SUNDS

-

Nano TiO_2 Coating

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Version log *[Add lines if needed]*			
Version	**Date**	**Author**	**Change**
1.0	01.10.2019	AZ, DH, PI	First draft
1.0	02.10.2019	AZ, DH, PI	Final version
Keywords			
Decision Support System, Human Health Risk Assessment, Environmental Risk Assessment, Life Cycle Impact Assessment, Economic Assessment, Social Assessment, Risk Management			

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 686239

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1 Tool description and use domain(s)

The SUNDS Decision Support System (DSS) is a nano-specific Decision Support Tool that enables its users to assess human and environmental risks and make risk management decisions based on input of technical data and expert judgement. In addition, it performs Socioeconomic Analysis (as required in the REACH authorization process) and allows the comparison of the risks of specific products to their possible economic and social impacts and benefits by means of a Multi Attribute Value Theory methodology.

It integrates models and tools for Risk Control and Sustainability Assessment, which are clustered in five modules as seen in Figure 1:

- Ecological/Environmental Risk Assessment
- Human Health (Public / Occupational / Consumer) Risk Assessment
- Life Cycle Impact Assessment
- Economic Assessment
- Social Impact Assessment

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Figure 1: SUNDS conceptual framework

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2 Description of case study

A single project folder representing the aim of the assessed product has been created in SUNDS under the name “Self-cleaning outside surface coating”. The project contains a single assessment scenario related to the specific nano particle used in implementing the selected product. The scenario is named “Nano TiO_2 Coating”.

In order to define the boundaries of the complete lifetime assessment SUNDS uses a meta-data structure named “Assessment tree”. The path starting from the root towards each leaf in the Assessment tree is named a “Lowest Unit of Assessment” (LUA) and represents something similar to an exposure route but with a larger interpretation. A LUA path contains information about the risk type, whether human or environmental, the Life Cycle stage, and more, which are not part of a standard exposure route definition.

For the presented case study, a representative subset of the complete decision tree has been selected basing on the information available in the different risk compartments. The final version of the decision tree both for human health and environmental assessment are reported below in Figure 2 and Figure 3.

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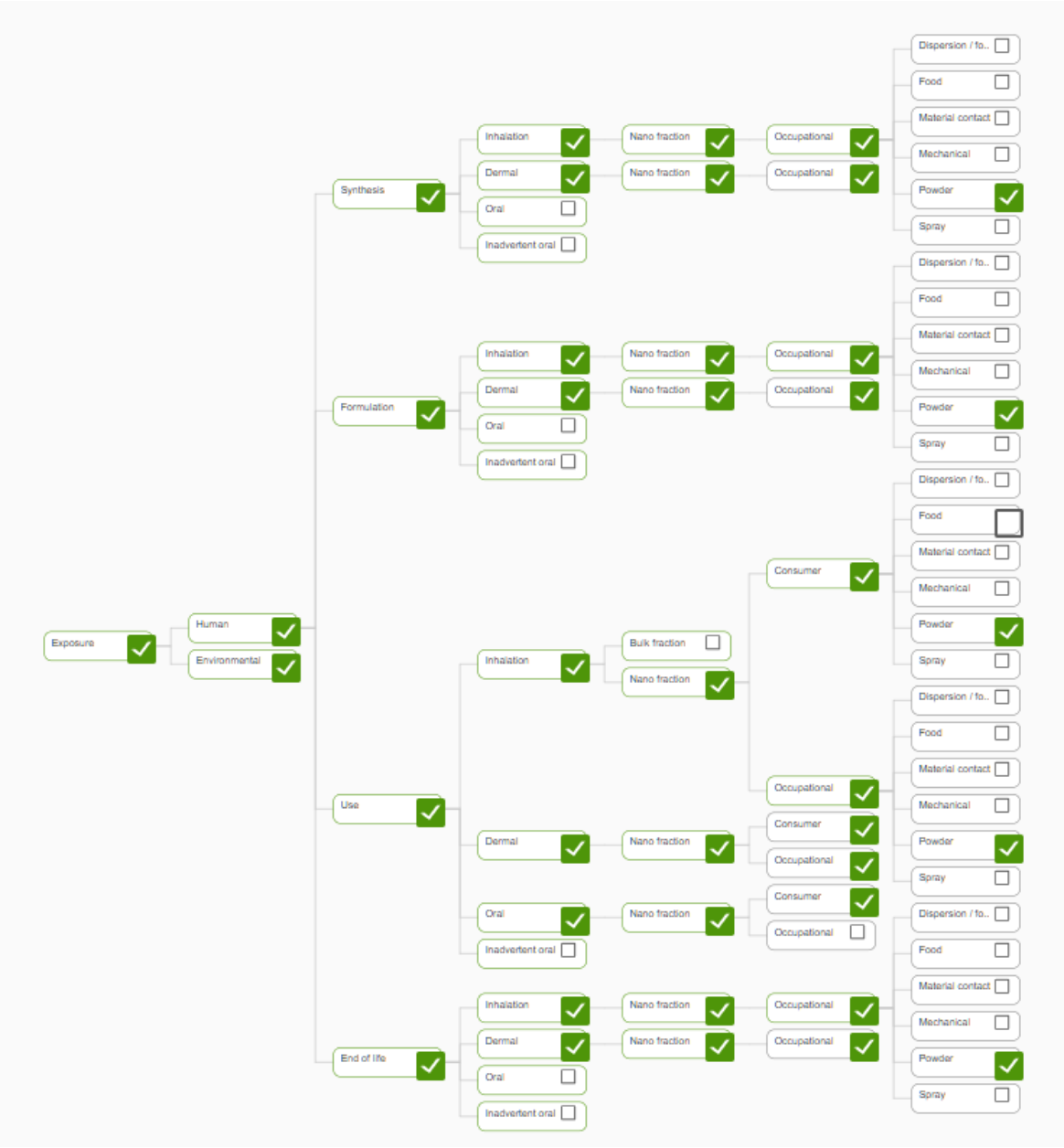

