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*Workshop on life cycle evaluation and
energy use for different production
processes of nanomaterials*

**LCA of nano-enabled products. Nanopolytox
and Ecotexnano case studies**

Dr. Vincent Jamier
LEITAT Technological Center
16 April 2015 - Turku, Finland



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Since 1906



Evolving its expanding activities and committed to knowledge generation and technology transfer toward the Industry



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VALUES:

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- Independence
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- Market orientation
- Global Perspective
- Talent



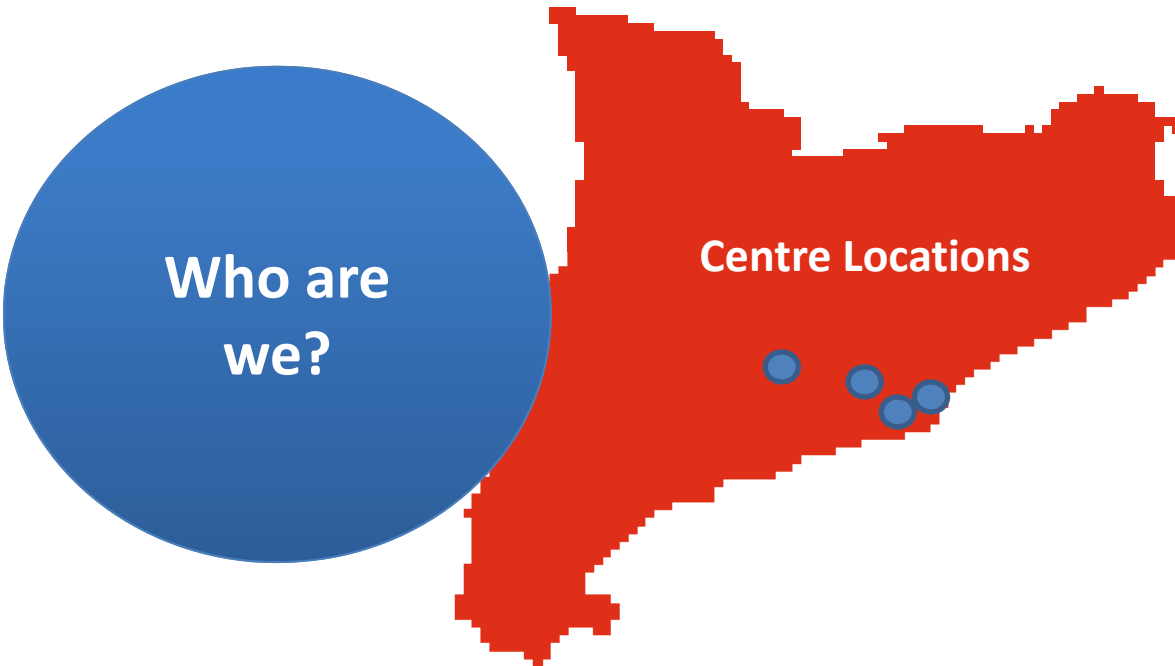
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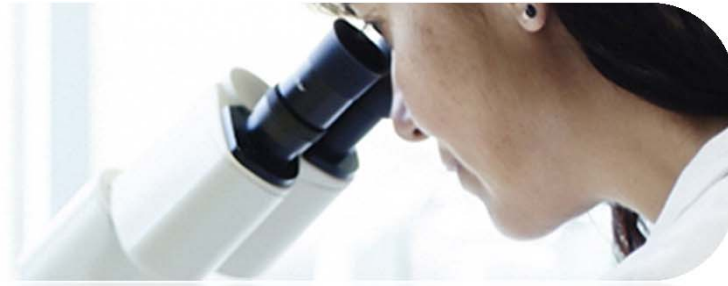


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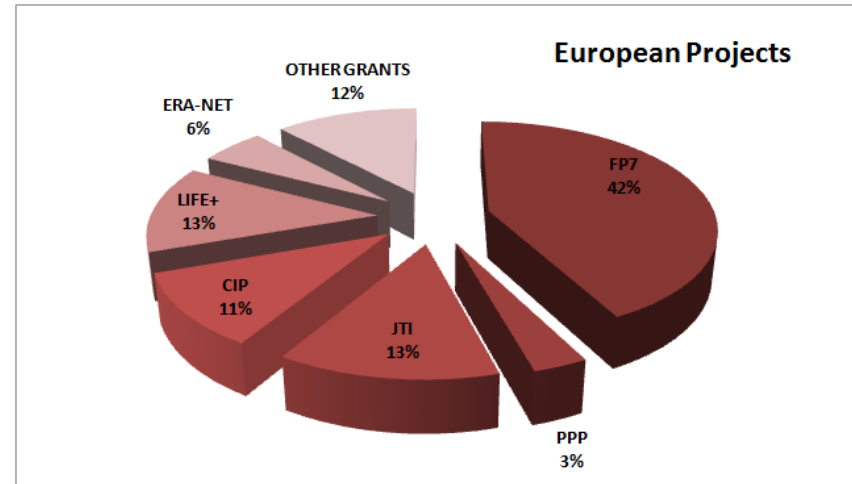
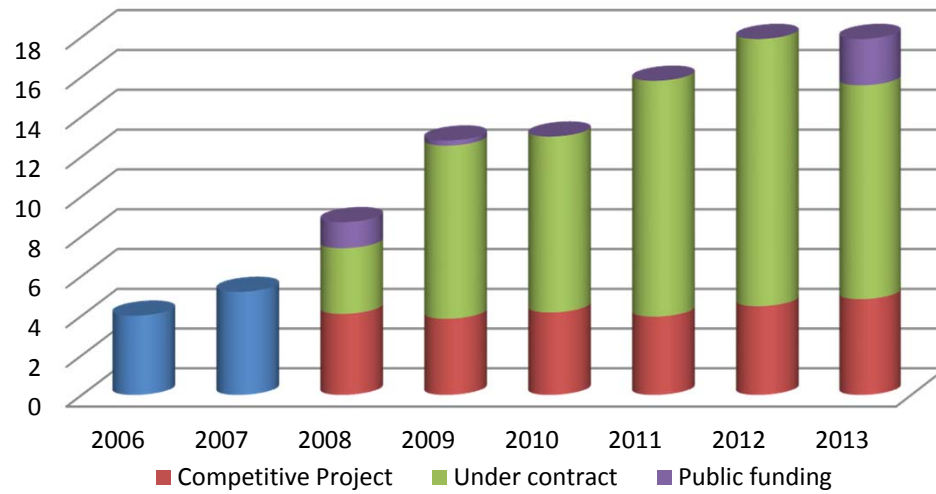
Centre Locations



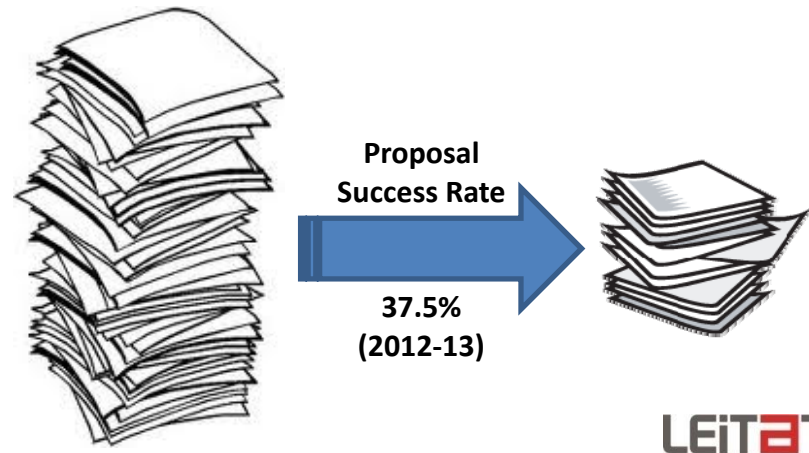
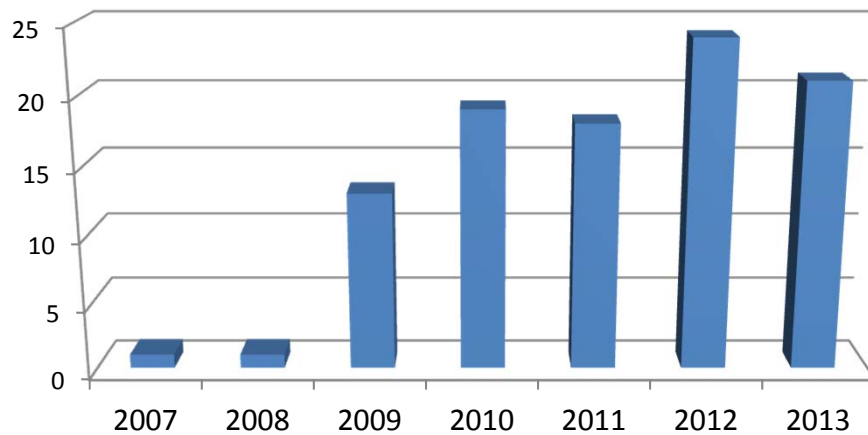
Barcelona



Income over the years (in M€)



Number of EU projects





LCA of nano-enabled products. Nanopolytox and Ecotexnano case studies

This presentation:

