nanopolytox

*Toxicological impact of nanomaterials derived from processing, weathering and recycling of polymer nanocomposites used in various industrial applications*

# Approach for Human Toxicity and Freshwater Ecotoxicity midpoints determination for their inclusion in Life Cycle Assessment of nanotechnology-based products

**Dr Socorro Vázquez-Campos**
Safety and Sustainability Division Leader
LEITAT TECHNOLOGICAL CENTER
svazquez@leitat.org

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SEVENTH FRAMEWORK PROGRAMME

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# Life Cycle Thinking for Nanotechnologies

**WHY???**

Scarce studies have generated data for the

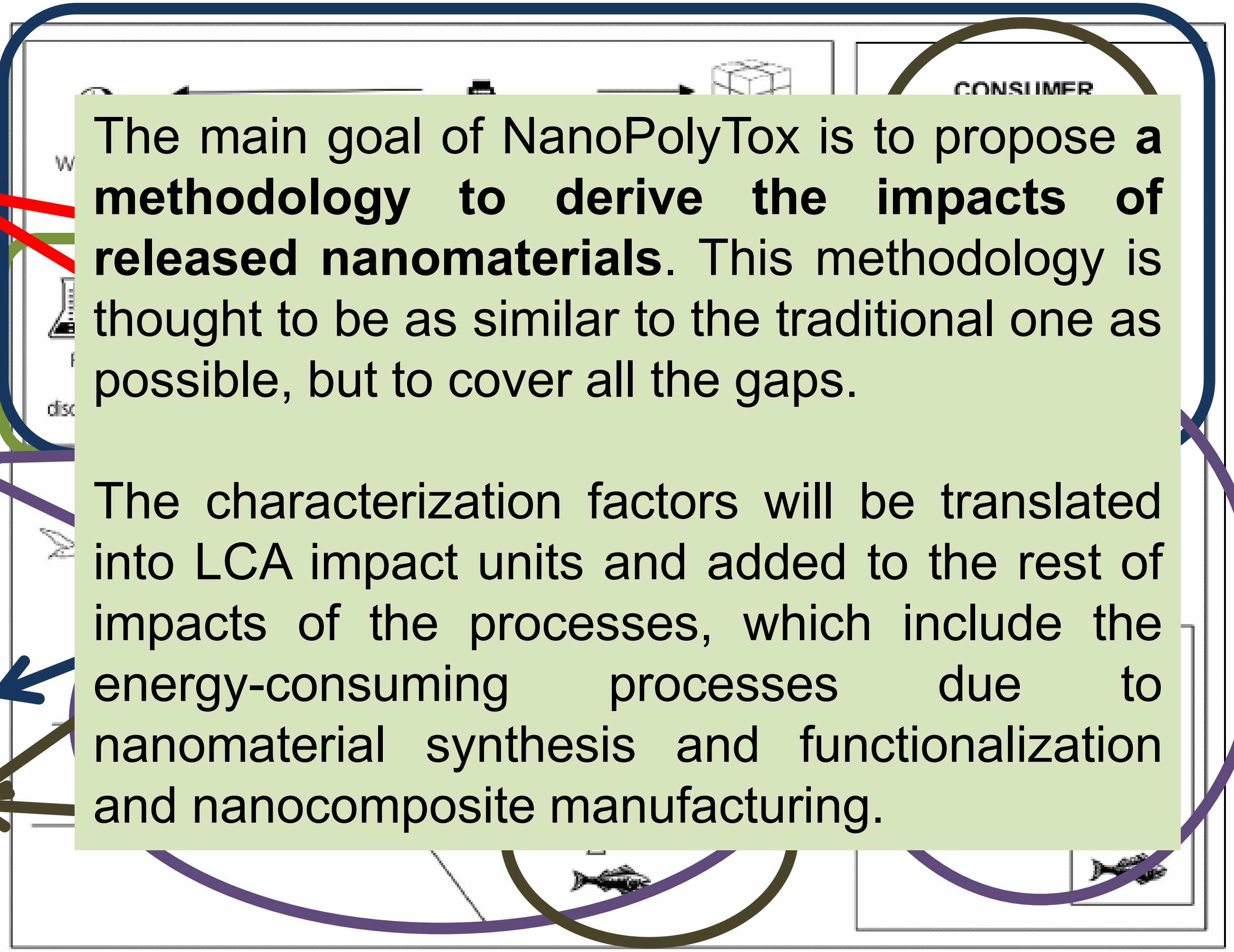
Difficulties in nanomaterial release determination

Absence of Fate and intake models for exposure factor determination

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

Lack of hazard data for the characterization factor determination

**LCA studies**

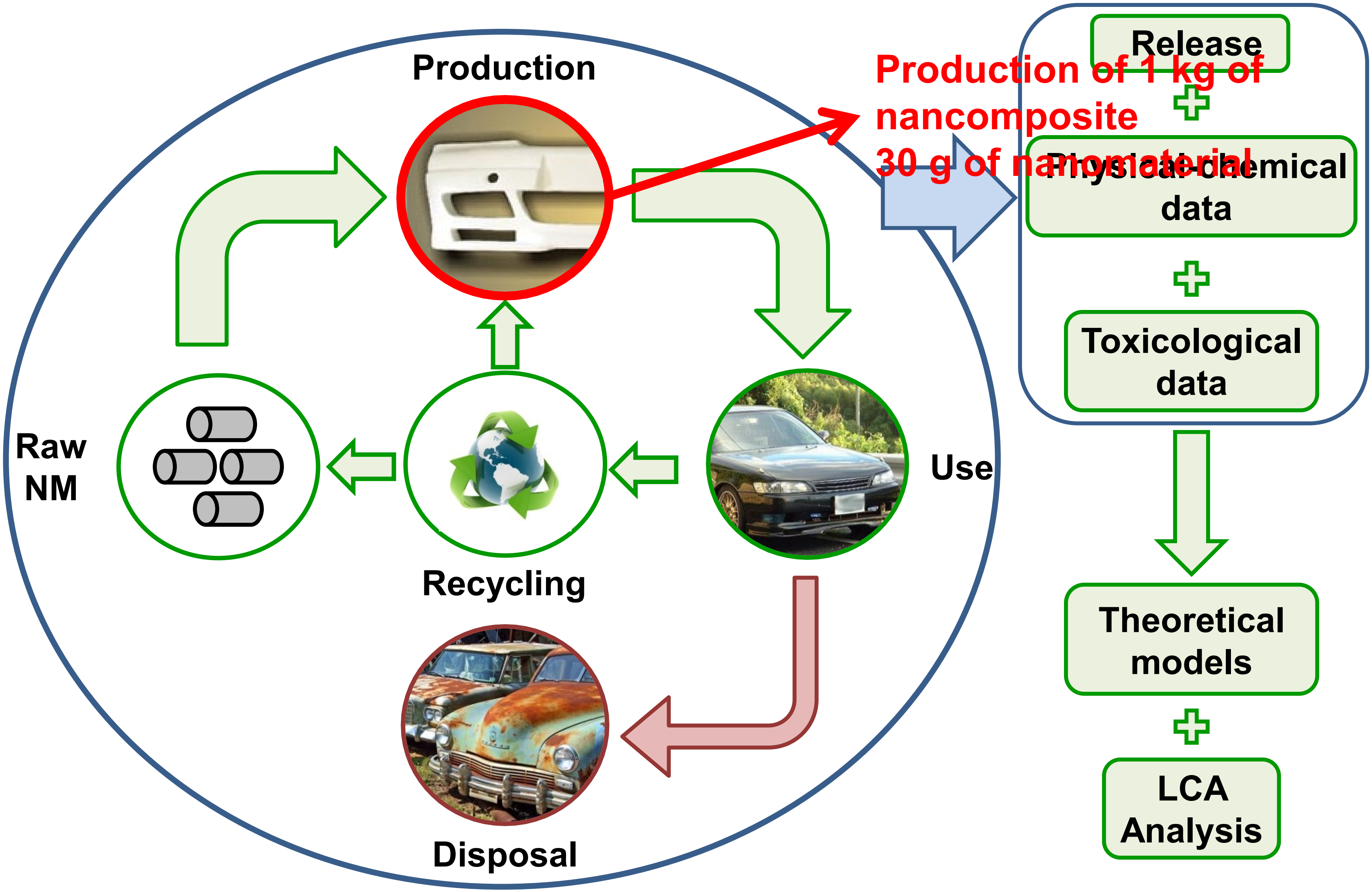


The main goal of NanoPolyTox is to propose **a methodology to derive the impacts of released nanomaterials**. This methodology is thought to be as similar to the traditional one as possible, but to cover all the gaps.