Figure 2: Assessment tree selections for Human Health Risk Assessment

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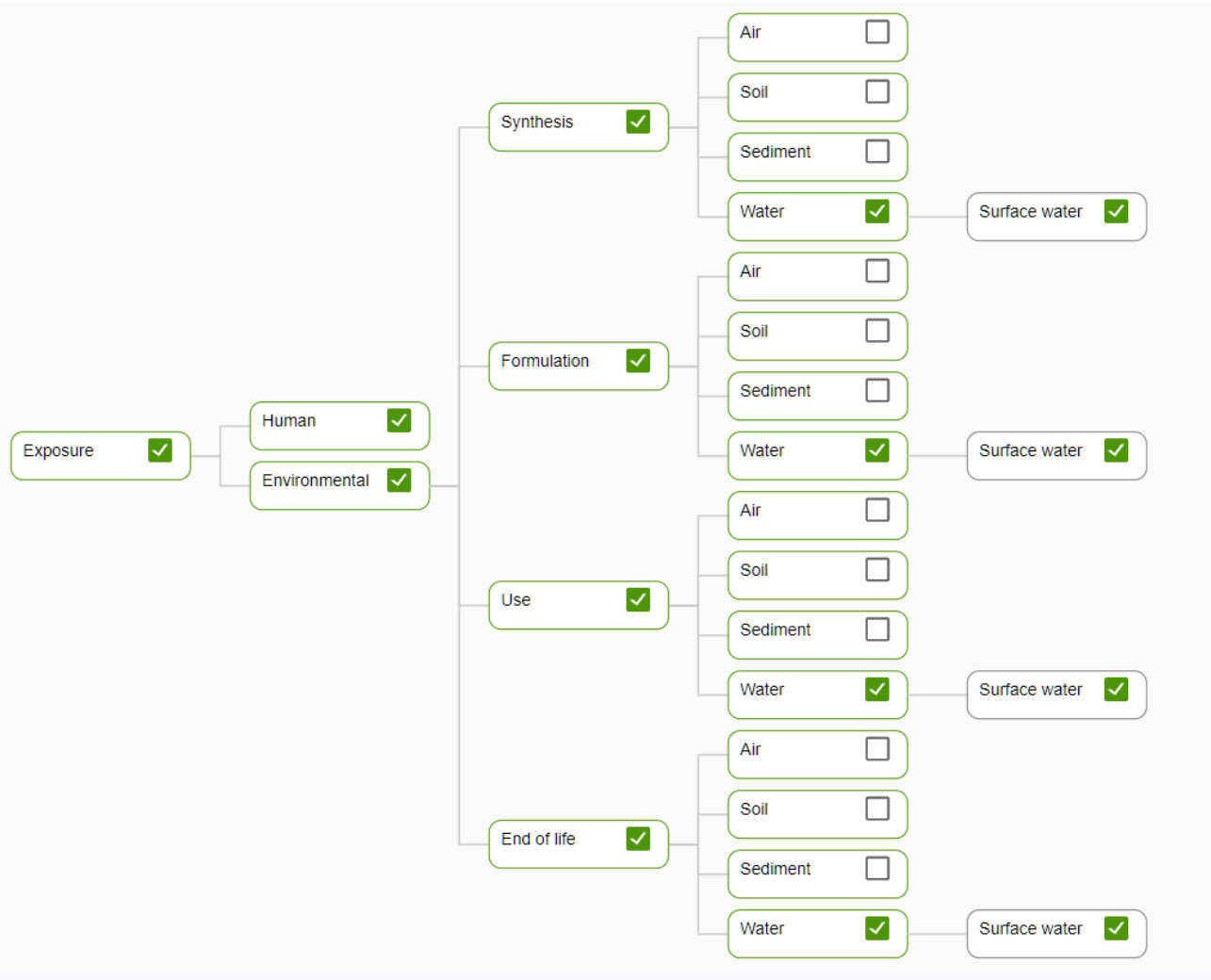

Figure 3: Assessment tree selections for Environmental Risk Assessment

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3 Input parameters

3.1 Environmental risk assessment

The utilized ERA inputs (exposure and effect) for the case study have been obtained by the application of embedded models within SUNDS, such as the PMFA and nSSWD models. They are presented in Table 1 and Table 2 below.

Table 1: ERA exposure input for the nano TiO_2 coating case study

Life cycle stage	Compartment		PNEC Type	Value (LCL) μg/L	Value (UCL) μg/L
Synthesis	Water	Surface water	Deterministic	0	
Formulation	Water	Surface water	Probabilistic	5.28E-04	4.28E-03
Use	Water	Surface water	Probabilistic	1.35E-04	1.23E-03
End of life	Water	Surface water	Probabilistic	2.10E-05	1.76E-04

Table 2: ERA effect input for the nano TiO_2 coating case study

Life cycle stage	Compartment		PNEC Type	Value (LCL) μg/L	Value (UCL) μg/L
Synthesis	Water	Surface water	Deterministic	0.34	
Formulation	Water	Surface water	Deterministic	0.34	
Use	Water	Surface water	Deterministic	0.34	
End of life	Water	Surface water	Deterministic	0.34	

3.2 Human Health risk assessment

The utilized HHRA inputs (exposure and effect) for the case study have been obtained by the application of embedded models within SUNDS, such as the Nanosafer, ConsExpo and dART models. They are presented in Table 3 and Table 4 below.

Table 3: HHRA exposure input for the nano TiO_2 coating case study

Life cycle stage	Compartment	Consumer / Occupational	PNEC Type	Value (LCL) μg/L	Value (UCL) μg/L
Synthesis	Inahalation	Occupational Powder	Negligible exposure	-	
Synthesis	Dermal	Occupational	Negligible exposure	-	
Formulation	Inahalation	Occupational Powder	Negligible exposure	-	
Formulation	Dermal	Occupational	Negligible exposure	-	
Use	Inahalation	Consumer Powder	Negligible exposure	-	
Use	Inahalation	Occupational	Negligible exposure	-	

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		Powder			
Use	Dermal	Consumer	Negligible exposure	-	
Use	Dermal	Occupational	Negligible exposure	-	
Use	Oral	Consumer	Deterministic	0.111	
End of life	Inahalation	Occupational Powder	Negligible exposure	-	
End of life	Dermal	Occupational	Negligible exposure	-	