- Life Cycle Thinking in nanotechnologies

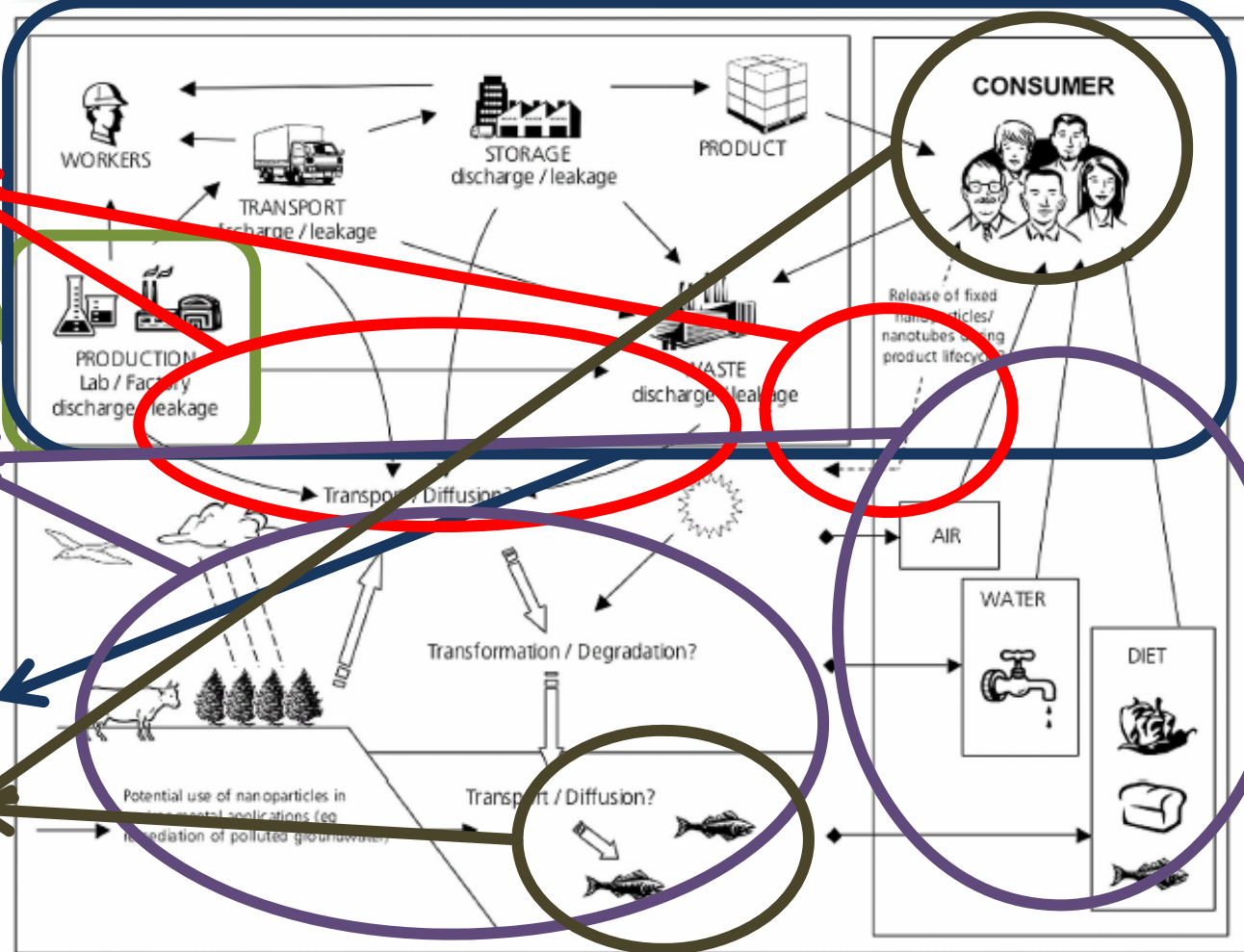
- 2 case studies:

1. NANOPOLYTOX project

2. ECOTEXNANO project



Life Cycle Thinking for Nanotechnologies



WHY???
 Scarce studies have generated data for the

Difficulties in nanomaterial release determination

As emerging products

Absence of Fate and intake models for exposure factor determination

and inventory data for the **whole life cycle** and include the

Lack of hazard data for the characterization factor determination

LCA studies

Adopted from The Royal Society & Royal Academy of Engineering 2004



Life Cycle Thinking for Nanotechnologies

MAIN GAPS AND SHORTCOMINGS OF LCA ON NANOTECHNOLOGY

- Synthesis and production processes:
 - wide variety in the production processes of nanomaterials and evolving fast
 - The information is also often confidential and proprietary
 - Different synthesis methods, different properties: CASE BY CASE
- Limited knowledge on Release of nanomaterials (especially during use phase and end-of-life phase).
- How to evaluate exposure from release data? EXPOSURE MODELLING
- Limited knowledge on the transformations and concentrations of nanomaterials in the environment.
- Environmental fate modelling of released nanomaterials: Need for adaptation of existing models (developed mainly for organic compounds)
- Uncertainty in toxicity: surface properties, functionalization, interaction with environmental media,



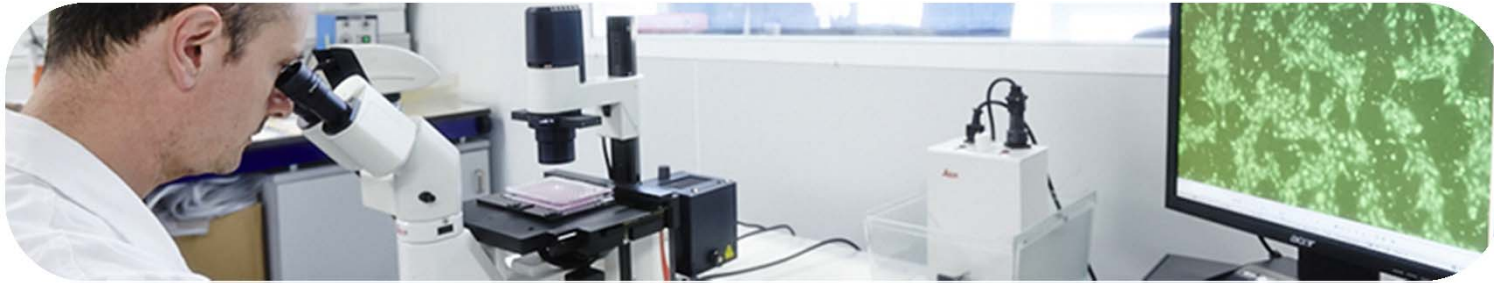
NANOPOLYTOX project

FP7-NMP-ENV-2009Project; Number: 247899; 2010-2013

Full Title: “Toxicological impact of nanomaterials derived from processing, weathering and recycling from polymer nanocomposites used in various industrial applications”

<http://www.nanopolytox.eu/>

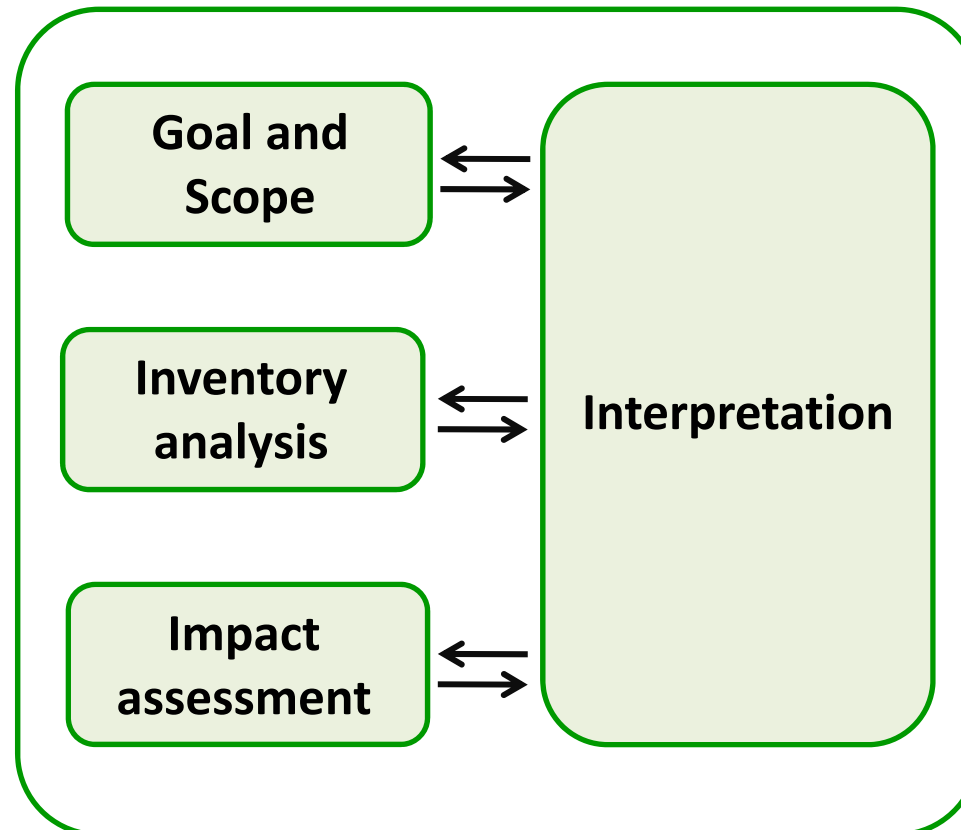
- The **main objective** of NANOPOLYTOX is the **monitoring of the life cycle** of three families of nanomaterials (**carbon nanotubes, nanoclays** and **metal oxide nanoparticles**) when embedded in selected polymeric hosts.
- The project included monitoring of the **chemical and physical properties** of the nanomaterials and their **toxicity** from the synthesis, processing, aging, and recycling to their disposal, covering their migration and/or release during their life cycle.
- The theoretical analysis of the data obtained during the project lead to the development of **predictive models to assess the biological and environmental fate of the studied nanomaterials.**
- The overall human health and environmental impact were assessed by **LCIA analysis**, specifically designed for nanomaterials.