The characterization factors will be translated into LCA impact units and added to the rest of impacts of the processes, which include the energy-consuming processes due to nanomaterial synthesis and functionalization and nanocomposite manufacturing.

Adopted from The Royal Society & Royal Academy of Engineering 2004

# LCA APPROACH IN NANOPOLYTOX



# Goal and scope definition

ReCiPe method

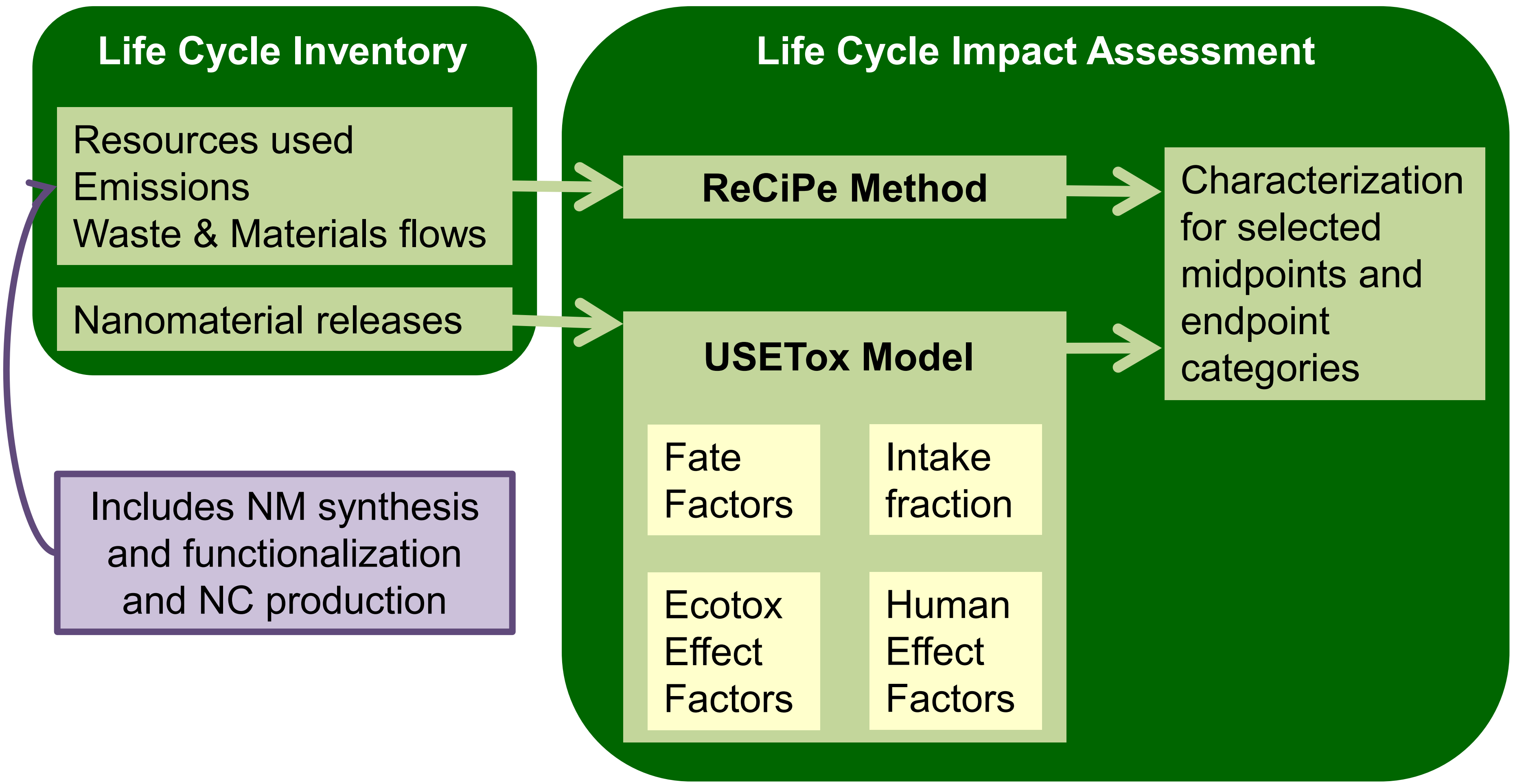
| Midpoint impact category name | Abbr. | Endpoint impact category* HH | ED | RA |
|---|---|---|---|---|
| climate change | CC | + | + | |
| ozone depletion | OD | + | – | |
| terrestrial acidification | TA | | + | |
| freshwater eurotrophication | FE | | + | |
| marine eurotrophication | ME | | – |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