Table 4: HHRA effect input for the nano TiO_2 coating case study

Life cycle stage	Compartment	Consumer / Occupational	DNEL Type	Value (LCL) mg/kg	Value (UCL) µg/L
Synthesis	Inahalation	Occupational Powder	Deterministic	0	
Synthesis	Dermal	Occupational	Deterministic	0	
Formulation	Inahalation	Occupational Powder	Deterministic	0	
Formulation	Dermal	Occupational	Deterministic	0	
Use	Inahalation	Consumer Powder	Deterministic	0	
Use	Inahalation	Occupational Powder	Deterministic	0	
Use	Dermal	Consumer	Deterministic	0	
Use	Dermal	Occupational	Deterministic	0	
Use	Oral	Consumer	Probabilistic	4.09E-02	2.35E+01
End of life	Inahalation	Occupational Powder	Deterministic	0	
End of life	Dermal	Occupational	Deterministic	0	

3.3 Life Cycle Impact Assessment

The LCIA results assessment is performed in SUNDS by comparison with a benchmark study and classification based on relative distance. For the presented case study application values were derived from previous SUNDS case studies performed during the SUN project and adapted for the specific situation under assessment.

The utilized LCIA results both for the case study and the benchmark situation have been obtained by the application of the Recipe Endpoint Hierarchical method. They've both been exported from the Simapro LCA software and are presented in Table 5 and Table 6 below.

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Table 5: LCIA results used as input for the nano TiO_2 coating case study

Calculation:	Analyse									
Results:	Impact assessment									
Product:	nano TO2 coating									
Current library:	Ecoinvent 3 - allocation, default - unit [U]									
Replacing library:	Ecoinvent 3 - allocation, default - system [S]									
Method:	ReCiPe Endpoint (H) V1.11 / Europe ReCiPe H/A									
Indicator:	Single score									
Skip categories:	Never									
Default units:	No									
Exclude infrastructure processes:	Yes									
Exclude long-term emissions:	No									
Per impact category:	No									
Sorted on item:	Damage category									
Sort order:	Ascending									
Damage category	Unit	Total	LC_CuCO3_	1a Product	1b Product	2 Manufac	3a Use of	3b Use of	4a End of l	4b End of l
Total	mPt	6.690756	0	6.079534	0	0.36658	0.029437	0	0.211714	0.003491
Human Health	mPt	3.313318	0	3.124656	0	0.174128	0.001962	0	0.011231	0.001341
Ecosystems	mPt	0.539344	0	0.269033	0	0.03892	0.027475	0	0.203163	0.000753
Resources	mPt	2.838094	0	2.685845	0	0.153532	0	0	-0.00268	0.001397

Table 6: LCIA results used as input for the non-nano TiO_2 coating benchmark study

Calculation:	Analyse									
Results:	Impact assessment									
Product:	non-nano TO2 coating									
Current library:	Ecoinvent 3 - allocation, default - unit [U]									
Replacing library:	Ecoinvent 3 - allocation, default - system [S]									
Method:	ReCiPe Endpoint (H) V1.11 / Europe ReCiPe H/A									
Indicator:	Single score									
Skip categories:	Never									
Default units:	No									
Exclude infrastructure processes:	Yes									
Exclude long-term emissions:	No									
Per impact category:	No									
Sorted on item:	Damage category									
Sort order:	Ascending									
Damage category	Unit	Total	LC_ACQ_\	1a Product	1b Product	2 Manufac	3a Use of	3b Use of	4a End of l	4b End of l
Total	mPt	6.750143	0	5.879461	0	0.323076	0.306474	0	0.237641	0.003491
Human Health	mPt	3.219668	0	2.906538	0	0.159434	0.006951	0	0.145404	0.001341
Ecosystems	mPt	0.82265	0	0.321362	0	0.029501	0.299523	0	0.171511	0.000753
Resources	mPt	2.707825	0	2.651561	0	0.134141	0	0	-0.07927	0.001397

3.4 Economic Assessment

The Economic assessment is performed in SUNDS by comparison with a benchmark study and classification based on relative distance. For the presented case study application values where derived from previous SUNDS case studies performed during the SUN project and adapted for the specific situation under assessment.

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The utilized inputs both for the case study and the benchmark situation have been obtained by the application of the Economic Assessment methodology developed during the SUNDS project as reported in (Subramanian et al. 2016).

The utilised input values are reported below both for the case study and benchmark in Table 7 and Table 8.

Table 7: Economic Assessment input for the nano TiO_2 coating case study

Synthesis		
Nanomaterial specific material Costs per year per functional unit	€	-
Non-Nanomaterial material costs per year for functional unit	€	-
Maintenance and purchasing cost of plant, machinery and equipment per year per functional unit	€	0.06
Worker training costs per year	€	-
Labor costs per year per functional unit	€	-
Production		
Nanomaterial specific material Costs per year per functional unit	€	0.14
Non-Nanomaterial material costs per year for functional unit	€	38.19
Maintenance and purchasing cost of plant, machinery and equipment per year per functional unit	€	19.13
Worker training costs per year	€	-
Labor costs per year per functional unit	€	-
Use		
Maintenance Cost per year per functional unit	€	2.12
Operating Costs per year per functional unit	€	-
Market margin for sold item	€	-
End of life		
Disposal and recycling costs per year per functional unit	€	0.01

Table 8: Economic Assessment input for the non-nano TiO_2 coating benchmark study

Production		
Nanomaterial specific material Costs per year per functional unit	€	-
Non-Nanomaterial material costs per year for functional unit	€	38.25
Maintenance and purchasing cost of plant, machinery and equipment per year per functional unit	€	19.13
Worker training costs per year	€	-
Labor costs per year per functional unit	€	-
Use		
Maintenance Cost per year per functional unit	€	2.13
Operating Costs per year per functional unit	€	-
End of life		
Disposal and recycling costs per year per functional unit	€	0.01

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3.5 Social Impact Assessment

The Social Impact assessment is performed in SUNDS by the application of the specific methodology developed during the SUN project and reported in (Subramanian et al. 2017). For the presented case study application values where derived from previous SUNDS case studies performed during the SUN project and adapted for the specific situation under assessment.

The utilised input values are reported below in Table 9.

