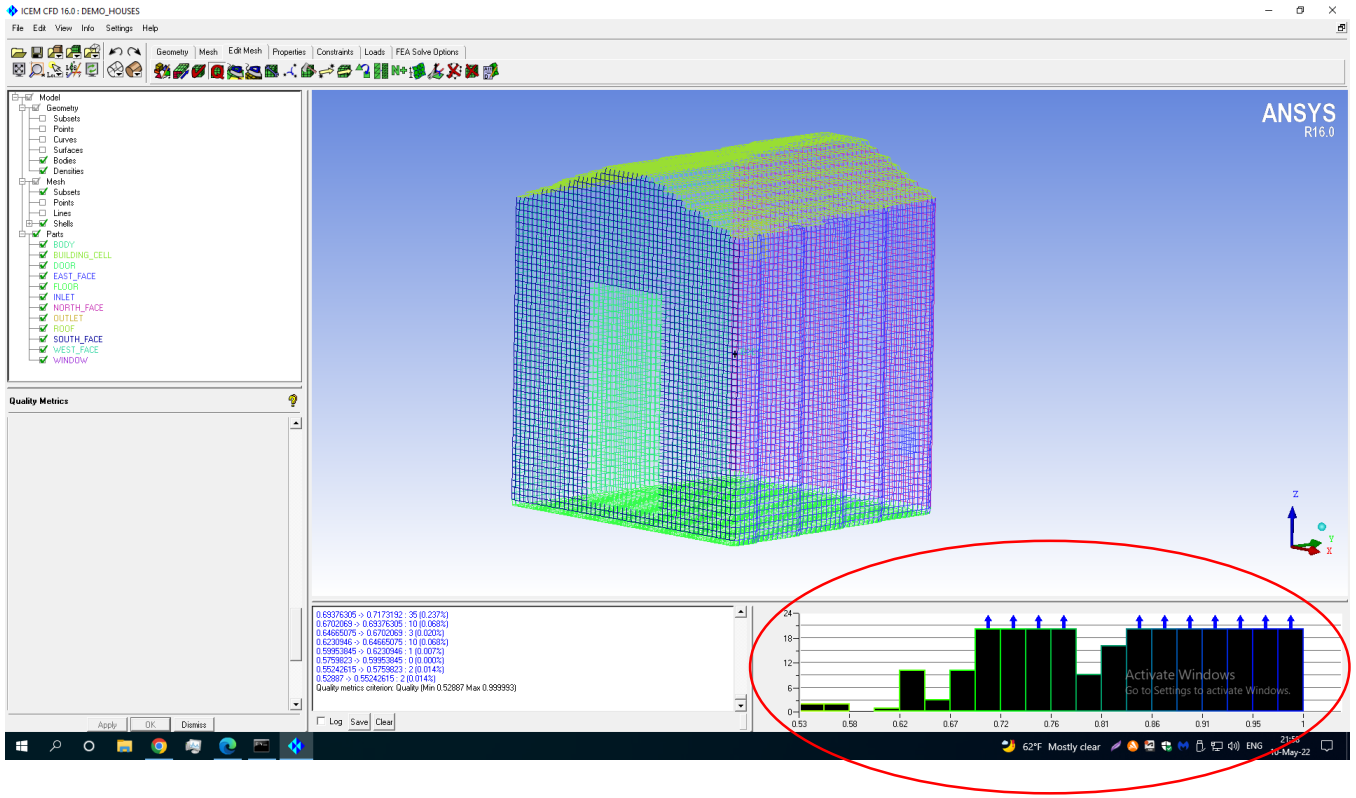
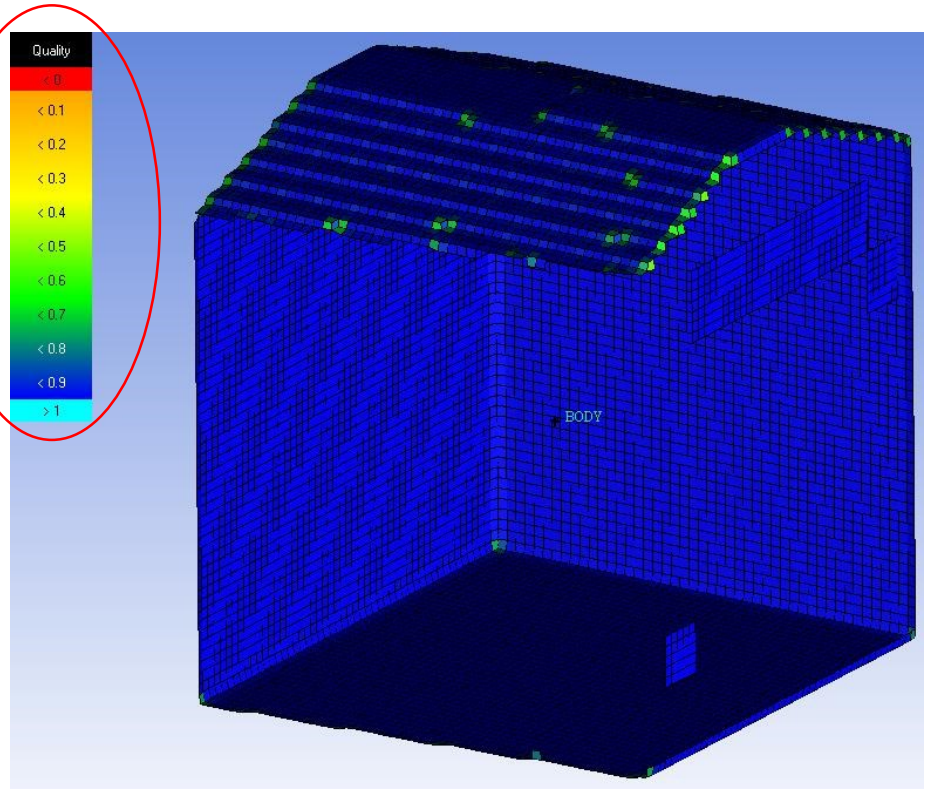
Depollution modelling