NM → human toxicity

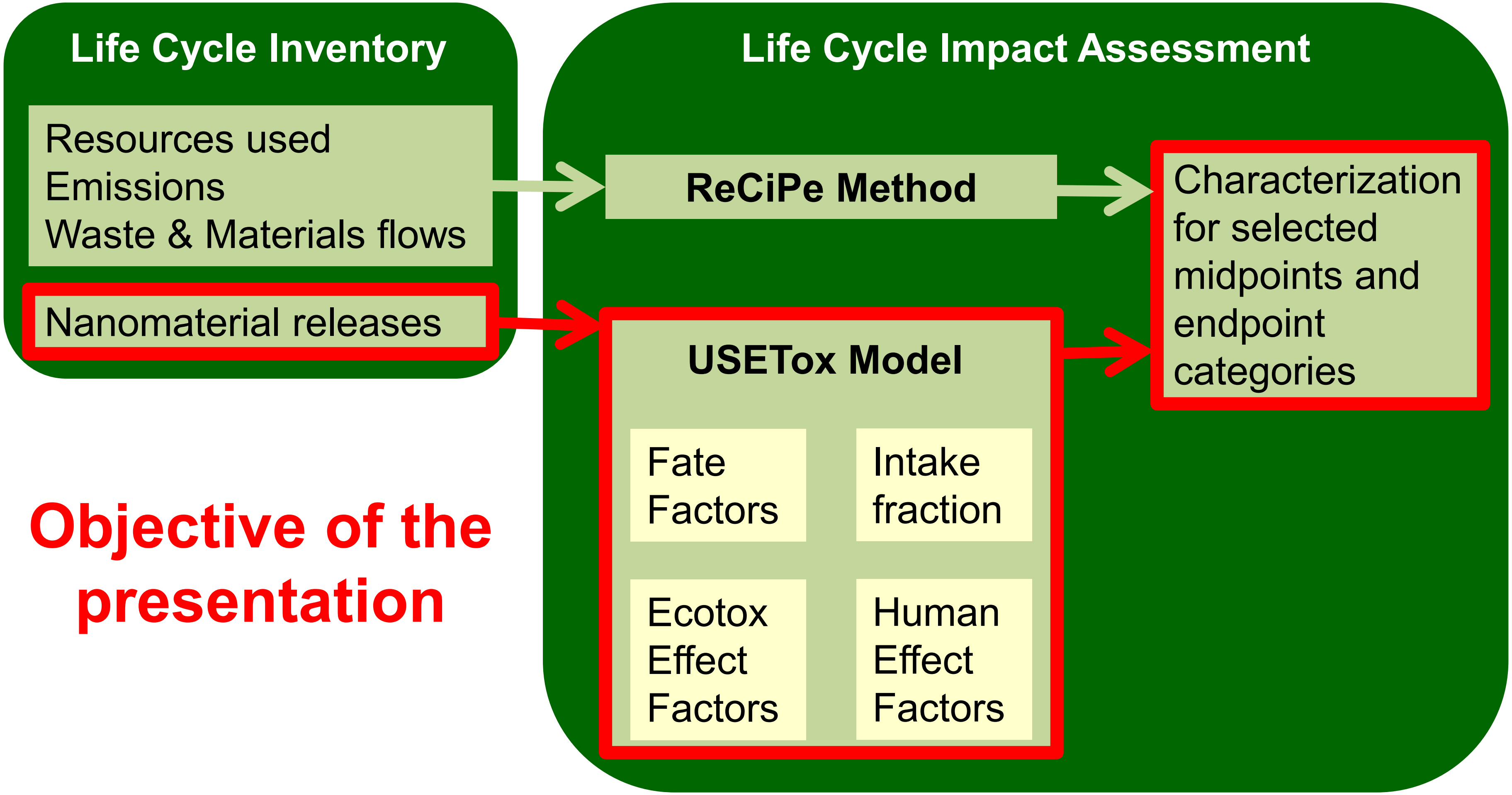
NM → freshwater ecotoxicity

* **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

# Goal and scope definition



# Goal and scope definition




**Objective of the presentation**

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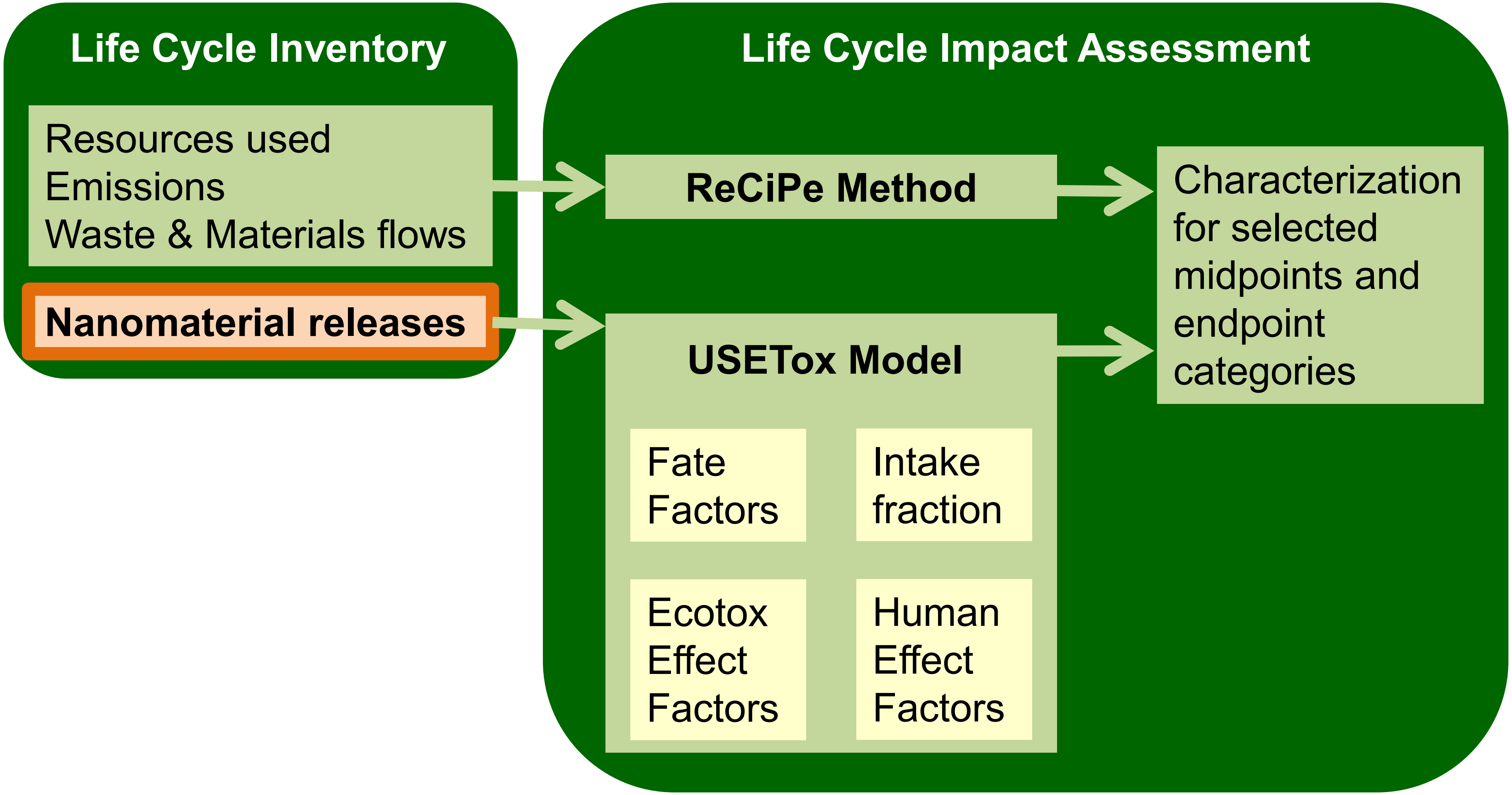
# Goal and scope definition