Table 9: Social Impact Assessment input for the nano TiO_2 coating case study

Preliminary	Value	Total	Weight
number of type SME companies	3700000		
number of type LI companies	10000		
Employment SME	16500625		
Employment LI	9900375		
Value added SME	7.3847E+11		
Value added LI	6.4703E+11		
Community weight	2		
Worker weight	4		
Benefit	**Value**	**Total**	**Weight**
Number of employees covered by collective agreements	33848	25600980	1
Number of employees who are trade union members	33697	6330000	1
Number of female employees who are part of senior management	6847	13923340	1
Number of employees with tertiary education	45070	1310100	1
Contribution to Social Benefits and Pension (in million Euros)	7380	1157041200	1
Employment (total number)	35848	44914000	1
Professional Training (days)	2.6	1.2	1
Number of handicapped employees	0	0	0
Number of patent applications	0	0	0
Number of employees in research and development	0	0	0
Cost	**Value**	**Total**	**Weight**
Number of non-fatal accidents	0	709940	1
Days not worked due to strikes and lockout	0	10	1
Number of employees who are paid below minimum wage (for developing countries)	0	0	1
Number of child employees	0	0	1
R&D expenditure (in million Euros)	1884	3139	1

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4 Results

The results of the evaluation of the selected case study scenario in SUNDS are presented below for each of the available assessment modules.

4.1 Environmental risk assessment

Comparison results to evaluate ERA case study performance are reported below in Figure 4, Figure 5 and Figure 6 as displayed in the SUNDS tool. These are examples of the exposure distribution and the Risk Assessment for the Formulation LC stage. Similarly, the software produces charts for all the LC stages for Exposure, Effect and Environmental Risk Assessment.

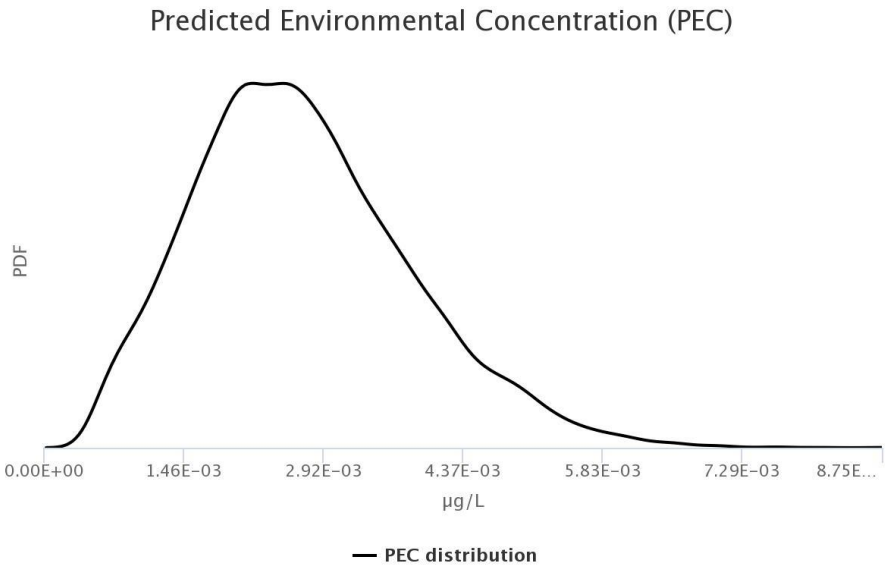

Figure 4: SUNDS ERA exposure (Formulation)

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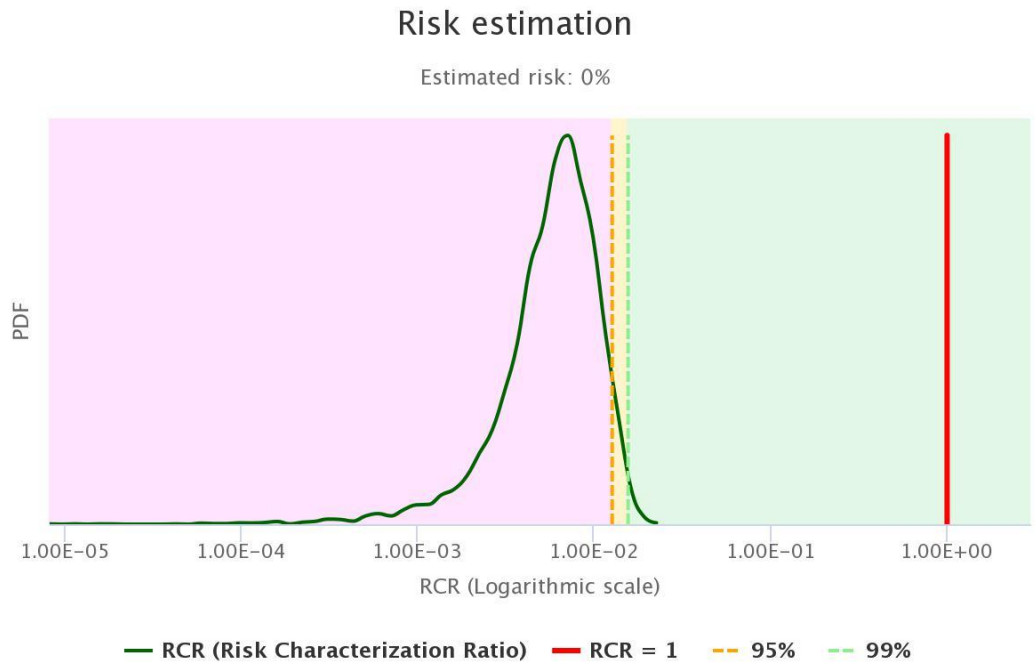

Figure 5: SUNDS ERA results (Formulation)