2. Quality assurance





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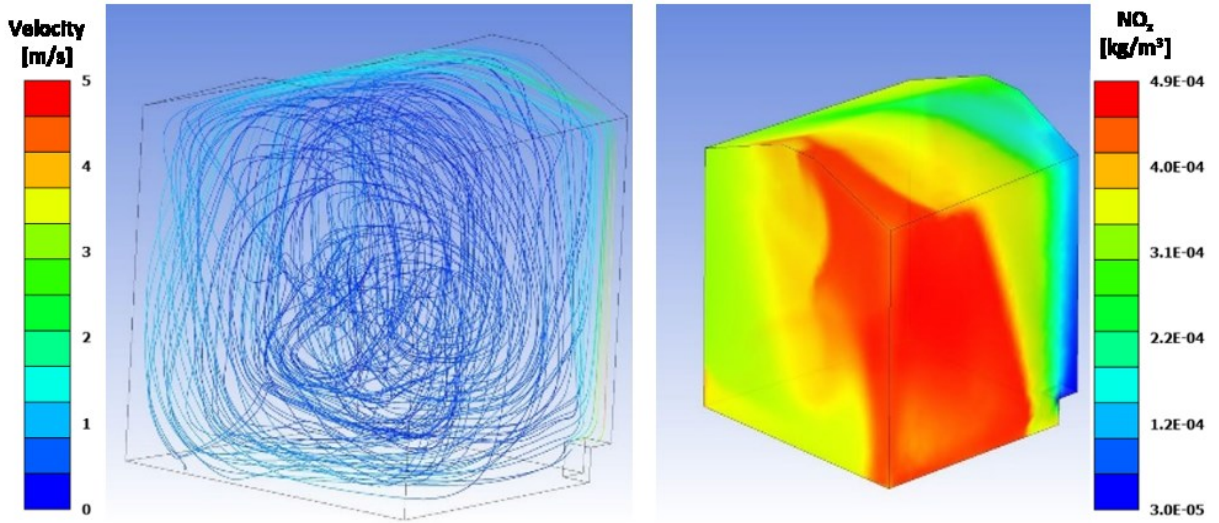
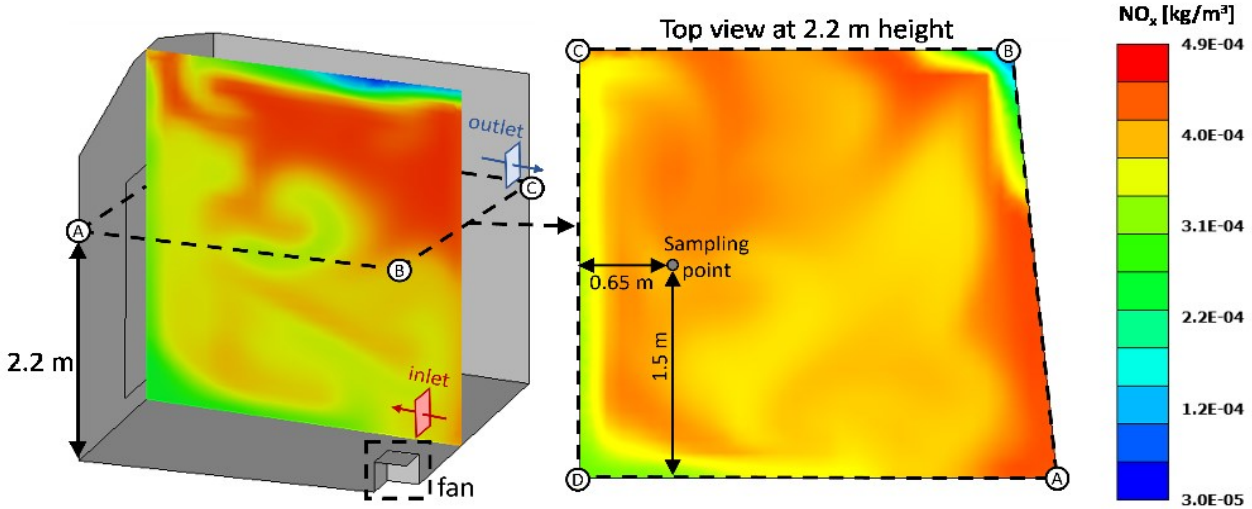
Depollution modelling – Demo house results

Table 1. Measured and numerically estimated NO_x removal for the two radiation scenarios

Pollutant	Radiation scenario	Removal (%)		U_{dep} ($cm\ s^{-1}$)
		Measured	Modelling	
NO_x	Natural light	61.7	70	0.028
	Natural + artificial light	70.1	85	0.034

- Both scenarios indicate a very high removal of NOx
- Good agreement with measurements
- For both scenarios modelling results seem to overestimate removal rates by 10% (natural light) to 15% (natural + artificial light)
- The fan operation is causing a very intense mixing inside the demonstration houses, rapidly accumulating Nox-rich air masses towards the treated walls





Thank you for your attention!

Acknowledgements
- This work has been carried out within the frame of the “LIFE VISIONS” Project, co-funded by the LIFE Programme of the European Union under contract number LIFE19 ENV/GR/000100