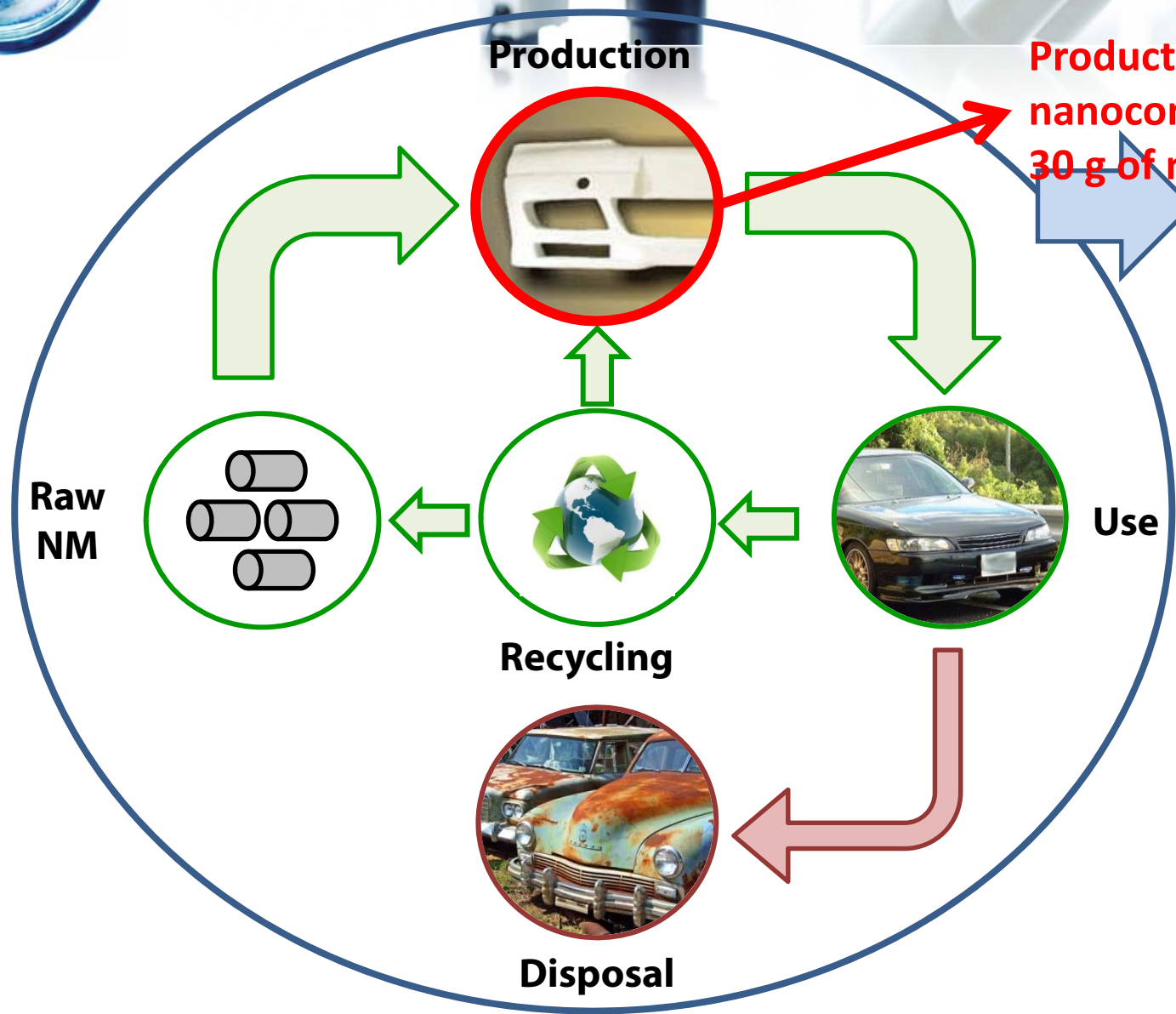


Life Cycle Assessment Framework (ISO 14044)

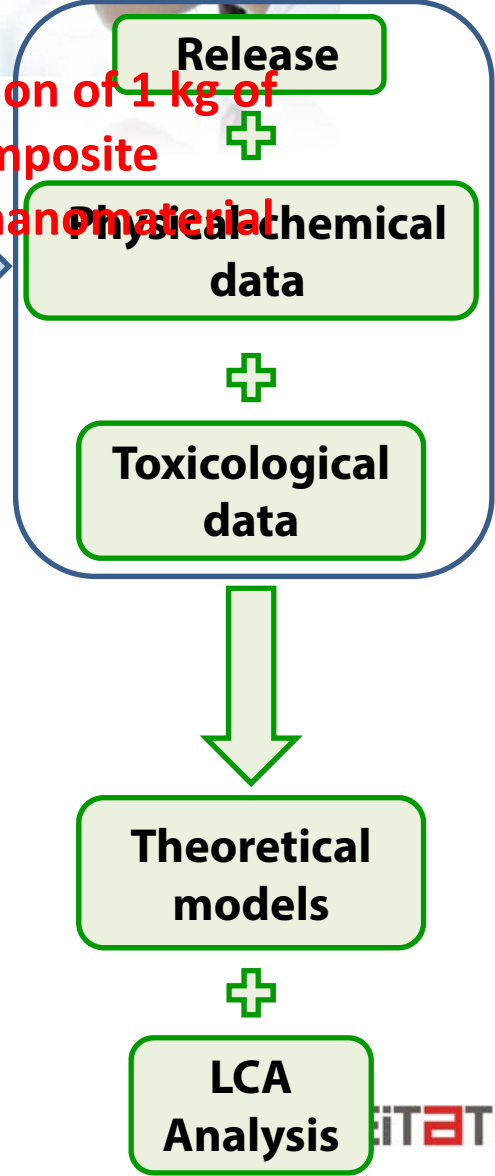
Standardized methodology: ISOs 14040 and 14044

European Platform on LCA: <http://ec.europa.eu/environment/ipp/lca.htm>





Production of 1 kg of nanocomposite
30 g of nanomaterial

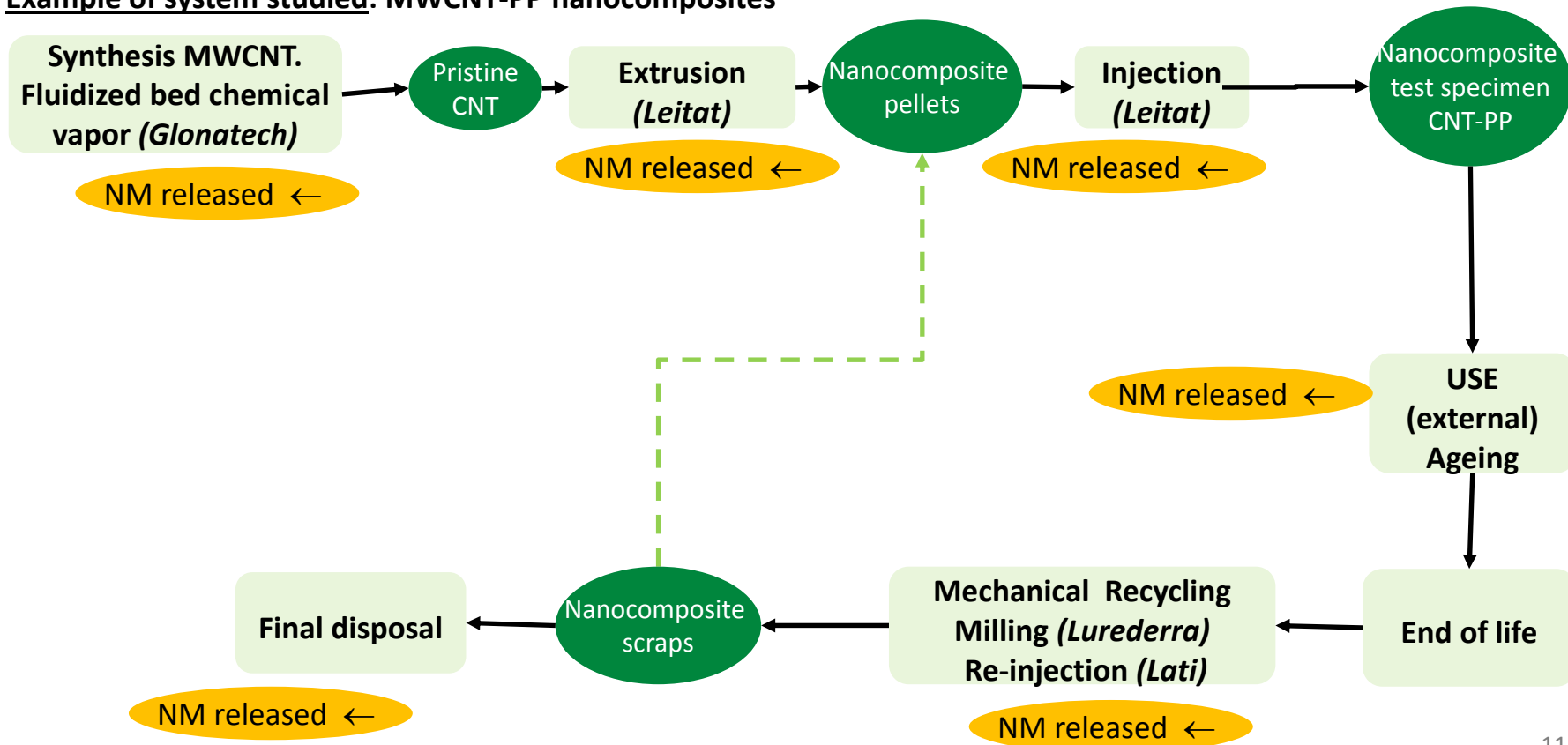




Four Selected nanomaterials to be studied in a comprehensive LCA:

- MWCNT-PP nanocomposite;
- Zinc Oxide – Ethylene vinyl acetate (EVA) nanocomposites;
- Clay – EVA nanocomposites;
- Titanium Dioxide – PA nanocomposite

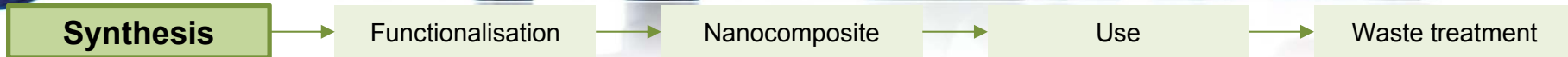
Example of system studied: MWCNT-PP nanocomposites





nanopolytox

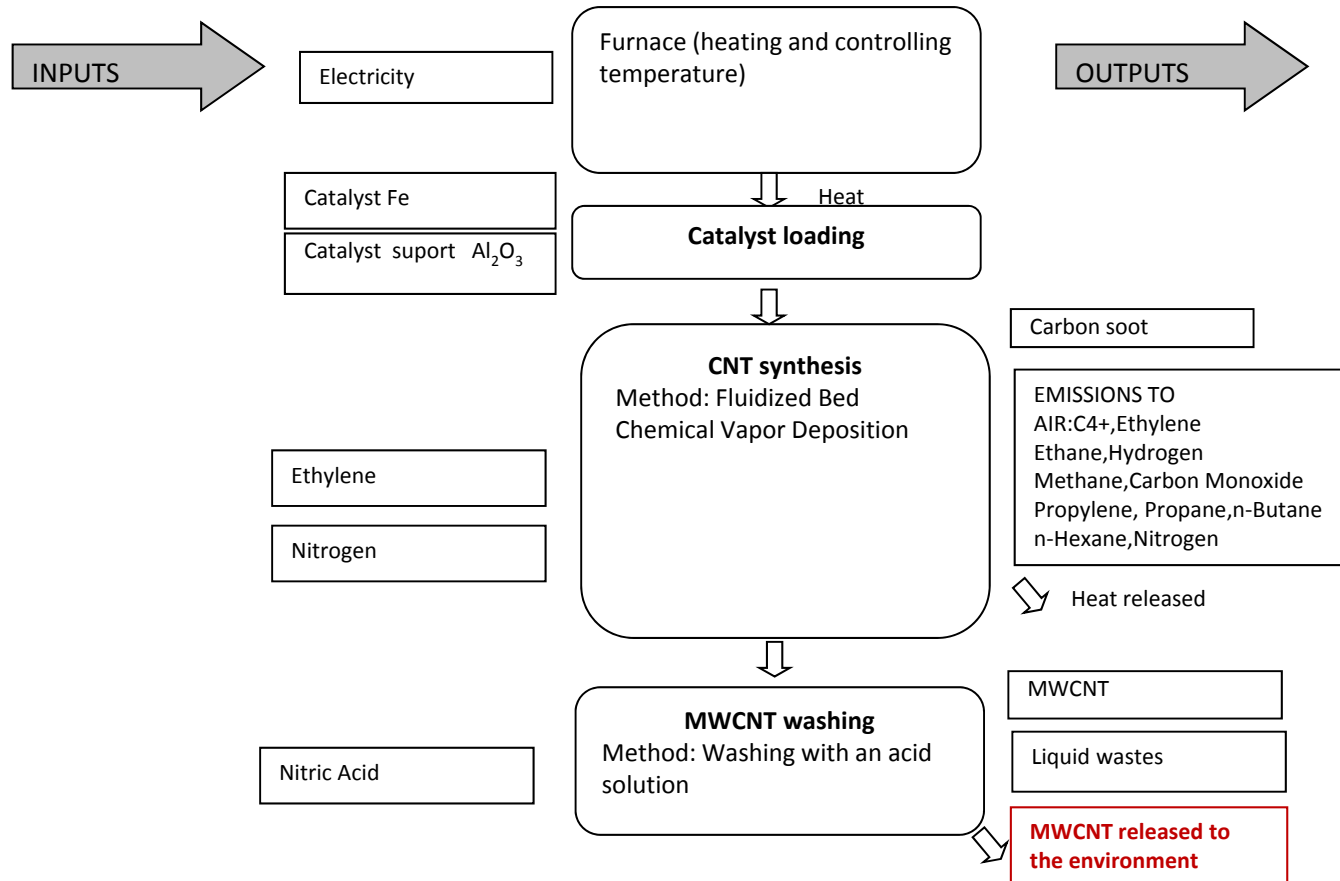
Life Cycle Inventory (LCI) MWCNT - Synthesis



Synthesis process: fluidized bed chemical vapour deposition (CDV),

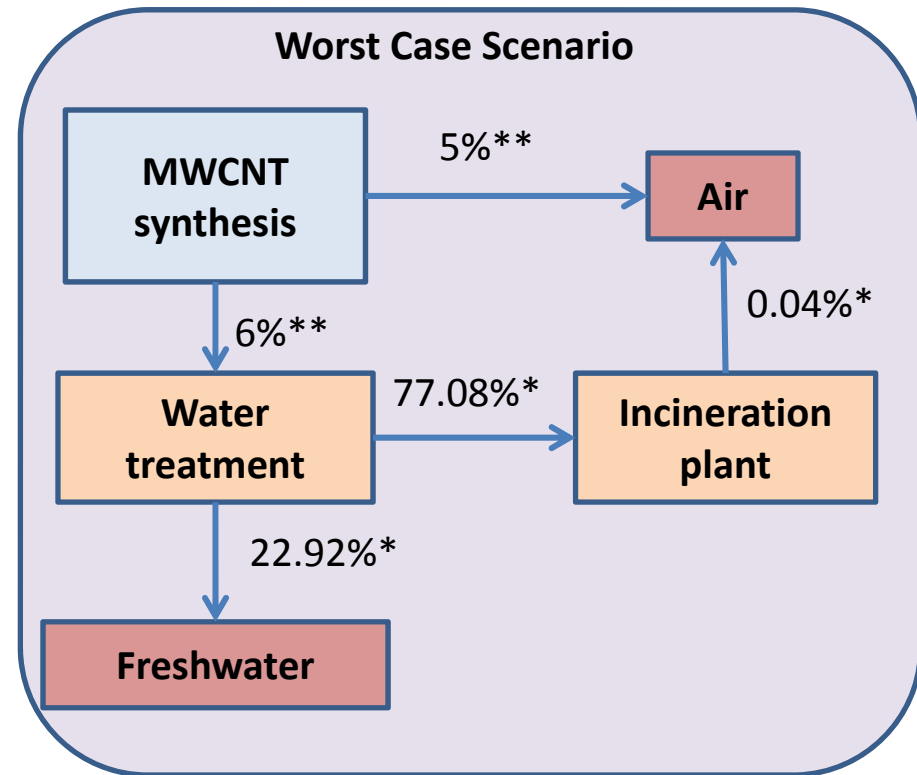
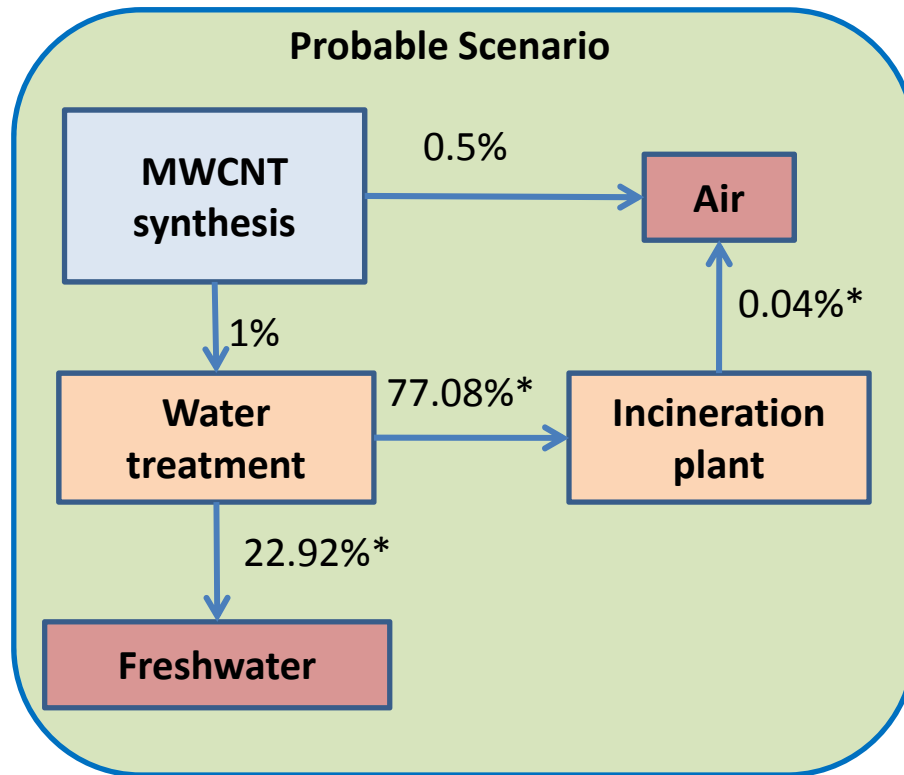
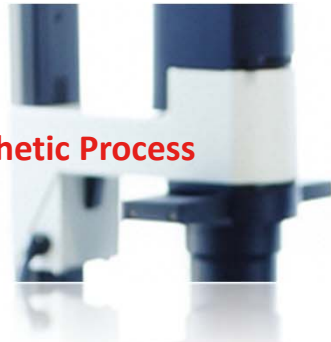
Reference flow: 30 g of multi-wall carbon nanotubes 97-98% (MWCNTs)