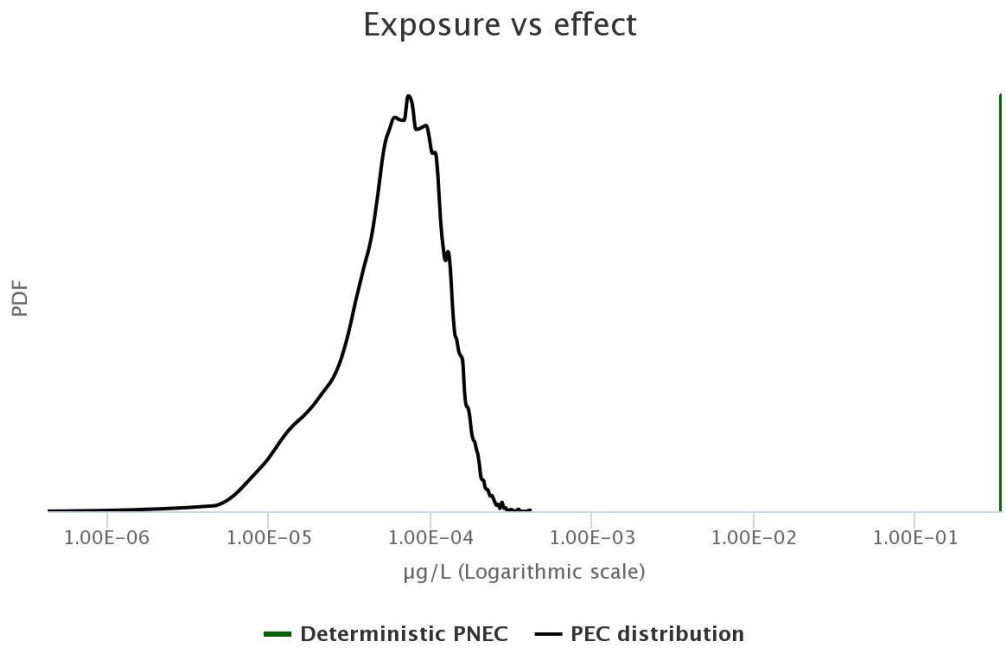

Figure 6: SUNDS ERA results comparison (Formulation)

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4.2 Human Health risk assessment

Comparison results to evaluate HHRA case study performance are reported below in Figure 7 and Figure 8 as displayed in the SUNDS tool. These are examples of the effect distribution and the Risk Assessment for the Oral LC stage. Similarly, the software produces charts for all the LC stages for Exposure, Effect and Human Health Risk Assessment.

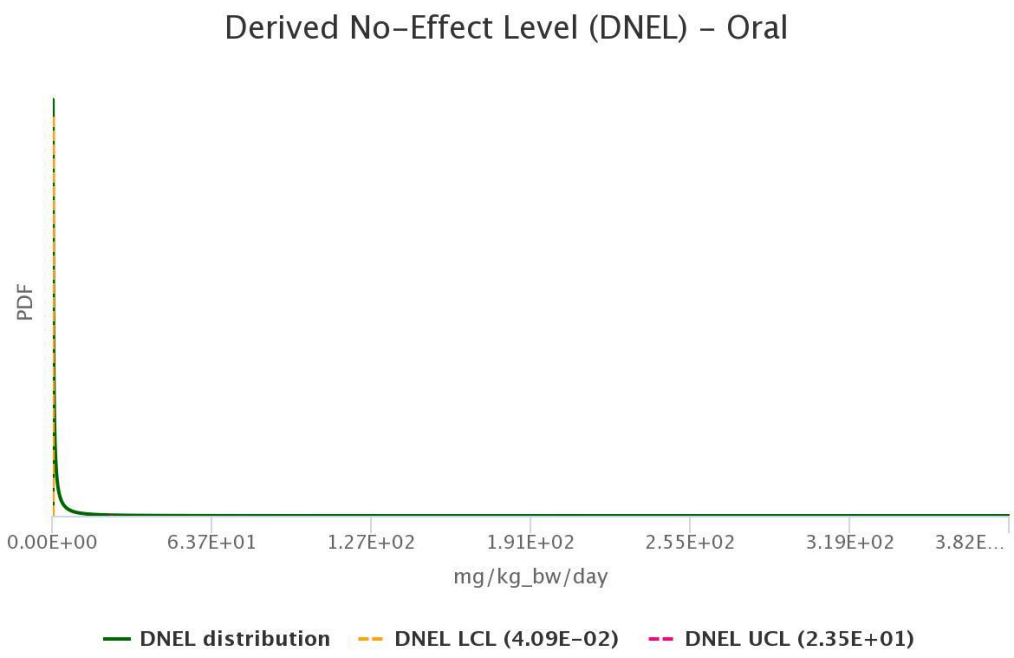

Figure 7: SUNDS HHRA effect (Oral)

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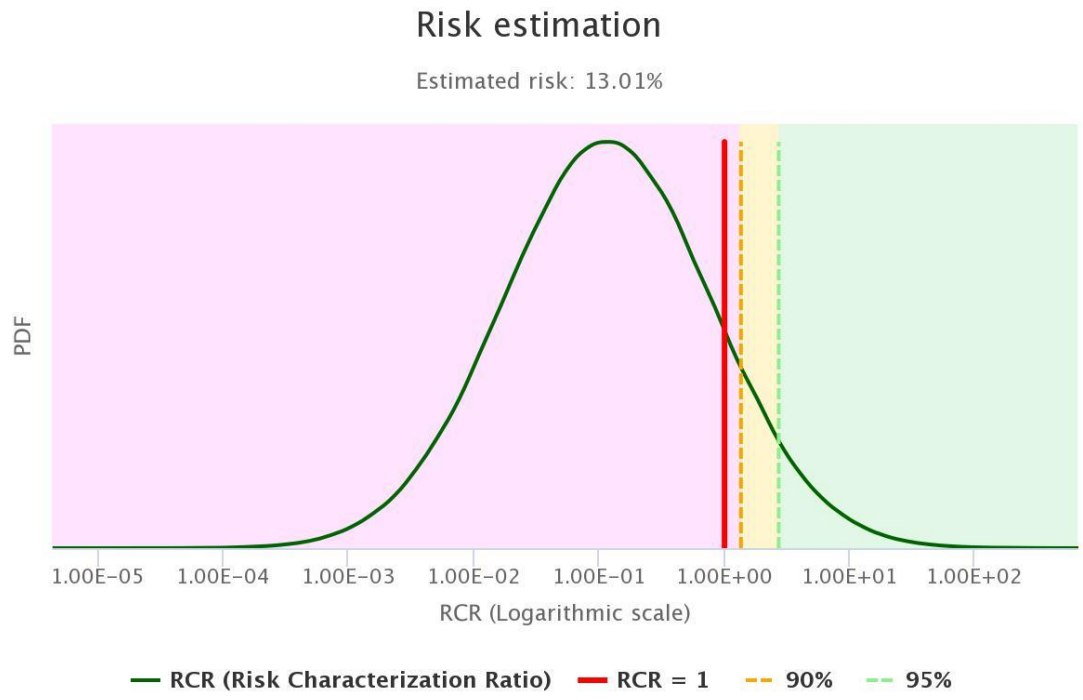

Figure 8: SUNDS HHRA results (Oral)

4.3 Risk Control

Apart from the individual results, the tool has overall comparison capabilities and provides fast and efficient communication of the Risk Assessment (ERA and HHRA) results to the user, as seen in Figure 9, Figure 10 and Figure 11. In the presented case study, the risk is considered at an "Unacceptable" level for one element of the HHRA, specifically at the Use LC stage and the oral compartment.