## Two scenarios proposed in the project

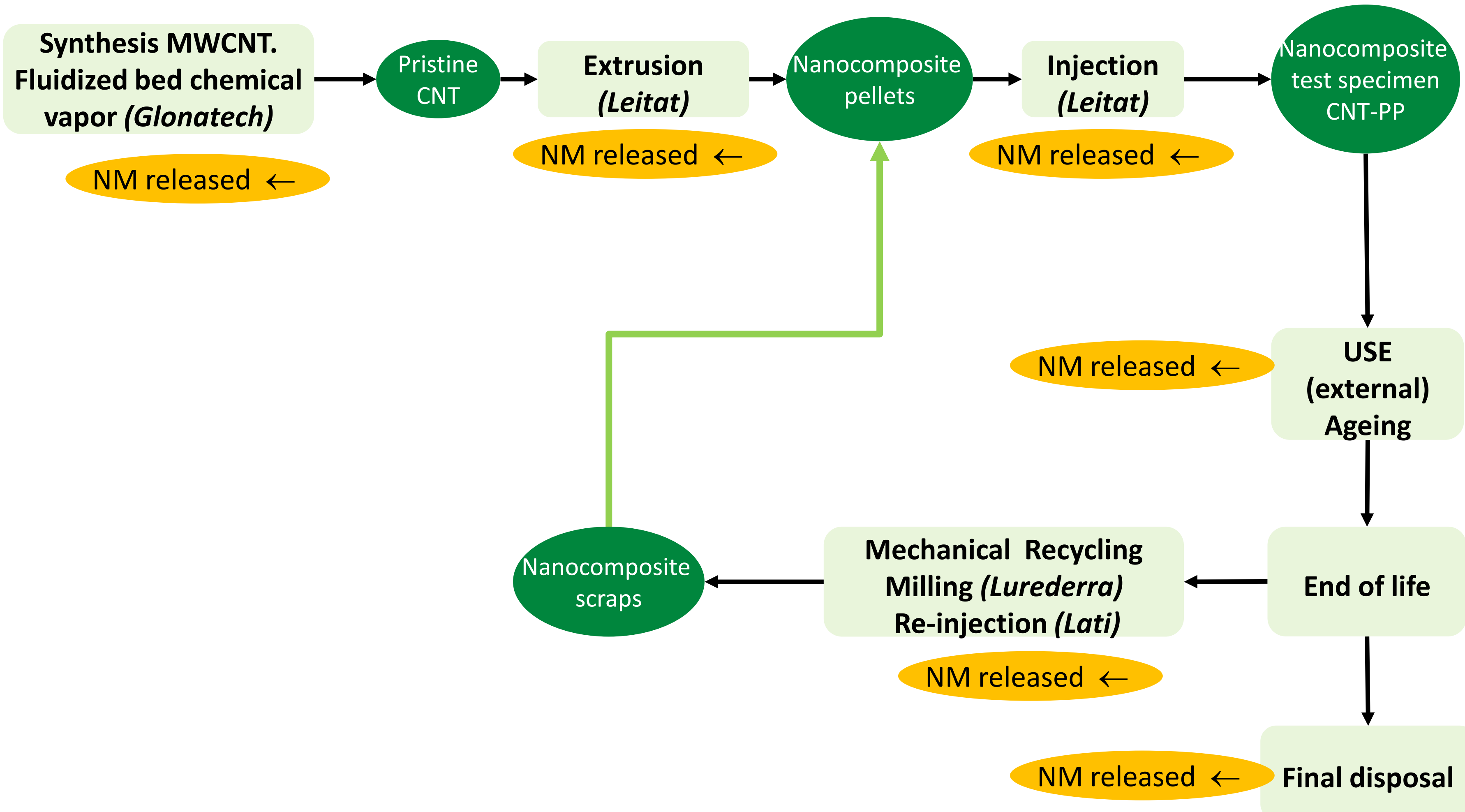
| Realistic | Worst-Case |
| --- | --- |
| Measured release | High release determined by ECHA Guidelines |
| Determined toxicity and ecotoxicity | Precautionary factors applied |
| Experimental characterization end-points or based on the media of results in the literature | Characterization end-points based on the worst-case in the literature (driving to longer persistence/bioaccumulation) |
| Low intake as shown in the literature | Precautionary factors applied |

# Goal and scope definition



# Life-Cycle Inventory

## Life-Cycle example: MWCNT-PP nanocomposites

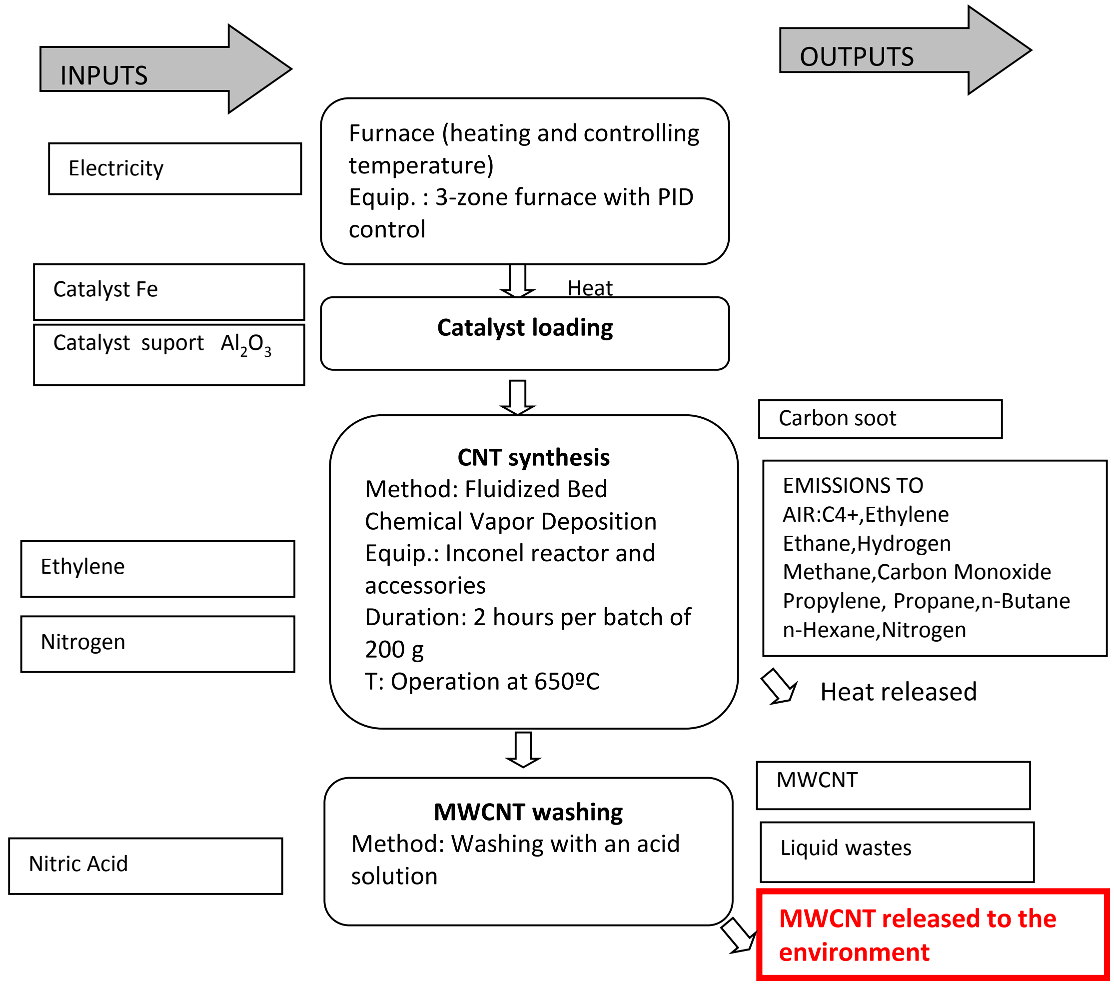


# Life-Cycle Inventory (LCI)
# Example: MWCNT - Synthesis

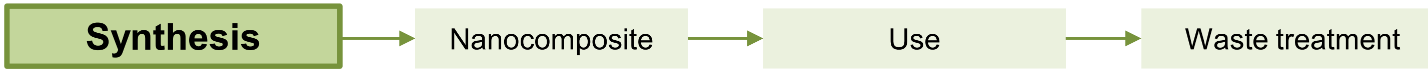
**Synthesis** → Functionalisation → Nanocomposite → Use → Waste treatment