Technology: Semi-pilot unit.





Released NM in the Synthetic Process



Environ. Sci. Technol.* **2008, 42, 4447; *Environ. Sci. Technol.* **2009**, 43, 9216

** 'Guidance on information requirements and chemical safety assessment'.Part D: R16. ECHA



nanopolytox

Estimated release of NM



Release of MWCNT during all life cycle of composites

-Production of 1 Kg nanocomposite (3% MWCNT in PP) [MWCNT synthesis + nanocomposite synthesis]

	Probable Scenario	Worst Case Scenario
Air	0.171 + 0.170 g	1.907 + 0.861 g
Freshwater	0.078 + 0 g	0.524 + 0.157 g

-1 year use of 1 kg nanocomposite (3% MWCNT in PP)

	Probable Scenario	Worst Case Scenario
Freshwater	0.017 g	0.068 g

-Waste treatment of 1 kg nanocomposite (3% MWCNT in PP)

	Probable Scenario	Worst Case Scenario
Air	0.005 g	0.012 g



nanopolytox

Life Cycle Impact Assessment (LCIA)



Life Cycle Inventory

Resources used
Emissions
Waste & Materials flows

Nanomaterials release

Life Cycle Impact Assessment

ReCiPe Method

USETox Model

Fate
Factors

Intake
fraction

Ecotox
Effect
Factors

Human
Effect
Factors

Characterization
for selected
midpoints and
endpoint
categories



Life Cycle Impact Assessment (LCIA)



ReCiPe method

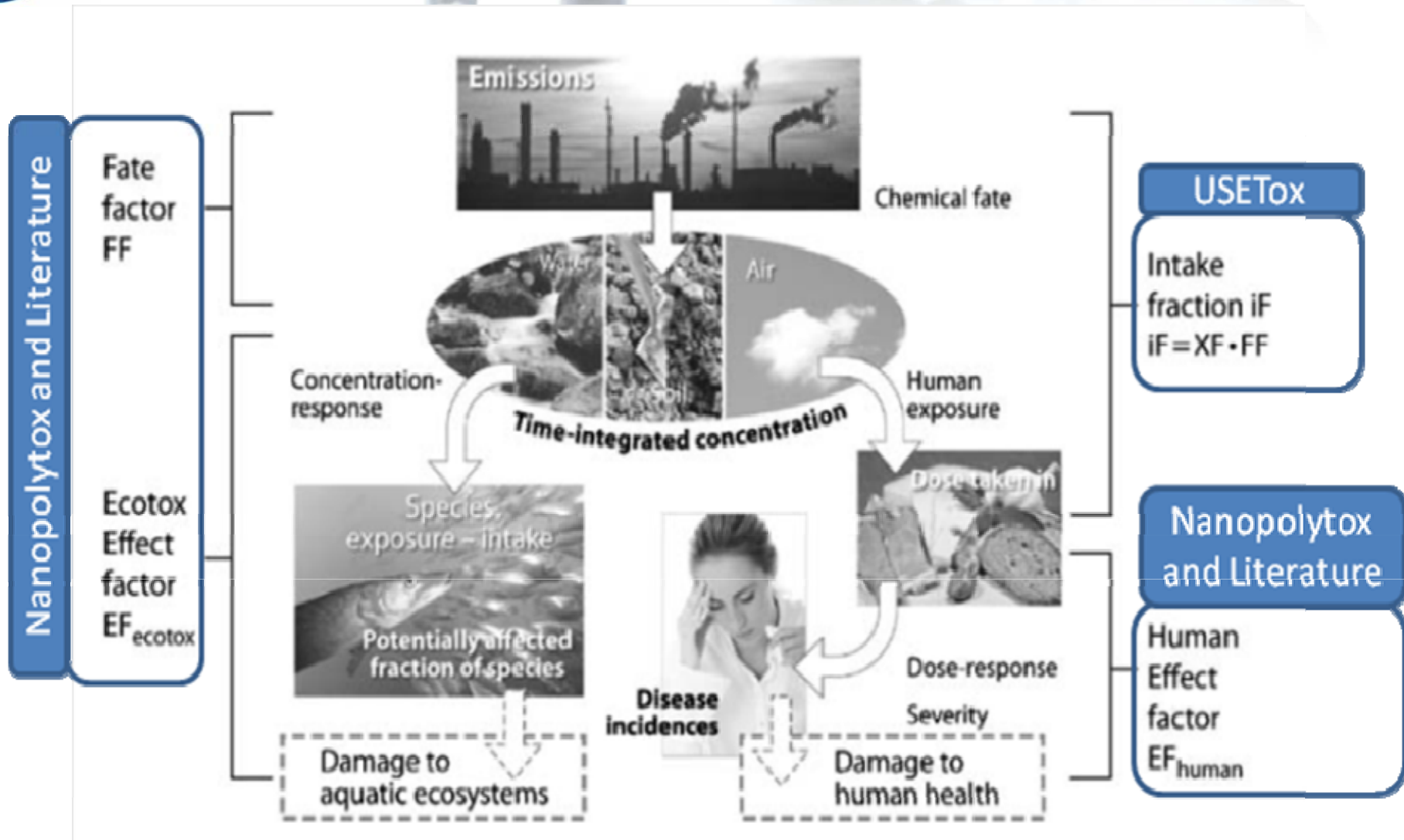
Midpoint impact category name	Abbr.	Endpoint impact category*		
		HH	ED	RA
climate change	CC	+	+	
ozone depletion	OD	+	-	
terrestrial acidification	TA		+	
freshwater eutrophication	FE		+	
marine eutrophication	ME		-	
human toxicity	HT	+		
Photochemical oxidant formation	POF	+	-	
particulate matter formation	PMF	+		
terrestrial ecotoxicity	TFT		+	
freshwater ecotoxicity	FET		+	
marine ecotoxicity	MET		+	
ionising radiation	IR	+		
agricultural land occupation	ALO		+	-
urban land occupation	ULO		+	-
natural land transformation	NLT		+	-
water depletion	WD			-
mineral resource depletion	MRD			+
fossil fuel depletion	FD			+

