

Safe-and-sustainable-by-design framework based on a prospective life cycle assessment: lessons learned from a nano-titanium dioxide case study

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Supplementary Material

The Supplementary Material contains Tables which were omitted from the manuscript:

Table S1 presents descriptions and units for the Effect Factor, Human Effect Factor and Exposure factor of Step 8 of the framework.

Table S2 shows the Life Cycle Inventory of reference system

Table S3 shows the Life Cycle Inventory of additional processes for original system

Table S4 shows the calculation of characterization factors for freshwater ecotoxicity and human toxicity

Table S1. Data needed from nano-toxicity studies

Parameter		Description	Unit
Effect Factor (EF)		Hazardous concentrations of a substance at which 50% of the species are exposed to a concentration above their EC_{50} (i.e. concentration of a nanoparticle that gives half-maximal response).	$kg.m^{-3}$
Human Effect Factor (HEF)		Change in lifetime disease probability due to change in lifetime intake of a pollutant. It is calculated based on ED_{50} values which are extrapolated from animal in vivo tests.	$case.kg_{intake}^{-1}$
Exposure Factor (XF)		Dissolved fraction of NPs in an environmental compartment, e.g. aquatic environment. Occurring transformation processes are important, such as agglomeration.	dimensionless

Table S2. Life Cycle Inventory of reference system

Input			Output		
TiO ₂ -NP production [1]					
Electricity	2.85	kWh	TiO ₂ -NP	1	kg
V–Ti magnetite ore	5.71	kg	GWP	5.53	kg CO ₂
Steel ball	0.001	kg			
Anthracite	10.076	MJ			
Coke	0.693	kg			
Liquid chlorine	0.25	kg			
Aluminum powder	0.06	kg			
Oxygen	0.693	kg			
Liquid caustic soda (30 %)	0.3	kg			
Saturated steam (1.3 MPa)	5.5	kg			
Petrol	0.017	kg			
Diesel	0.011	kg			
Hydrogen production					
TiO ₂ -NP	2.4	mg	H ₂	63.012	μmol
Light (from lamp)	500	W	H ₂	0.00012	g
Water	21.6	ml	Waste methanol (O ₂ bound)	23.9998	g
Methanol	2.4	ml			
Catalyst	1	unit	Factor for 1 g H ₂	7872.4	

Table S3. Life Cycle Inventory of additional processes for original system

Input			Output		
Copper acetate [2]					
Copper(II) carbonate	247.1098	kg	Cu(CH ₃ COO) ₂	363.26	kg
Acetic acid	180.156	kg			
Sodium hydroxide	147.2	kg			
Copper(II) hexafluoroacetylacetonate hydrate (C ₁₀ H ₄ CuF ₁₂ O ₅) [2]					
Cu(CH ₃ COO) ₂	181.63	kg	C ₁₀ H ₄ CuF ₁₂ O ₅	569.84	kg
Hexafluoroacetylacetone dihydrate	388.21	kg			
Nanocoating with ALD					
TiO ₂ -NP	1.5	g	TiO ₂ coated with CuO	1.554484	g
C ₁₀ H ₄ CuF ₁₂ O ₅	0.3395	g	CO ₂	0.105096	g
Dionized water	5	L			
Pressurized nitrogen liquid	544.6952	g			
Cooling water		L			
Electricity for heating tapes	945	Wh			
Hydrogen production					
TiO ₂ coated with CuO	2.484	mg	H ₂	319.3335	μmol
Light (from lamp)	500	Wh	Waste methanol (O ₂ bound)	23.99936	g
Water	21.6	ml			
Methanol	2.4	ml			

Table S4. Calculation of characterization factors for freshwater ecotoxicity and human toxicity

Freshwater ecotoxicity	P25	CuO	Human toxicity	P25	CuO
EF	26.9	7.025	EF	2.70	0.045
FF	128	2520	FF	130	22
XF	1	1	XF	1	1

References

1. Liao, W.; Heijungs, R.; Huppes, G. Thermodynamic Resource Indicators in LCA: A Case Study on the Titania Produced in Panzhihua City, Southwest China. *Int J Life Cycle Assess* **2012**, *17*, 951–961, doi:10.1007/s11367-012-0429-4.
2. Zhang, T.; Gu, H.; Ding, F.; Qu, F.; Dai, S. Synthesis, Characterization, and Thermostability of Bis(2,2,6,6-Tetramethyl-3, 5-Heptanedionato)Copper(II). *Rare Metals* **2012**, *31*, 343–349, doi:10.1007/s12598-012-0518-3.