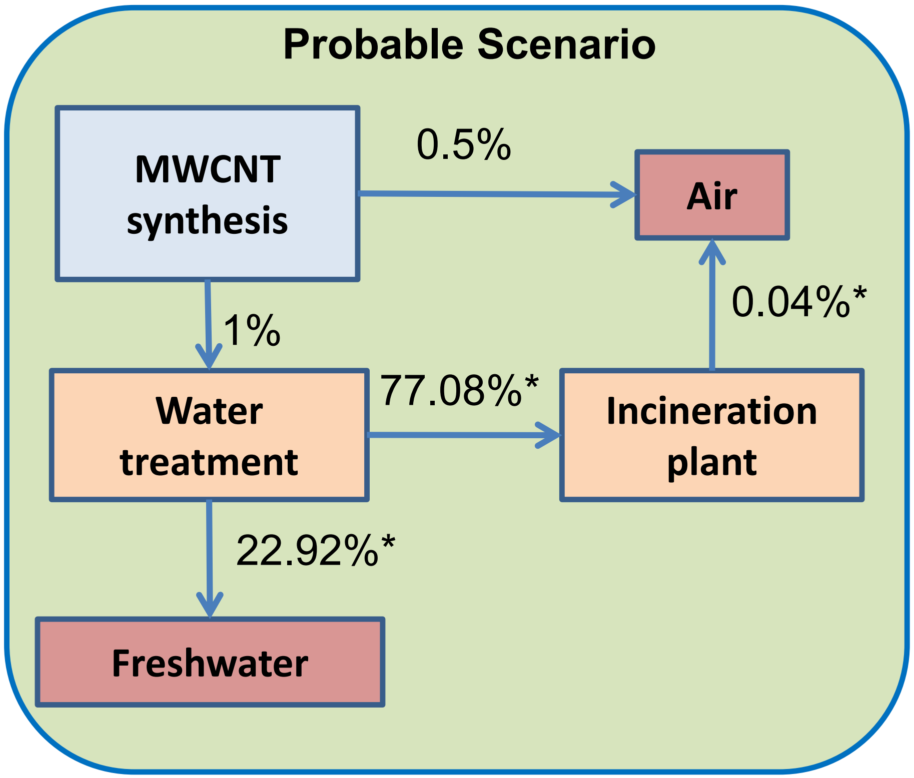
**Synthesis process**: fluidized bed chemical vapour deposition (CDV),

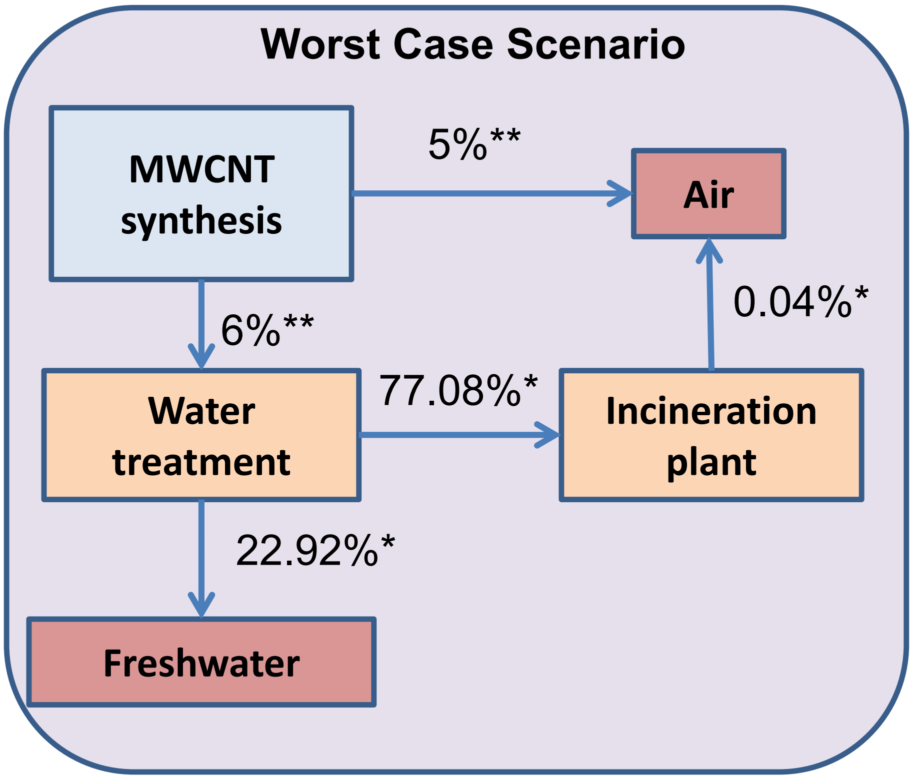
**Reference flow:** 30 g of multi-wall carbon nanotubes 97-98% (MWCNTs)
**Technology:** Semi-pilot unit. Glonatech



# 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

# Life-Cycle Inventory (LCI)
# Example: MWCNT@PP

## Release  of MWCNTduring 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 |

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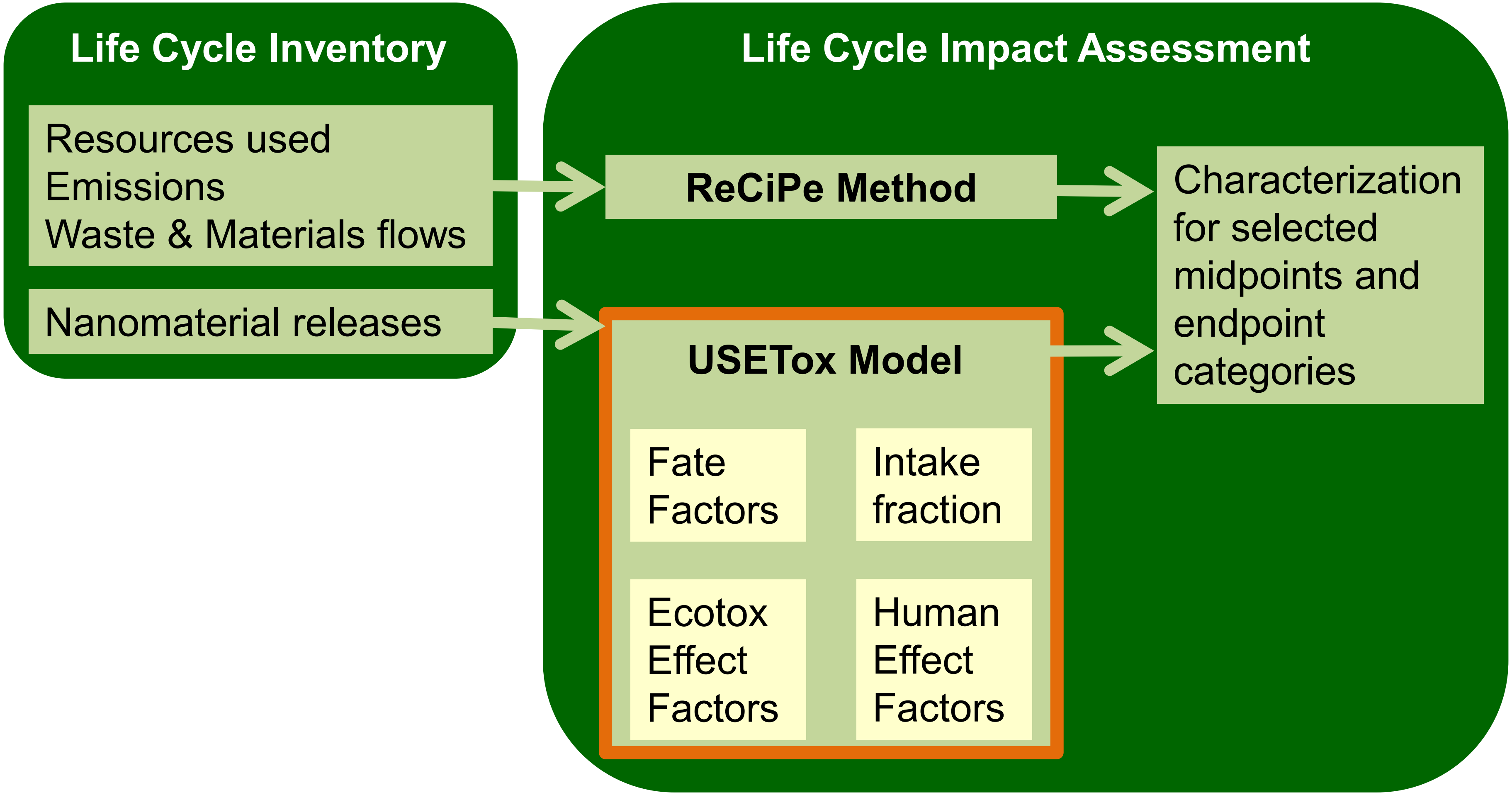
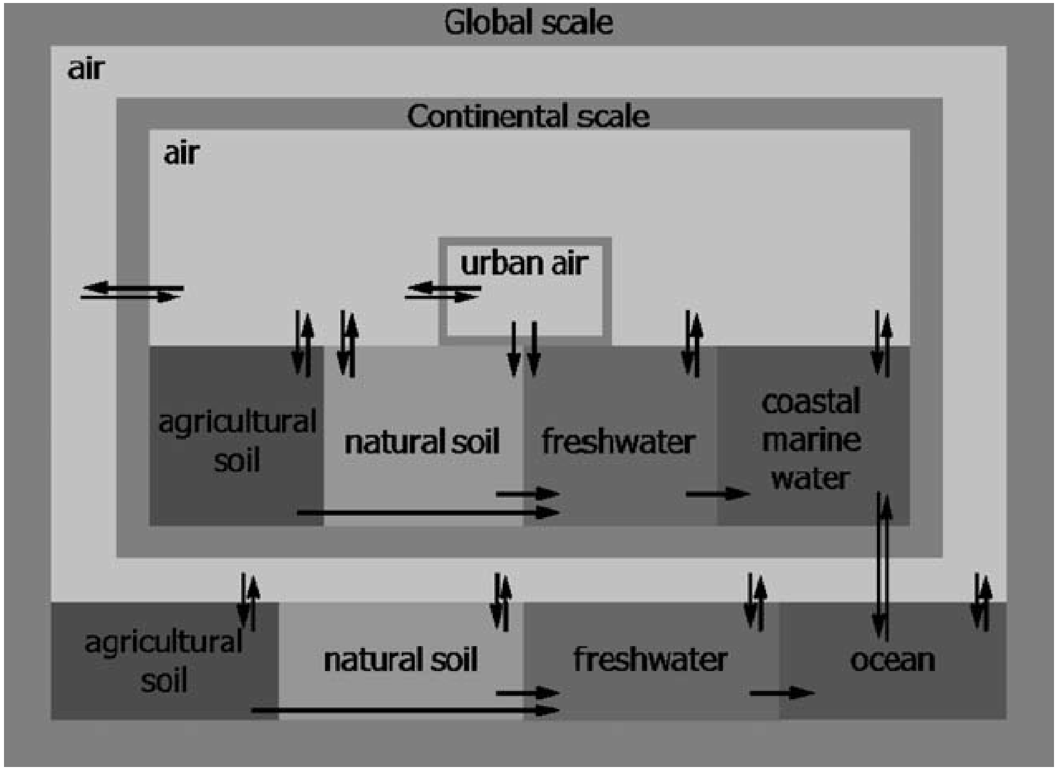
# Goal and scope definition



