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National Institute for Public Health
and the Environment
Ministry of Health, Welfare and Sport

SimpleBox4nano
Extension of regulatory accepted screening level fate model for use with nanomaterials

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2. From SimpleBox to SimpleBox4nano
3. Application of the model
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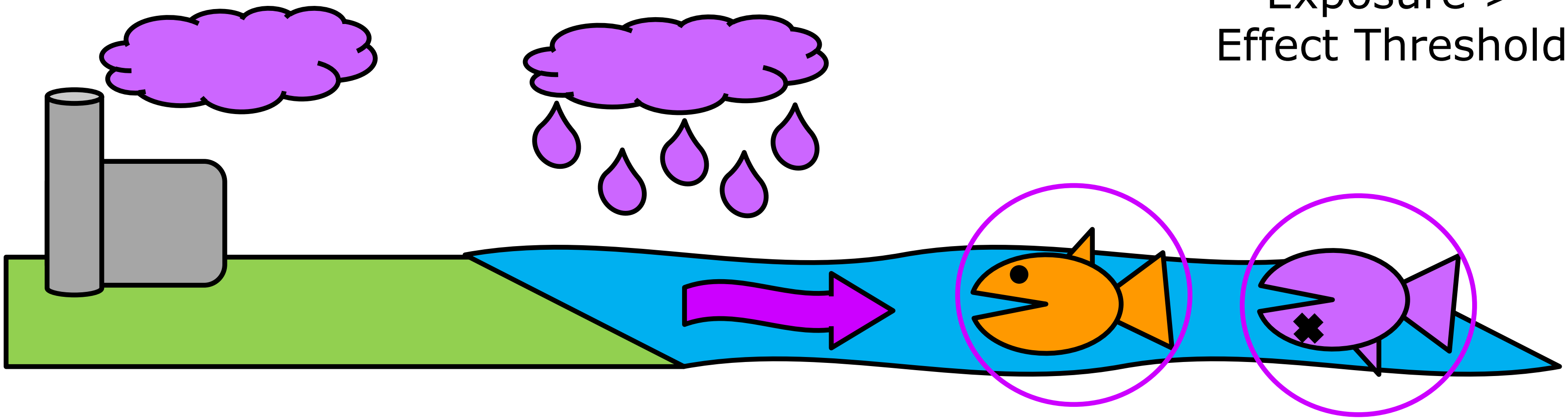
Environmental risk assessment of chemicals

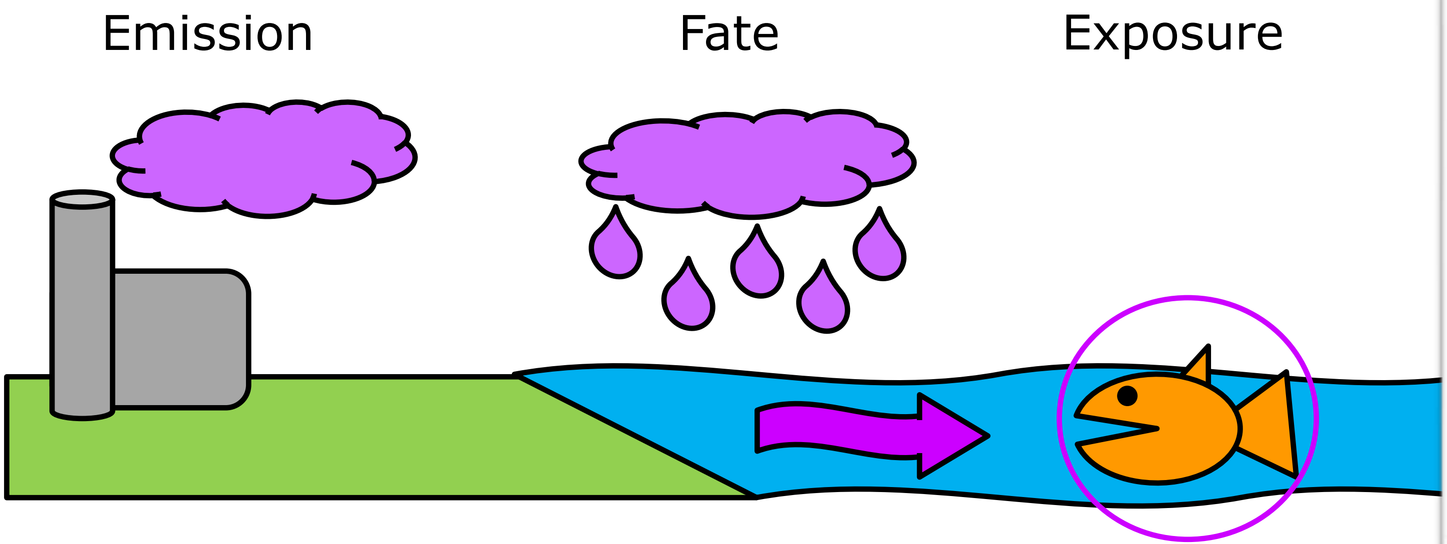
Emission | Fate | Exposure | Risk: Exposure > Effect Threshold