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Figure 9: SUNDS Risk control global results

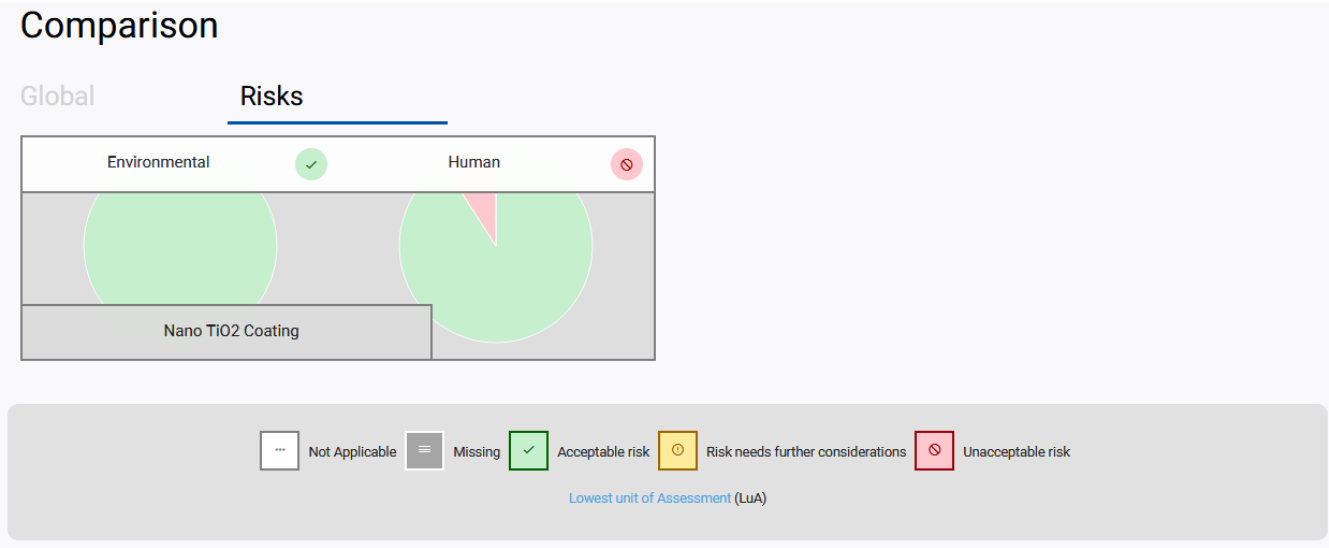

Figure 10: SUNDS Risk control overview results

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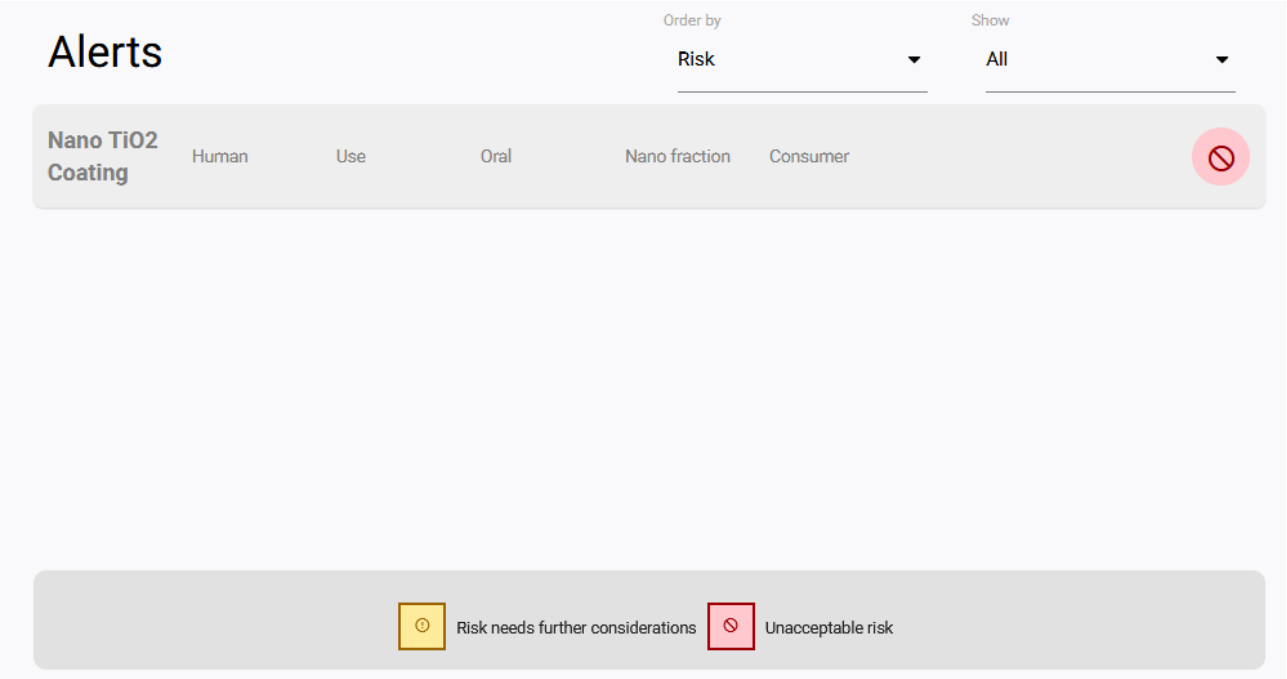

Figure 11: SUNDS Risk control alert results

4.4 Life Cycle Impact Assessment

Comparison results to evaluate LCIA case study performance are reported below in Figure 12 as displayed in the SUNDS tool. Results demonstrates the two case studies are very close in global impacts, nevertheless the nano TiO_2 scenario performs slightly better (i.e. has lower impacts). By examining the right side of the results in Figure 12 it's easy to understand that the main reason for the reduced impacts is related to the almost absent impacts in the TiO_2 use phase which falls into the green Low Impact (LI) category as opposed to all other phases where a yellow Medium impact (MI) category is reached.