# Environmental distribution and intake

**USEtox™ is a toxicity model that integrates a multicompartimental fate model to calculate the environmental distribution of chemical compounds**: The tool combines the calculated Fate Factors (FF) with the Intake Factors (IF) to calculate the Human and Freshwater Ecosystem Exposures

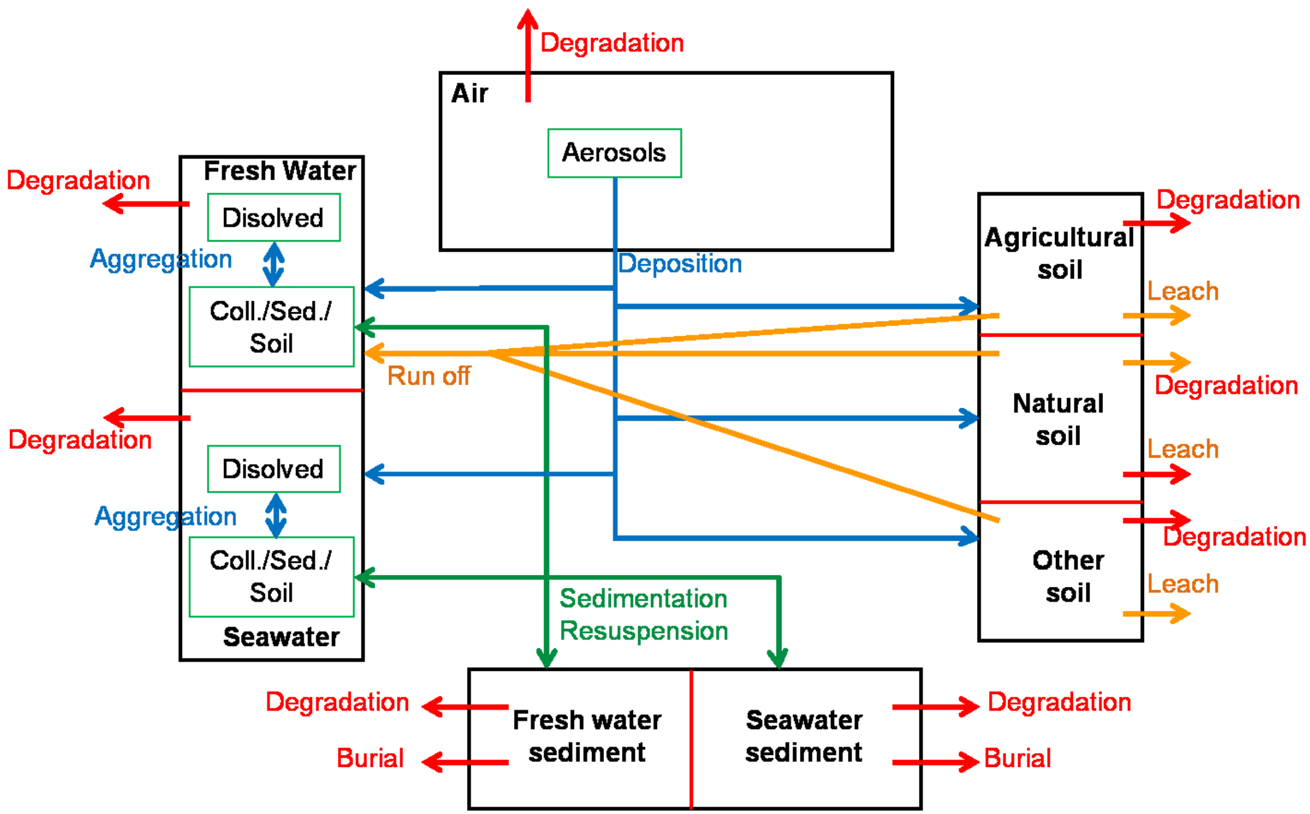



From Rosenbaum *et al*. Int. J. LCA, **2008,** 13, 532-546

# Environmental fate modelling

**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

Trans
mec
Dry De
Wet D
Gas a
Water
Run o
Degra
Metal




e,
rate

# Ecotoxicity and Human Toxicity Effect Factors

**Derivation following the general USEtox methodology.**

Main problems:

- (Eco)toxicity studies focused on most common nanomaterials.
- Tests done with the same material but different form (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/$kg_{emitted}$]:

| | *Emission to **urban air*** | | | *Emission to **cont. rural air*** | | | *Emission to **cont. freshwater*** | | |
|---|---|---|---|---|---|---|---|---|---|
| | 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/$kg_{emitted}$]:

| | *Emission to **urban air*** | | | *Emission to **cont. rural air*** | | | *Emission to **cont. freshwater*** | | |
|---|---|---|---|---|---|---|---|---|---|
| | 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·$m^3$·day/kg]:

| | *Emission to **urban air*** | *Emission to **cont. rural air*** | *Emission to **cont. freshwater*** |
|---|---|---|---|
| Average | 1,8E+02 | 1,8E+02 | 4,5E+02 |
| Worth Case | 4,6E+02 | 4,6E+02 | 1,2E+03 |