NM →

NM →

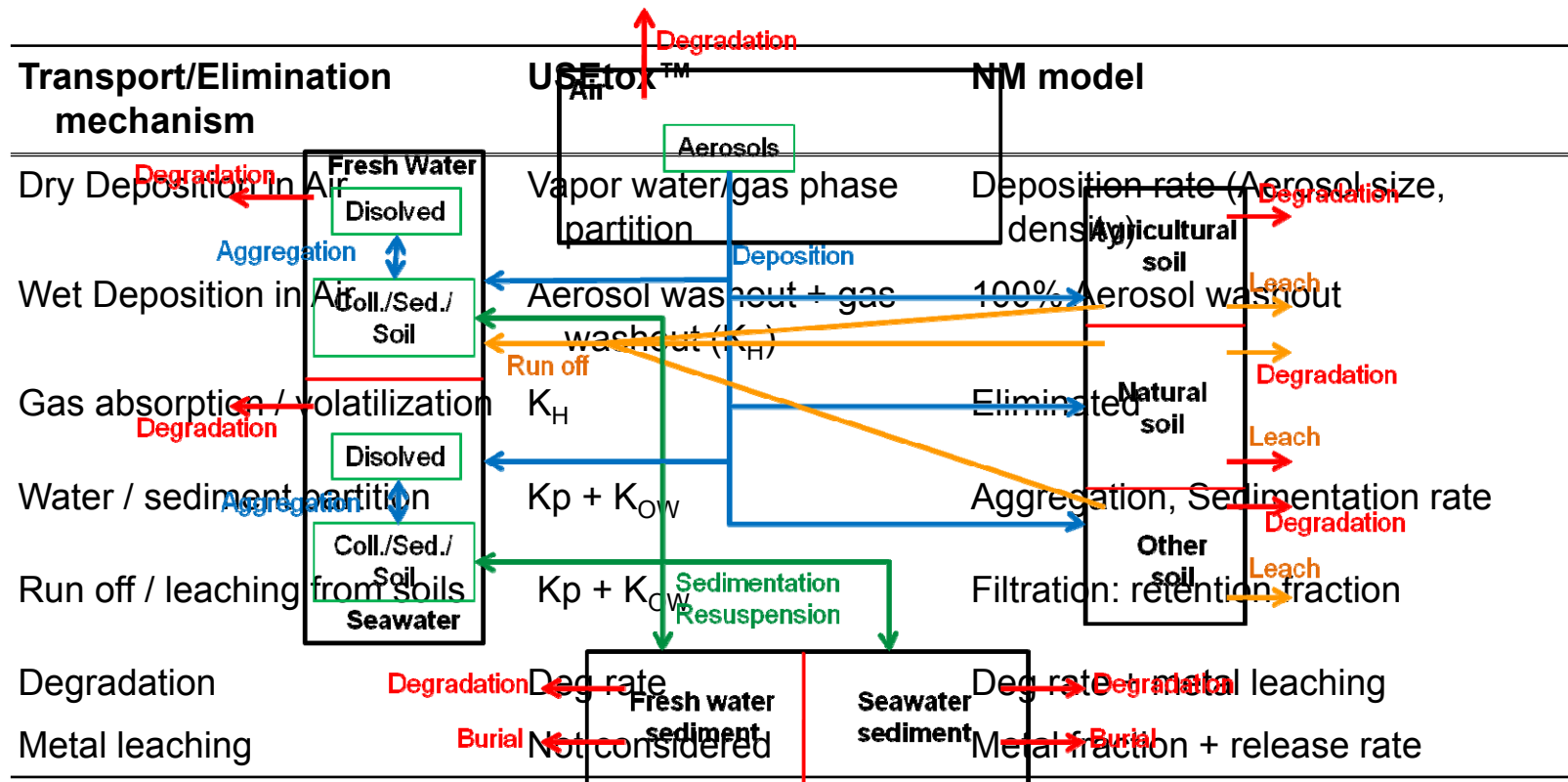
* **HH**: Human Health Damage; **ED**: Ecosystems damage; **RA**: Resource Availability Damage

+ : Quantitative connection has been established in ReCiPe 2008 for this link; - : No quantitative connection has been established for this link in ReCiPe 2008





USEtox™ Fate model is basically designed for organic compounds and derives most distribution and biodistribution factors from few physico-chemical endpoints. This is not possible with nanomaterials, so we modified the model using different distribution equations. Moreover, **bioaccumulation and intake parameters cannot be derived** from K_{OW} and have to be introduced case by case





Ecotoxicity and Human Toxicity Effect Factors



Derivation following the general USEtox methodology

For example, for ecotoxicity:

1. Collection of available toxicity data for MWCNTs in freshwater organisms and estimation of single species EC_{50}
2. Derivation of HC50 following this formula :
$$\text{Log HC50} = 1/n \text{ species} \cdot \text{SUM} (\text{log } EC_{50} \text{ for each tropic level})$$

HC50 values = 12.7 mg/L (best estimate); 4.9 mg/L (worst-case)

3. Derivation of Ecotoxicity Effect Factor:
$$EF = (0.5/HC50)$$

EF = 39 m³/kg (best estimate) and 102 m³/kg (worst-case)

Main problems:

- (Eco)toxicity studies focused on most common nanomaterials.
- Tests done with the same compound but different material (size, shape, surface chemistry).
- Absence of clear SOP. Comparison between studies is difficult.
- Absence of dosimetry studies. Real exposure vs. supposed exposure.



MWCNT Characterisation factors



Characterization Factor = Fate Factor x Intake Factor x Effect Factor

Human health characterization factor

[cases/kg_{emitted}]:

	<i>Emission to urban air</i>			<i>Emission to cont. rural air</i>			<i>Emission to cont. freshwater</i>		
	cancer	non-canc.	total	cancer	non-canc.	total	cancer	non-canc.	total
Average	1,5E-05	1,5E-05	2,9E-05	1,7E-06	1,7E-06	3,4E-06	1,4E-07	1,4E-07	2,7E-07
Worth case	1,5E-04	1,5E-04	2,9E-04	1,6E-05	1,6E-05	3,3E-05	1,4E-07	1,4E-07	2,7E-07

[DALY/kg_{emitted}]:

	<i>Emission to urban air</i>			<i>Emission to cont. rural air</i>			<i>Emission to cont. freshwater</i>		
	cancer	non-canc.	total	cancer	non-canc.	total	cancer	non-canc.	total
Average	5.7E-05	5.7E-05	1,1E-04	6,5E-06	6,5E-06	1,3E-05	5,3E-07	5,3E-07	1,0E-06
Worth case	5.7E-04	5.7E-04	1,1E-03	6,1E-05	6,1E-05	1,2E-04	5,3E-07	5,3E-07	1,0E-06

Ecotoxicological characterization factor

[PDF·m³·day/kg]:

	<i>Emission to urban air</i>	<i>Emission to cont. rural air</i>	<i>Emission to cont. freshwater</i>
Average	1,8E+02	1,8E+02	4,5E+02
Worth Case	4,6E+02	4,6E+02	1,2E+03



**Effect of released MWCNT
(release x charac. factors)**



Human health effect

		Probable scenario DALY	Worst case scenario DALY
MWCNT synthesis	cancer	1,15E-09	1,17E-07
	non-cancer	1,15E-09	1,17E-07
	total	2,31E-09	2,33E-07
Nanocomposite synthesis	cancer	1,11E-09	5,26E-08
	non-cancer	1,11E-09	5,26E-08
	total	2,22E-09	1,05E-07
Use	cancer	9,01E-12	3,60E-11
	non-cancer	9,01E-12	3,60E-11
	total	1,80E-11	7,21E-11
Waste treatment	cancer	2,85E-10	6,84E-09
	non-cancer	2,85E-10	6,84E-09
	total	5,70E-10	1,37E-08
Total	cancer	2,55E-09	1,76E-07
	non-cancer	2,55E-09	1,76E-07
	total	5,11E-09	3,53E-07

Ecotoxicological characterization factor

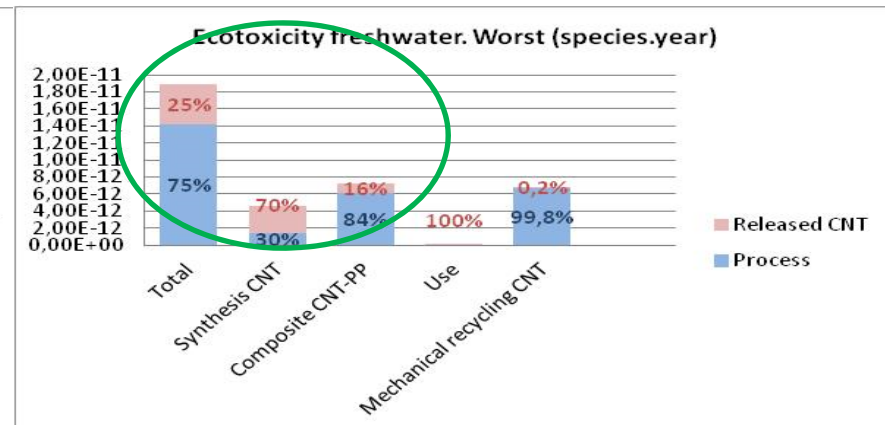
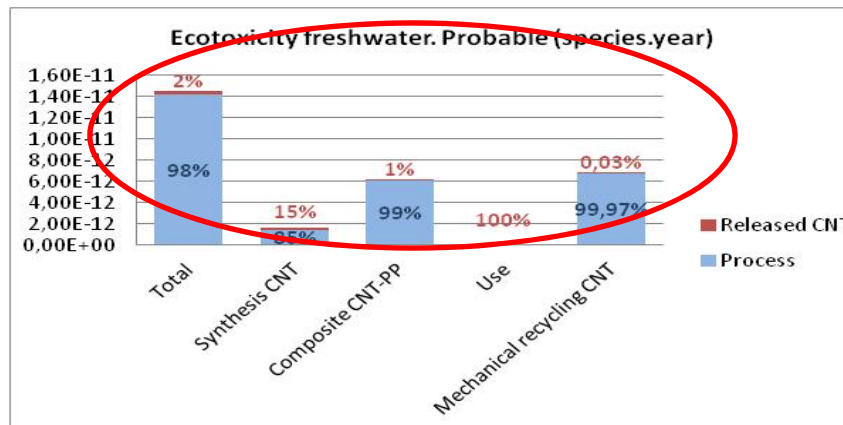
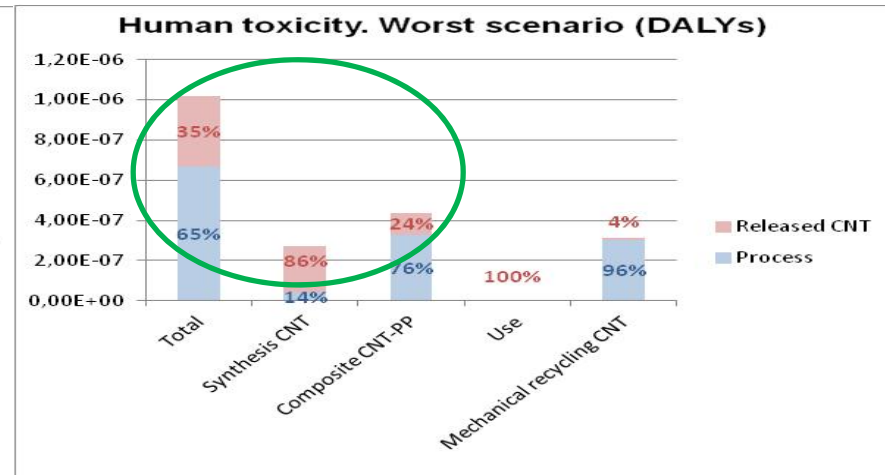
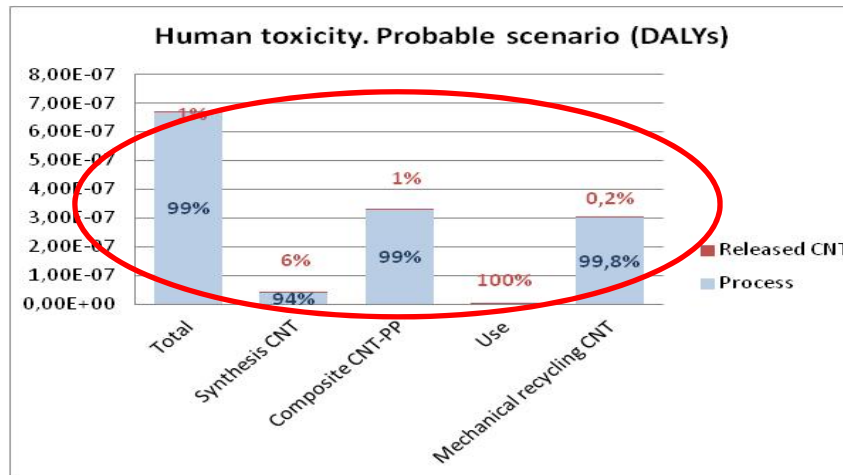
	Probable scenario		Worst case scenario	
	PDF·m ³ ·day	species·year	PDF·m ³ ·day	species*year
MWCNT synthesis	6,58E-02	2,39E-13	1,51E+00	3,25E-12
Nanocomposite synthesis	3,06E-02	6,61E-14	5,84E-01	1,20E-12
Use	7,65E-03	1,65E-14	8,16E-02	1,76E-13
Waste treatment	9,00E-04	1,95E-15	5,52E-03	1,19E-14
Total	1,05E-01	3,24E-13	2,18E+00	4,64E-12