Part of REACH, REACH annexes being adapted for nanomaterials

ECHA EUROPEAN CHEMICALS AGENCY Anticipated that these changes come into force by 1-1-2020 v.d. Meent, et al. 2014

Environmental Exposure assessment

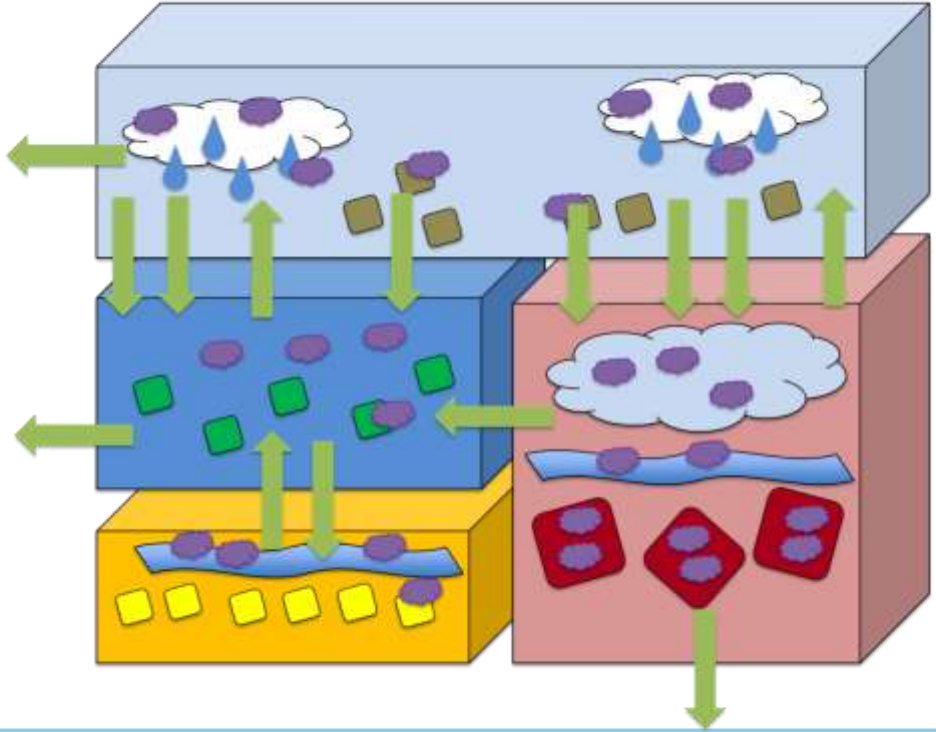


Tools available: the **European Union System for the Evaluation of Substances (EUSES)**, implemented also in ECETOC TRA and Chesar.

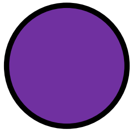
SimpleBox basis for EUSES Multimedia fate module

Multimedia fate model – SimpleBox 4.0

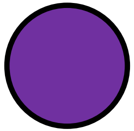
- Fate processes of chemicals
- Distribution over gas, liquid and solid media by thermodynamic equilibrium (partitioning)
- Not applicable to nanomaterials
  1. Thermodynamically unstable
  2. Dissolution as removal
  3. Transformation products