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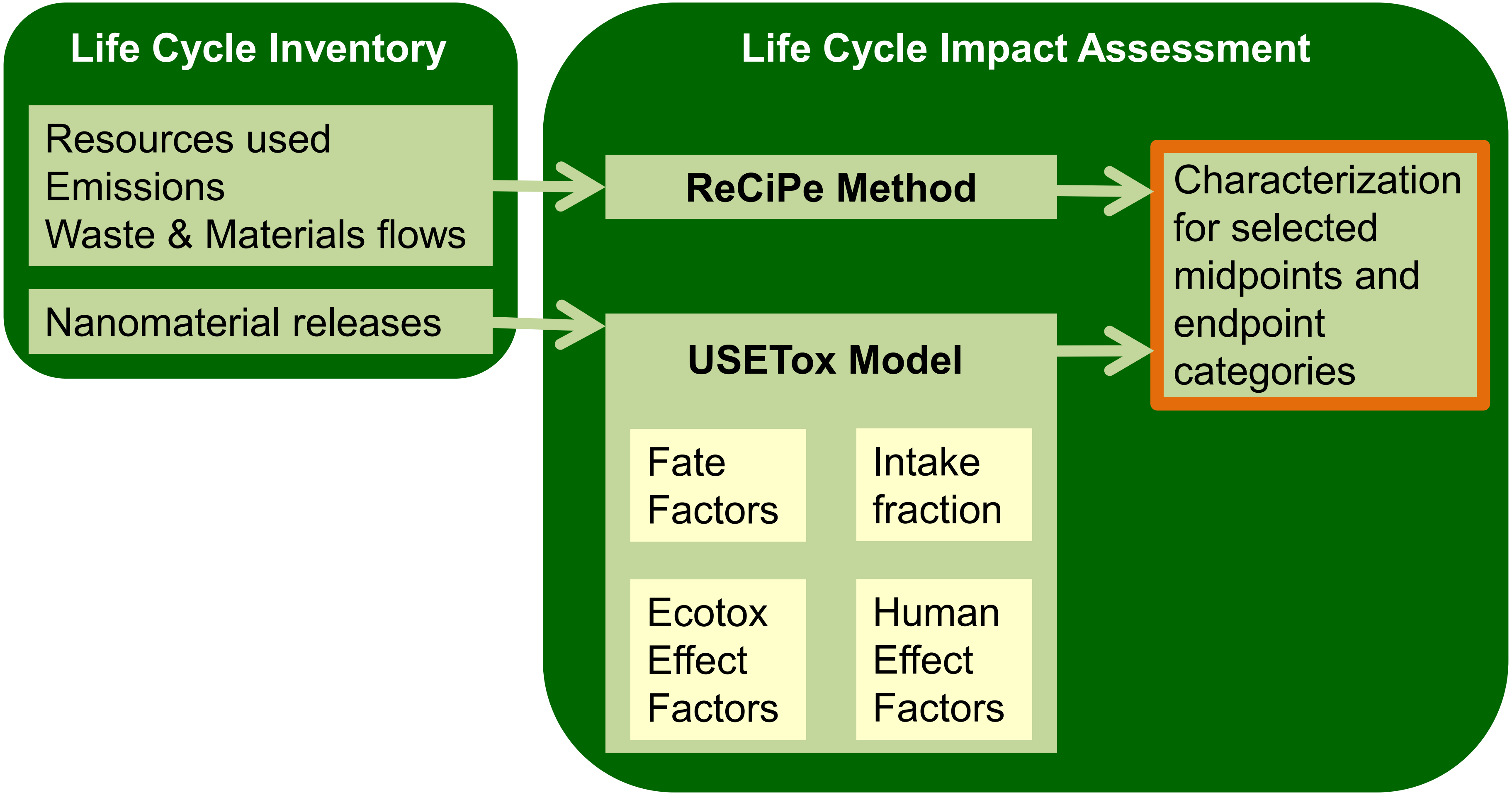
# Goal and scope definition