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Figure 12: SUNDS LCIA comparison results

4.5 Economic Assessment

Comparison results to evaluate Economic Assessment case study performance are reported below in Figure 13 as displayed in the SUNDS tool. Results demonstrates the two case studies are basically identical both in global and single stage comparison. By examining the right side of the results in Figure 13 it results clearly that only nano TiO_2 production comprehends a Synthesis phase, nevertheless as all other phases fall in the yellow Medium impact (MI) category also the global result does.

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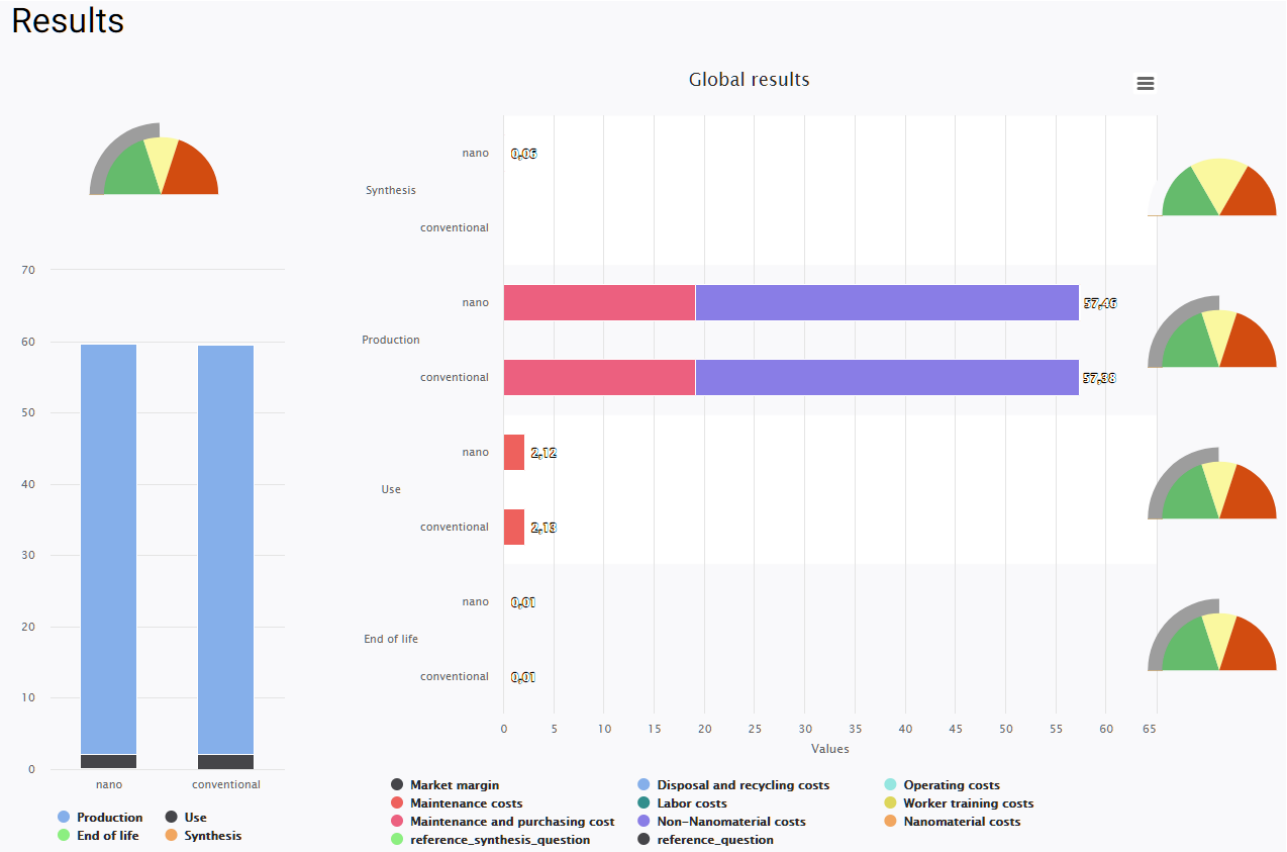

Figure 13: SUNDS Economic Assessment comparison results

4.6 Social Impact Assessment

Results to evaluate Social Impact Assessment of nano TiO_2 case study performance are reported below in Figure 14 as displayed in the SUNDS tool. Results demonstrates the nano TiO_2 case study presents a High Benefit (HB) global classification. The final classification is obtained by a cost benefit ratio, where as it clearly depicted in Figure 14 benefits highly overcome costs.

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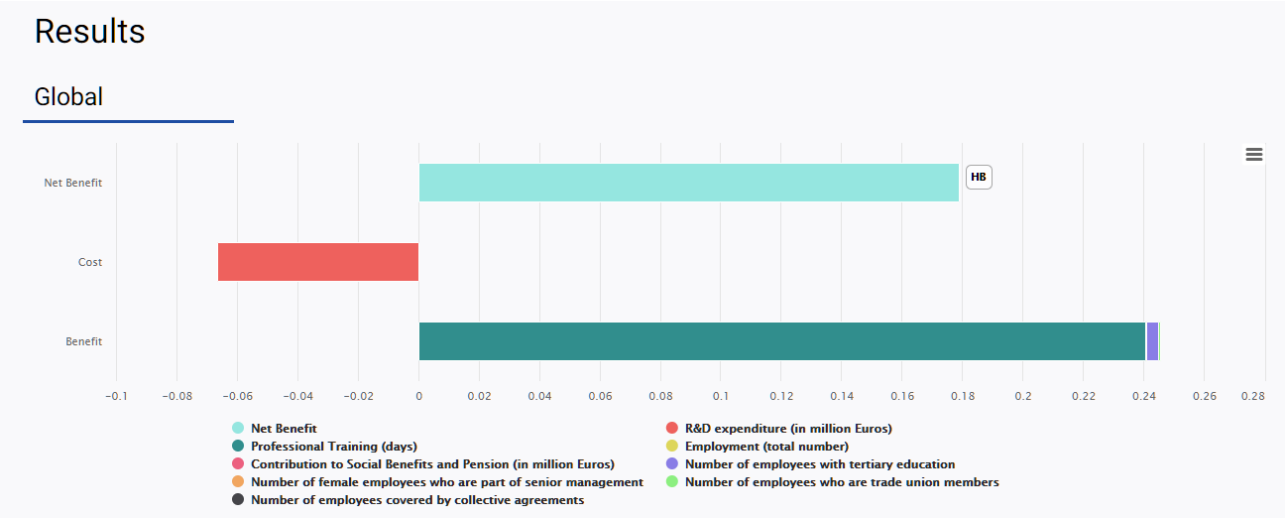