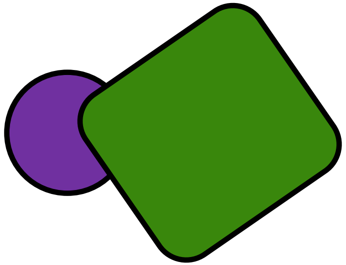
Adapting to fate of nanomaterials



Deposition



Dissolution

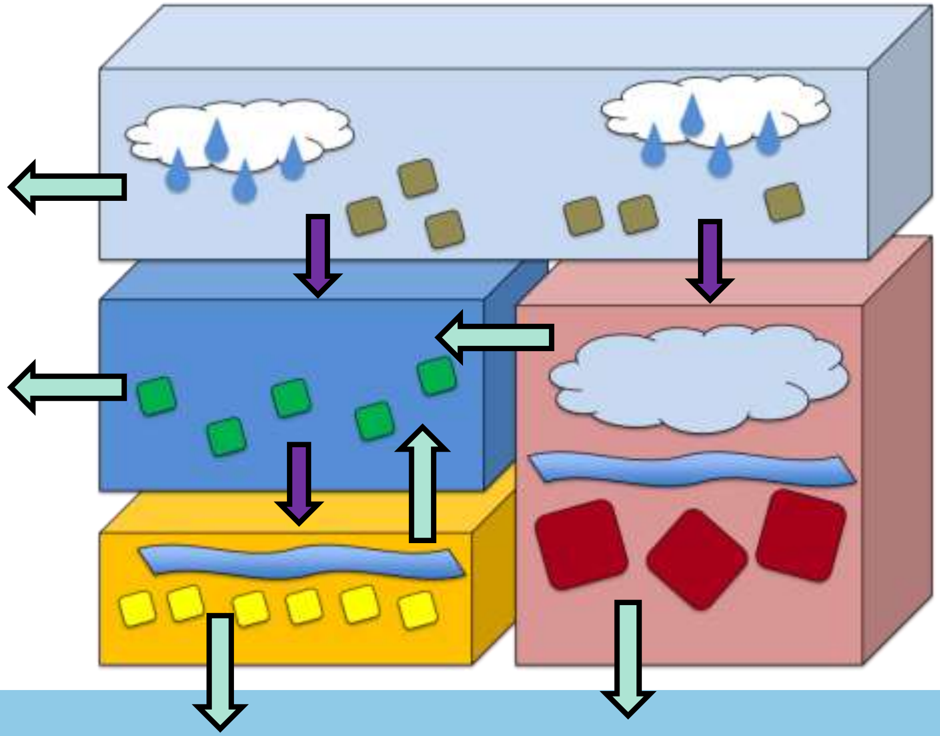


Attachment to natural particles

Use of process rate constants!

SimpleBox4.0-nano: Transport

- Deposition
- Advection
- No evaporation



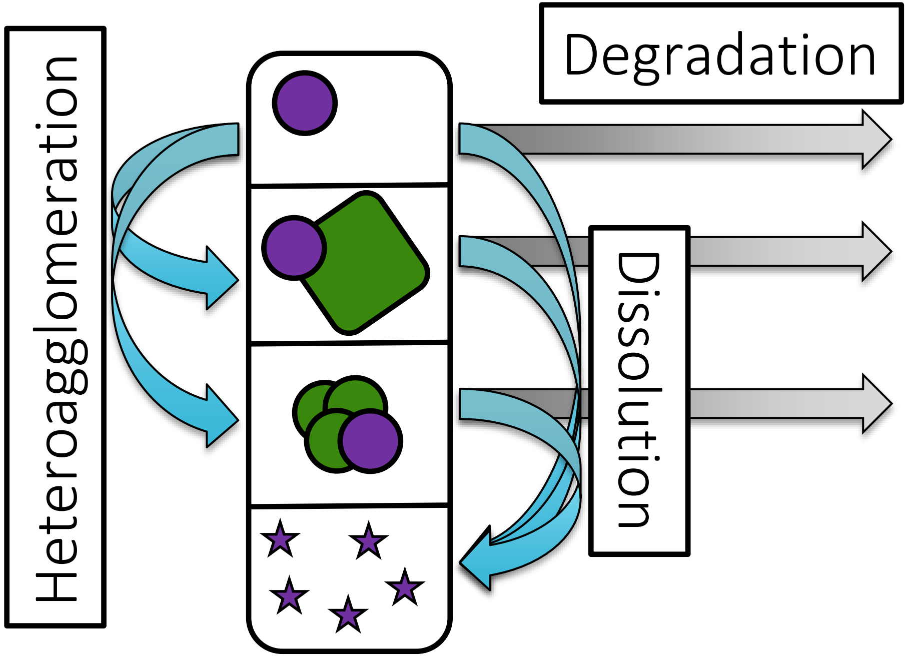
SimpleBox4.0-nano: Transformation

Nanoparticle (1-100 nm)