**LCIA (ReCiPe)
MWCNT - Nanocomposite**



The contribution over Human Toxicity and Ecotoxicity Freshwater is small in the **probable scenario** but quite important in the **Worst Case**



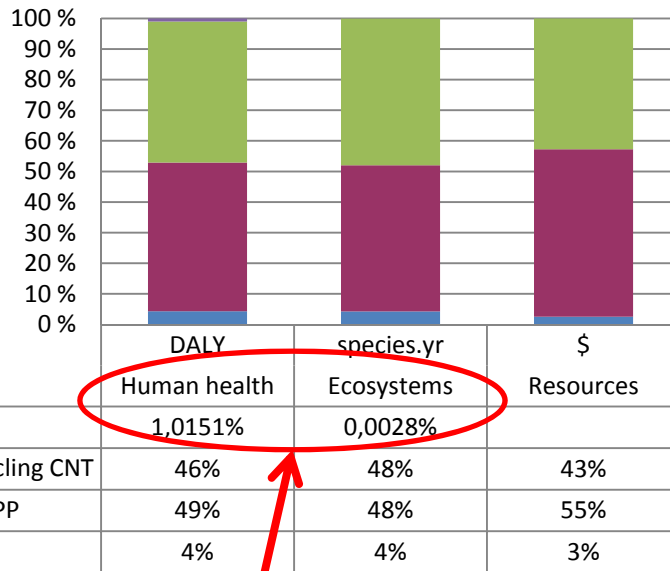


LCIA (ReCiPe)
MWCNT - Nanocomposite



Damage on Human Health and Distribution of impacts at endpoint level (damage) incorporating the effect of released MWCNT in toxicity categories

(Endpoint indicators. Worst case scenario)



	DALY	species.yr	\$
■ CNT released	1,0151%	0,0028%	
■ Mechanical recycling CNT	46%	48%	43%
■ Composite CNT-PP	49%	48%	55%
■ Synthesis CNT	4%	4%	3%

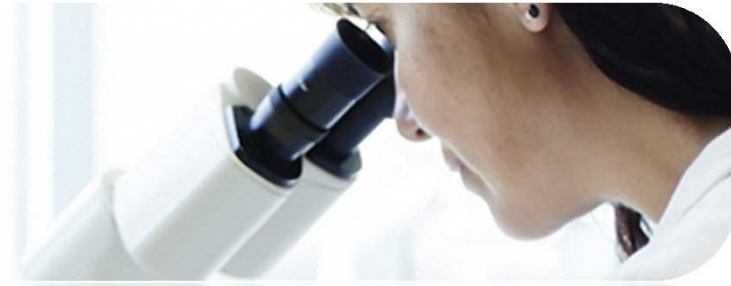
But the contribution to the total Damage on Human Health and Damage on the Ecosystems is low even in the Worst Case Scenario

Contribution of the different impact categories to the three damage levels (endpoint, worst case scenario)

	Unit category	Units	Contribution
DAMAGE ON HUMAN HEALTH	Climate change Human Health	DALY	84%
	Ozone depletion	DALY	0,01%
	Human toxicity	DALY	3%
	Photochemical oxidant formation	DALY	2%
	Particulate matter formation	DALY	0,01%
	Ionising radiation	DALY	0,3%
	DAMAGE ON ECOSYSTEMS	Climate change Ecosystems	species.yr
Terrestrial acidification		species.yr	0,2%
Freshwater eutrophication		species.yr	0,01%
Terrestrial ecotoxicity		species.yr	0,1%
Freshwater ecotoxicity		species.yr	0,01%
Marine ecotoxicity		species.yr	0,00002%
Agricultural land occupation		species.yr	1,0%
Urban land occupation		species.yr	0,4%
Natural land transformation		species.yr	1,2%
DAMAGE ON RESOURCES		Metal depletion	\$
	Fossil depletion	\$	99,996%



Conclusions



- LCA approach for nanotechnology and nano-products can provide useful information about the main environmental impacts and benefits of this emerging technology.
- At inventory stage, it should be kept in mind that experimental and **lab scale processes can vary from industrial scale processes.**
- When nano-based products are assessed through life cycle assessment, **it is important to include nanoparticles flows and the changes/modifications that these nanoparticles can have during the product life**, since the impact that these nanoparticles can cause if they are released to the environment can be relevant in some stages.
- Potential **impacts of released nanoparticles should be included in the impact assessment step.** Prospective LCA approaches are needed and experimental data on characteristics and toxicity of nanoparticles coming from research projects should be included in LCA methodologies.
- Adapted **exposure and fate modelling are needed** in order to have complete results on the environmental performance of nano-products during all life cycle stages.
- **Adapted Standard Operating Procedure (SOP) for hazard, intake and bioaccumulation are necessary** to have good impact determination,



ECOTEXNANO project

LIFE12ENV/ES/000667; Start date: 01/10/2013 End date: 30/09/2016

Full Title: “Innovative tool to improve risk assessment and promote the safe use of nanomaterials in the textile finishing industry”

<http://www.life-ecotexnano.eu/>



Key objectives:

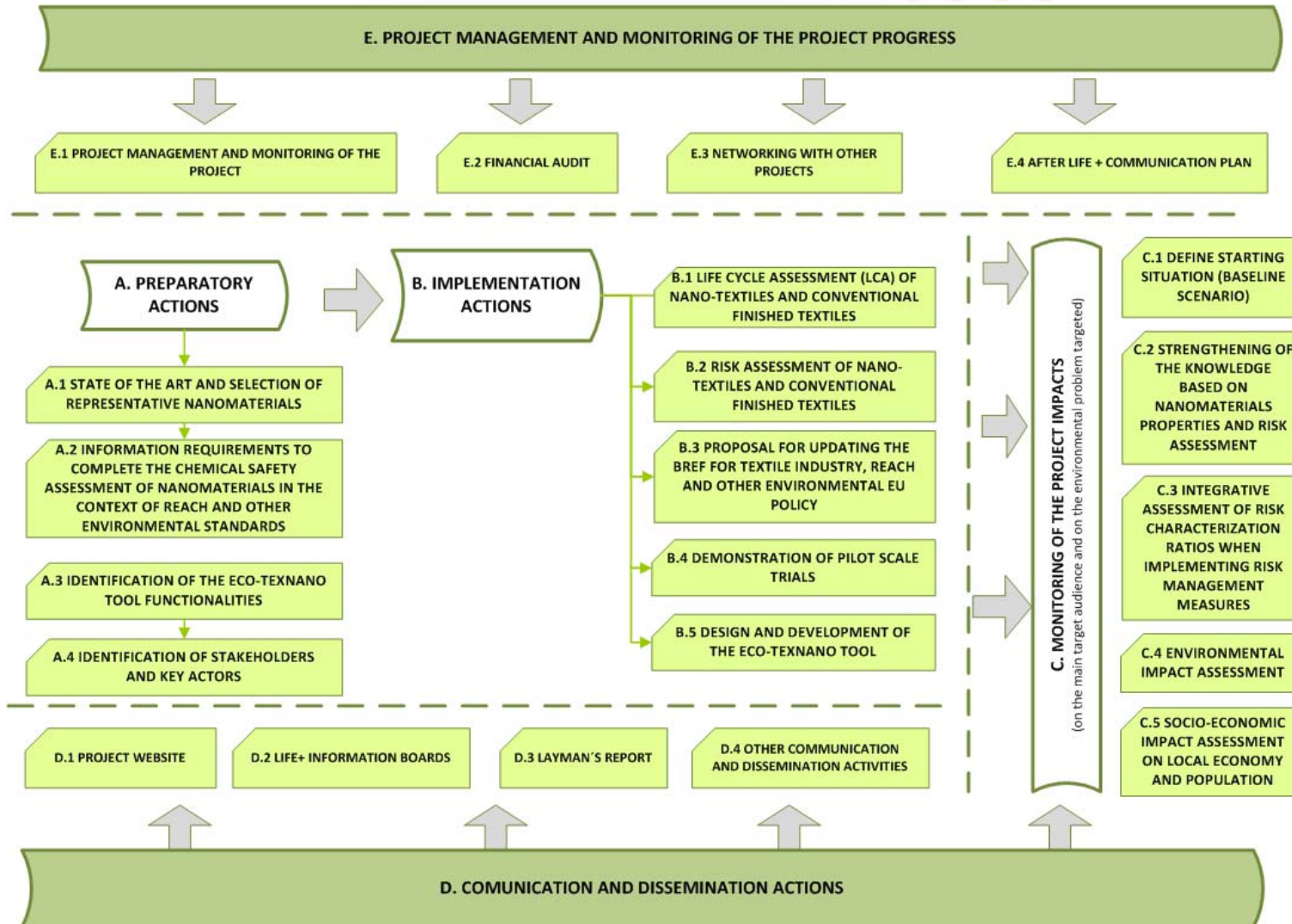
1. Provide the textile finishing industry a user-friendly tool to improve the knowledge on risk assessment of nanomaterials and to promote the safe use along their life cycle.
2. Identify and reduce the environmental, health and safety impacts carrying out a comprehensive Life Cycle.



Work Programme

ecotex

nano
young





LCA Scope



✓ 4 textile technical properties:

Soil-release
UV protection
Antibacterial
Flame retardant

✓ Pilots scale trials:

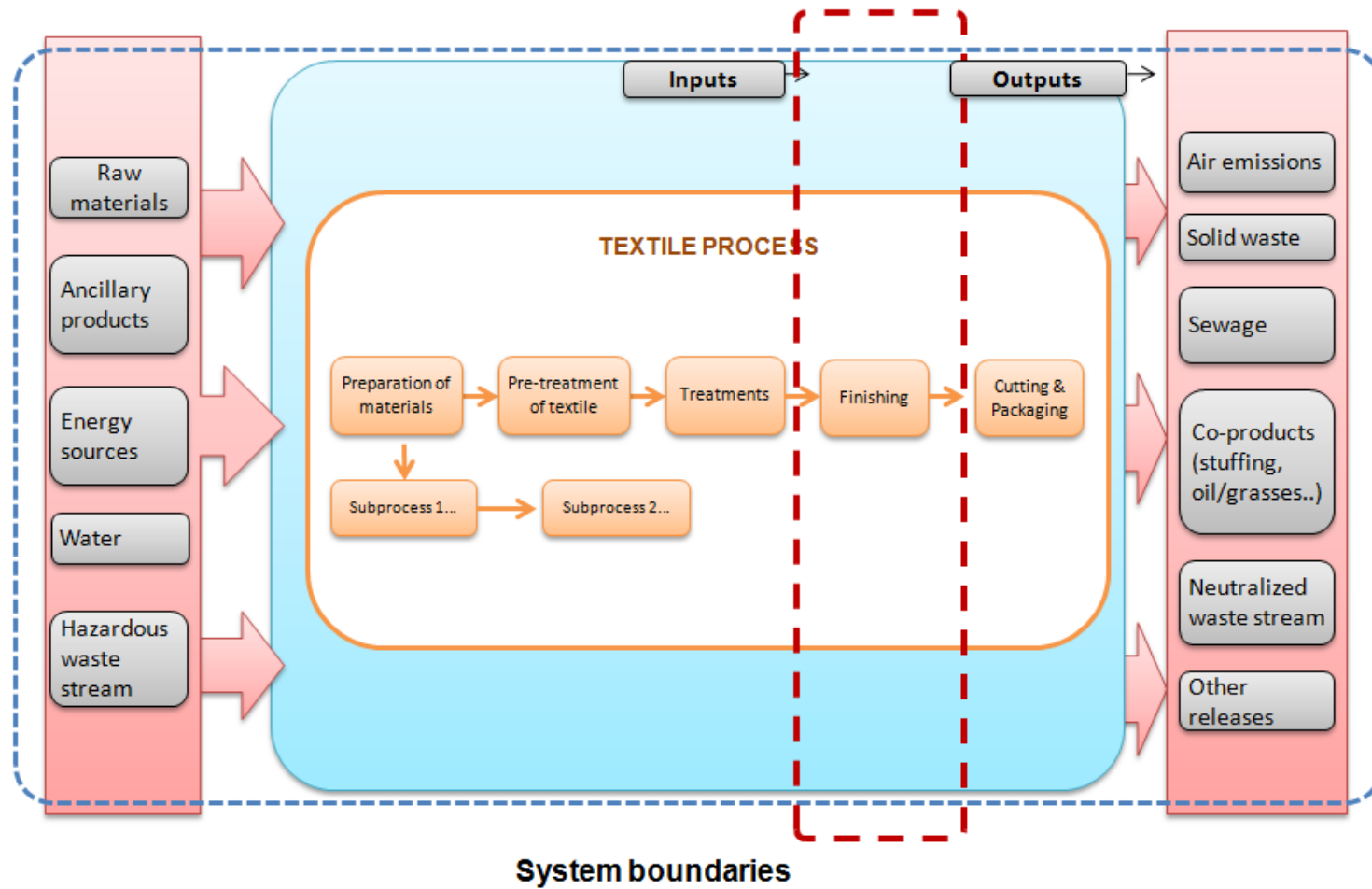
PIACENZA (Italy)	VINCOLOR (Spain)
Soil-release	Soil-release
UV protection	Flame retardant
Antibacterial	



LCA Scope



✓ Focused on finishing textile process:

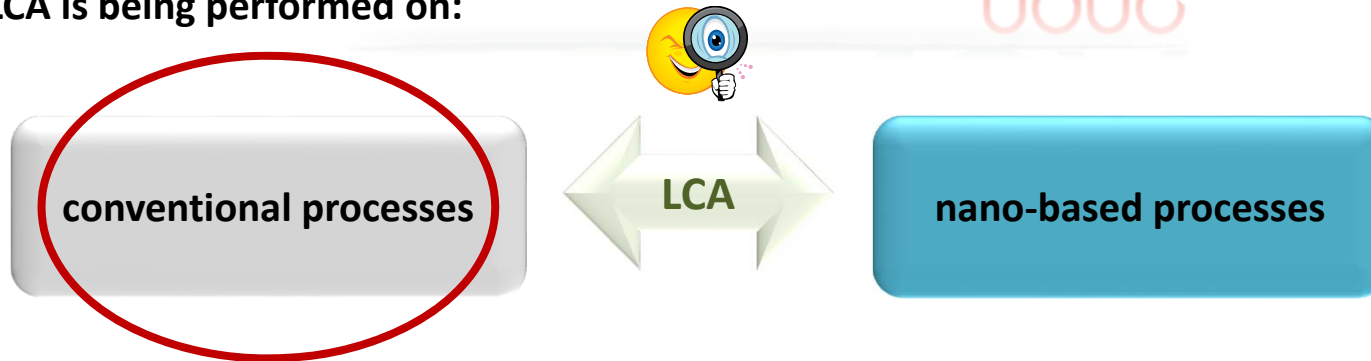




LCA Scope



LCA is being performed on:



Environmental assessment					
PILOT	PIACENZA			VINCOLOR	
PROPERTY	Antibacterial	UV protection	Soil release	Soil release	Flame retardant
Conventional	x	x	x	x	x
Nanomaterial*	Silver	TiO2	C6 based fluorochemical	C6 based fluorochemical	Montmorillonite nanoclay / Silica

*Selection criteria based on both “commercially available” and “technically demonstrated on the selected textile applications”

At this stage we have obtained **preliminary results** on the environmental performance of the **conventional processes** used for **soil release** applications in two fabrics from **Vincolor (MIRAGE and DIVINE)**



LCA future results



- ✓ Identification of the **significant impacts** related to the process analyzed
- ✓ Evaluation of impacts in accordance with the objectives and scope of the study to draw **conclusions** and / or **recommendations**.
- ✓ Environmental impact contribution among different stages
- ✓ Environmental impacts compared to conventional process
- ✓ Specific results are translated into:



- ✓ Expected end date: **March 2016**

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