Figure 14: SUNDS Social Assessment results

4.7 Socio Economic Assessment

The final stage of SUNDS assessment involves the integration of all the previously assessed Lines of Evidence (LoE): Human Health Risk Assessment, Environmental Risk Assessment, Life Cycle Impact Assessment, Economic Assessment and Social Impact Assessment.

Each LoE is evaluated into a single performance class and all the classes are displayed together in an assessment matrix both at global level and by life cycle stage as reported in Figure 15 and Figure 16.

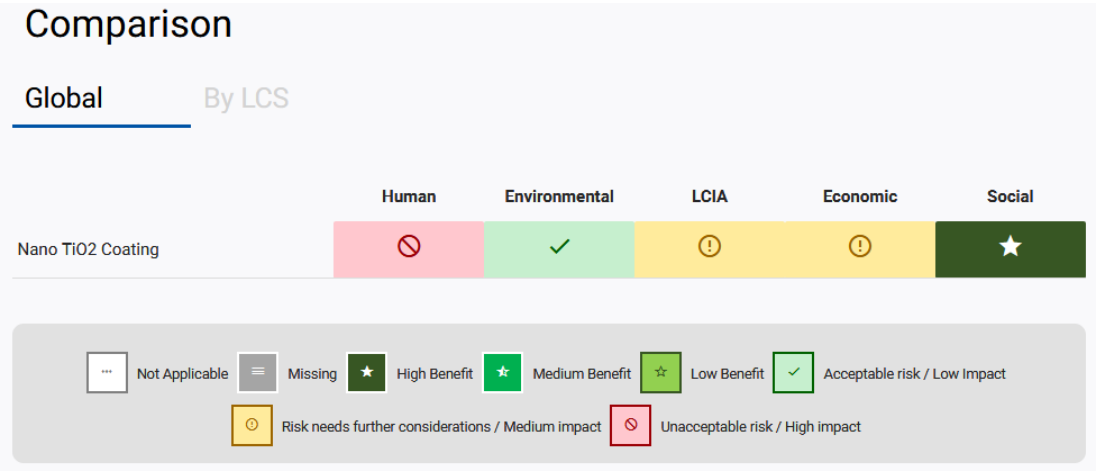

Figure 15: SUNDS Socio Economic Assessment global results

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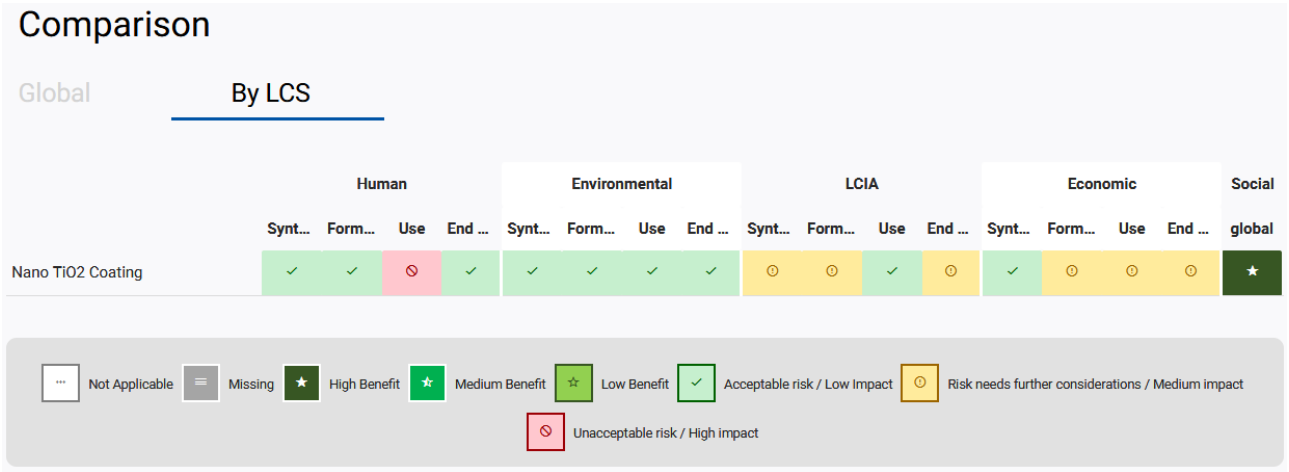

Figure 16: SUNDS Socio Economic Assessment results by Life Cycle Stage

The final result of the proposed case study application is characterised by an unacceptable risk level in Human Health Risk assessment, due to the condition in Use case life cycle stage. Environmental Risk assessment and Social Impact Assessment does not present any kind of issue while both LCIA and Economic assessment are in acceptable conditions as classified in the Medium impact category.

5 References / Selected sources of information

Subramanian, V., Semenzin, E., Hristozov, D., Zabeo, A., Malsch, I., McAlea, E., Murphy, F., Mullins, M., van Harmelen, T., Ligthart, T., Linkov, I., Marcomini, A. – Journal Nanoparticle Research (2016) 18: 89. https://doi.org/10.1007/s11051-016-3375-4

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6 List of abbreviations

DSS: Decision Support System

LUA: Lowest Unit of Assessment

ERA: Environmental Risk Assessment

HHRA: Human Health Risk Assessment

LCIA: Life Cycle Impact Assessment

EA: Economic Assessment

SEA: Socio Economic Assessment

LoE: Lines of Evidence

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