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

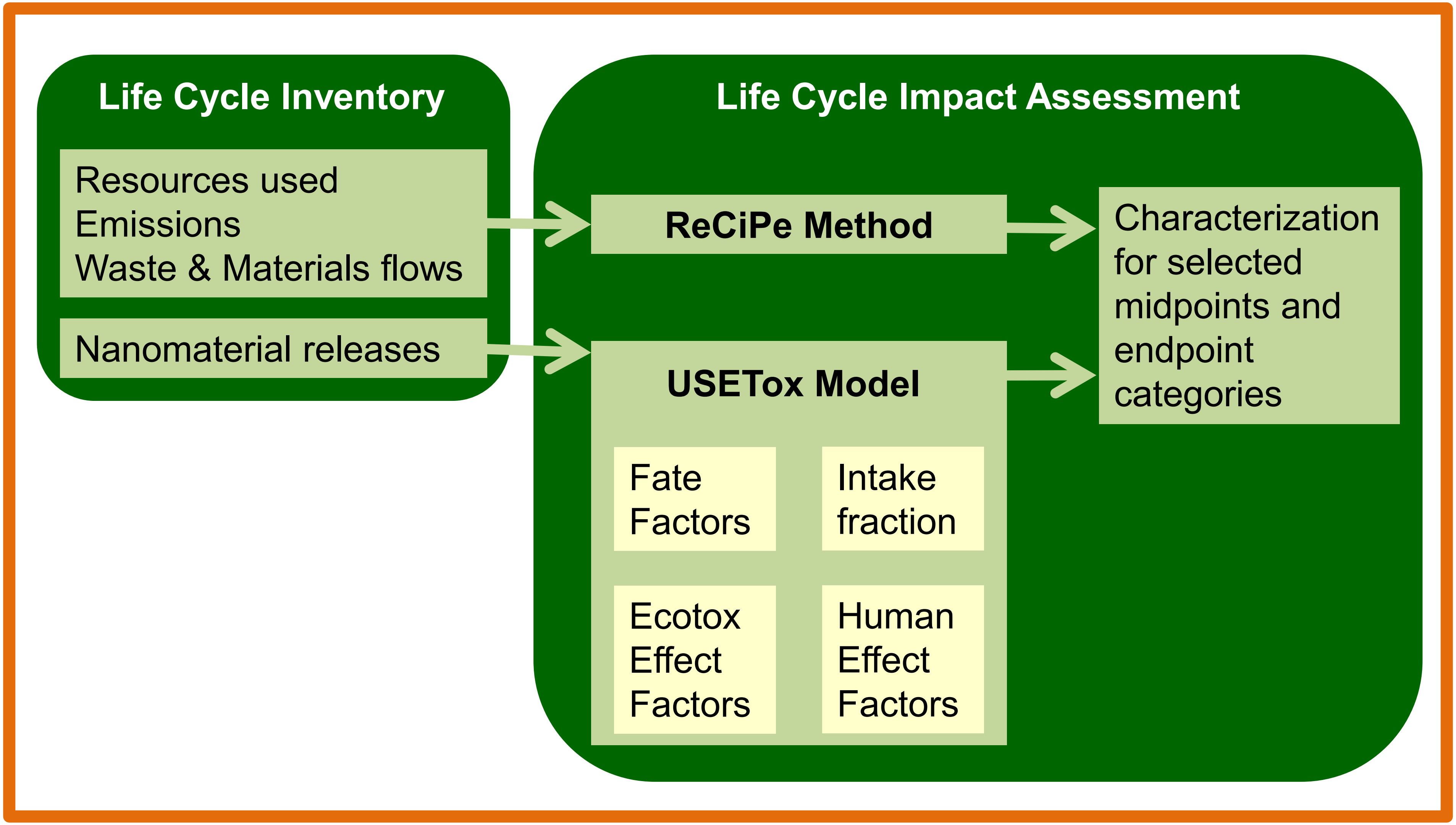
## Human health effect

| | | 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

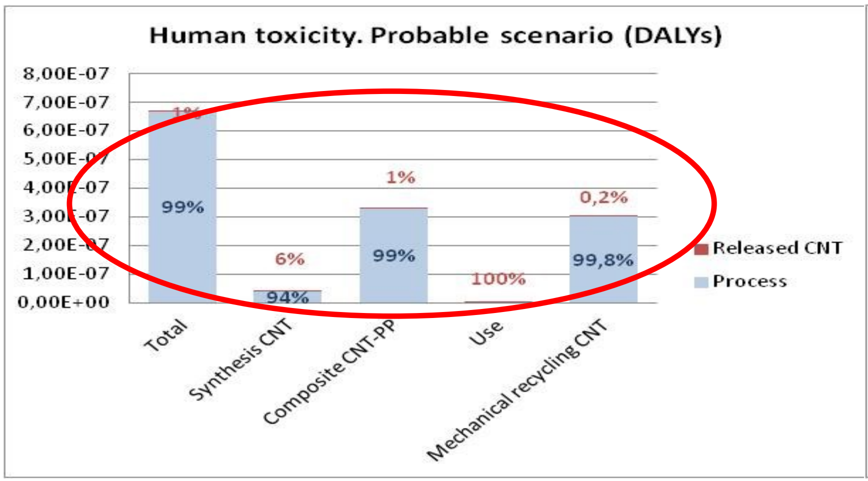
| | Probable scenario | | Worst case scenario | |
|---|---|---|---|---|
| | PDF·m³·day | species·year | PDF·m³·day | species*year |
| MWCNT synthesis | 6,58E-02 | 2,39E-13 | 1,51E+00 | 3,25E-12 |
| Nanocomposite synthesis | 3,06E-02 | 6,61E-14 | 5,84E-01 | 1,20E-12 |
| Use | 7,65E-03 | 1,65E-14 | 8,16E-02 | 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 |

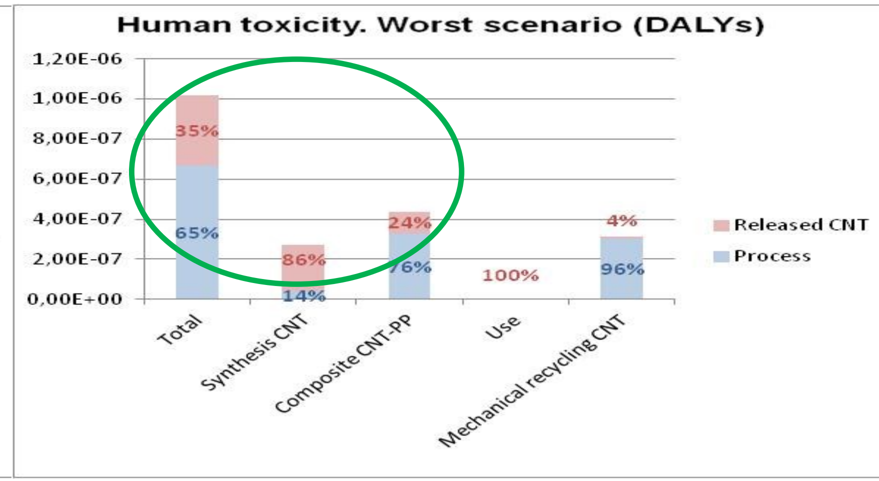
# Goal and scope definition

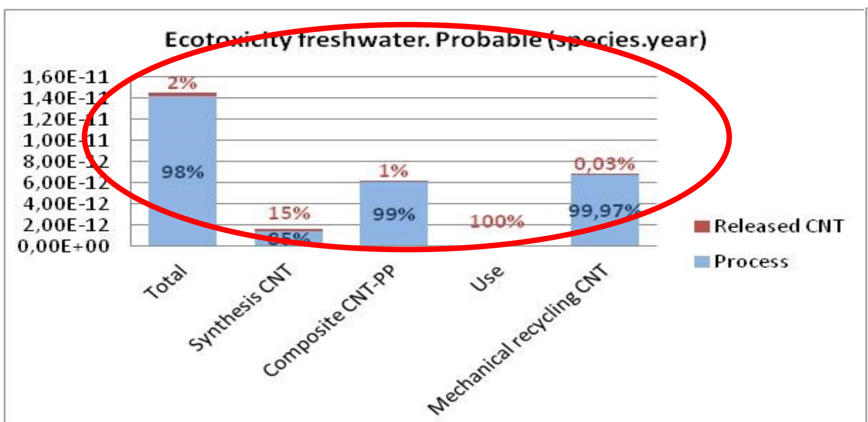


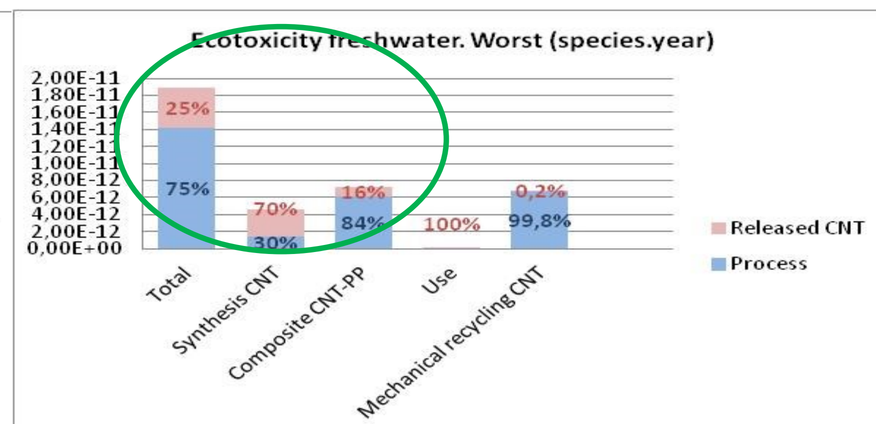
# LCIA (ReCiPe) MWCNT - Nanocomposite

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



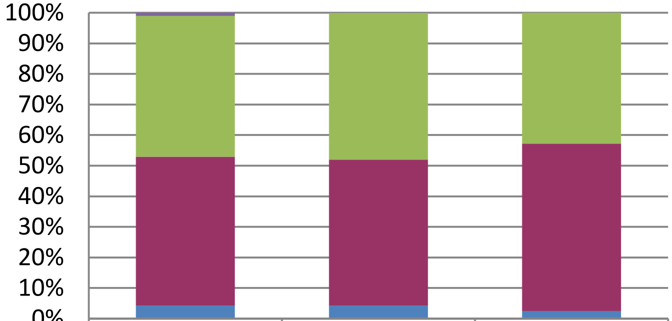



# LCIA (ReCiPe)
# MWCNT - Nanocomposite

**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<br>Human health | species.yr<br>Ecosystems | $<br>Resources |
|---|---|---|---|
| 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 | 97% |
| | 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 | $ | 0,004% |
| | 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 SOP for hazard, intake and bioaccumulation are necessary** to have good impact determination

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# ACKNOWLEDGMENTS


## Consortia

| | |
|---|---|
| L'Urederra Technological Centre (L'UREDERRA) | SPAIN |
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