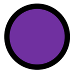
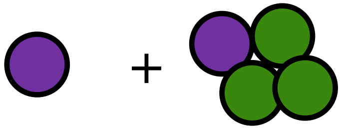
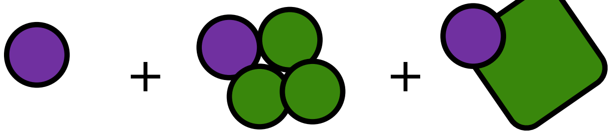
Colloidal heteroagglomerate (<450 nm)

Coarse heteroagglomerate (>450 nm)

Ion or dissolved metal



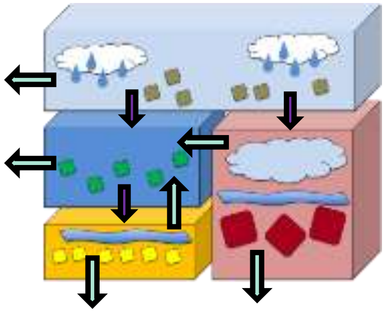
Nanomaterial concentrations

- Free: 
- Bioavailable:  (< 450 nm)
- Total: 
- Dissolved:  is no longer nanomaterial

SimpleBox4.0-nano - input

- Emission volumes to air, water, soil

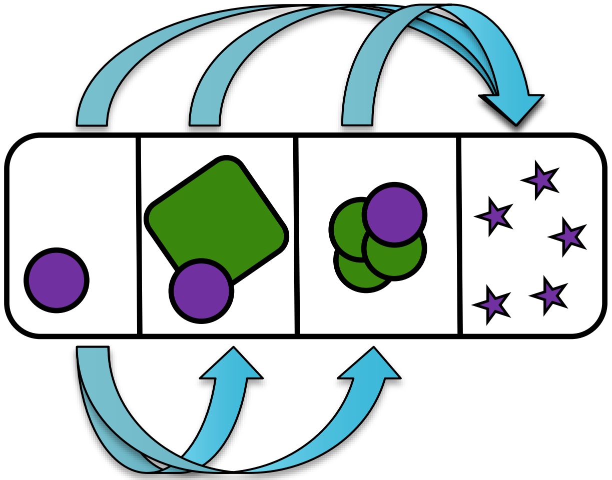
- Physicochemical properties
  - Size
  - Density
  - Attachment efficiency
  - Dissolution rate
  - Hamaker constant



- Landscape characteristics:
  - Natural particles
  - 3 scales: regio, continent, global
  - 3 water types: lake, river, sea
  - 3 soil types: agri., natural, other

Uncertainty/sensitivity of new aspects

- Uniform distributions:
  - Size of ENP (1 – 100 nm)
  - Attachment efficiency (10^{-4} – 1)*
  - Dissolution rate (s^{-1})*
    - Ag: 10^{-20} – 10^{-5}
    - TiO_2: 10^{-20} – 10^{-13}
    - C_{60}: 0
- Size and density PM (realistic)*



*Independent for each compartment and particle type ($PM_{<0.45}$ $PM_{>0.45}$)

Results

Variation in exposure concentration explained by:

ENP size

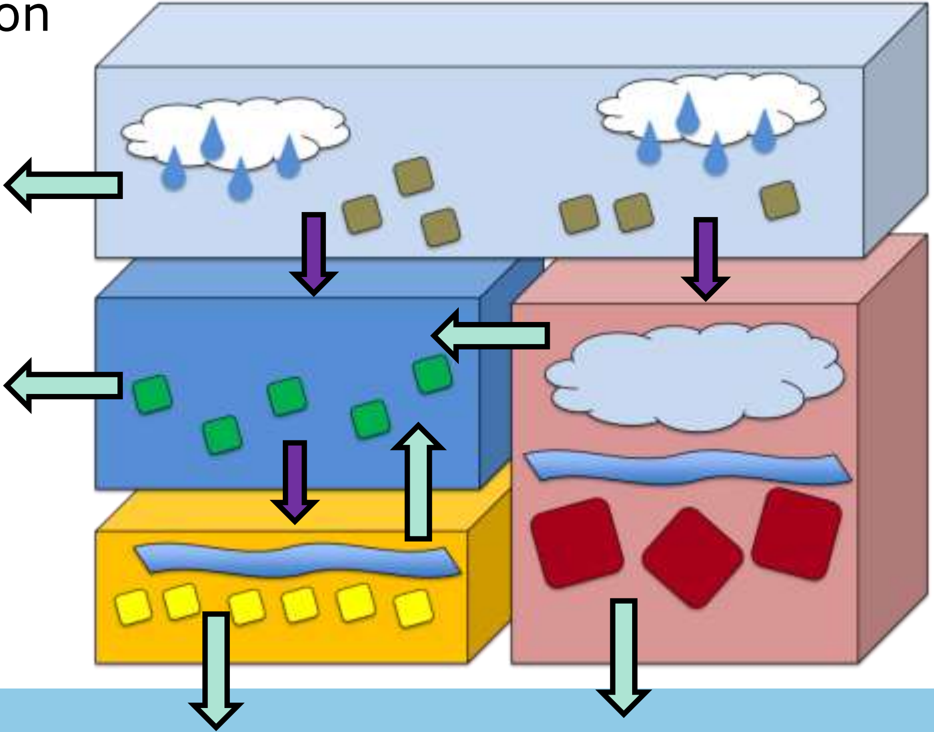
Aerosol size

Attachment Efficiency

Natural PM size and density

Dissolution rate (Ag only)

ENP size



How to find input parameters

- Attachment efficiency
  - Measure or calculate, base on methods in scientific literature and OECD dispersion stability TG 318
- Dissolution rate
  - Measure or expert judgement based on OECD TG (work in progress)
- Size and density primary ENP
  - Manufacturer data based on definition of nanomaterial
- Size and density heteroagglomerate/natural particle
  - measure and/or calculate, base on monitoring data and defaults
- Emission rates
  - Calculate from Production Volume, based on scientific literature (Sun et al. 2014 and Keller et al. 2013), in future update of EUSES emissions module.

Case Study – input parameters TiO_2, C_{60}, Ag ENPs

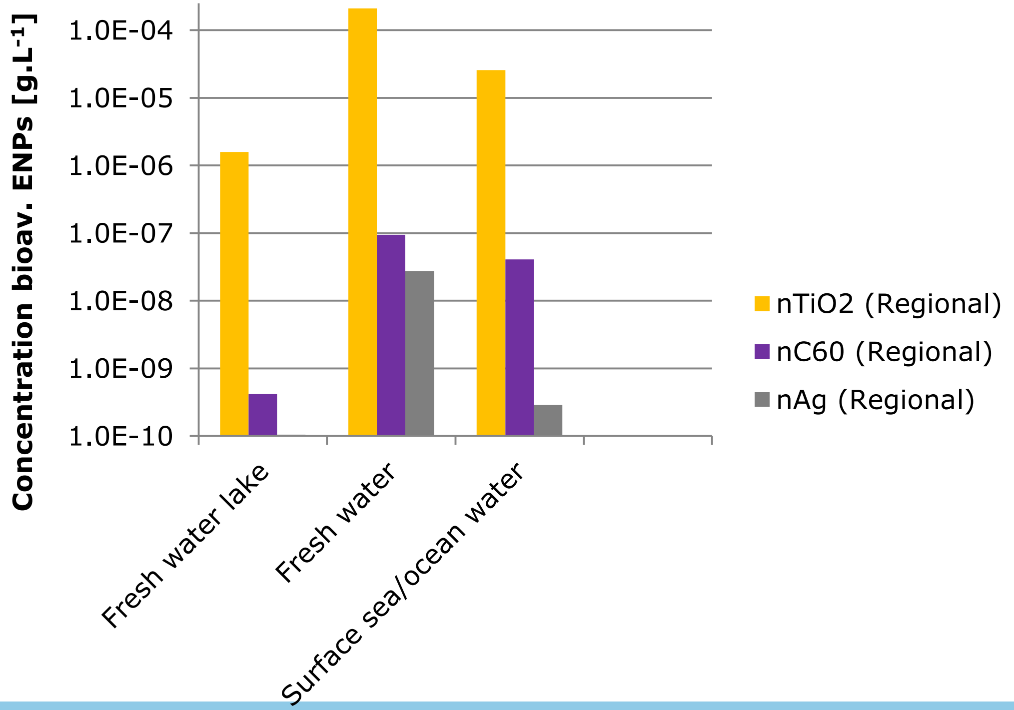
Hypothetical	$nTiO_2$	nC_{60}	nAg
Diameter (nm)	10	10	10
Density ($kg\ m^{-3}$)	4230	1650	10500
Hamaker (J)	6.9×10^{-21}	2.76×10^{-20}	2.02×10^{-20}
Attach. Eff. (ENP-PM)	0.02 – 1	0.01 – 1	0.045 – 1
Dissol. rate (s^{-1})	10^{-13}	0	10^{-7} – 10^{-5}
Production Volume (t/y)	42000	90	90

Best estimate

Results – water compartments

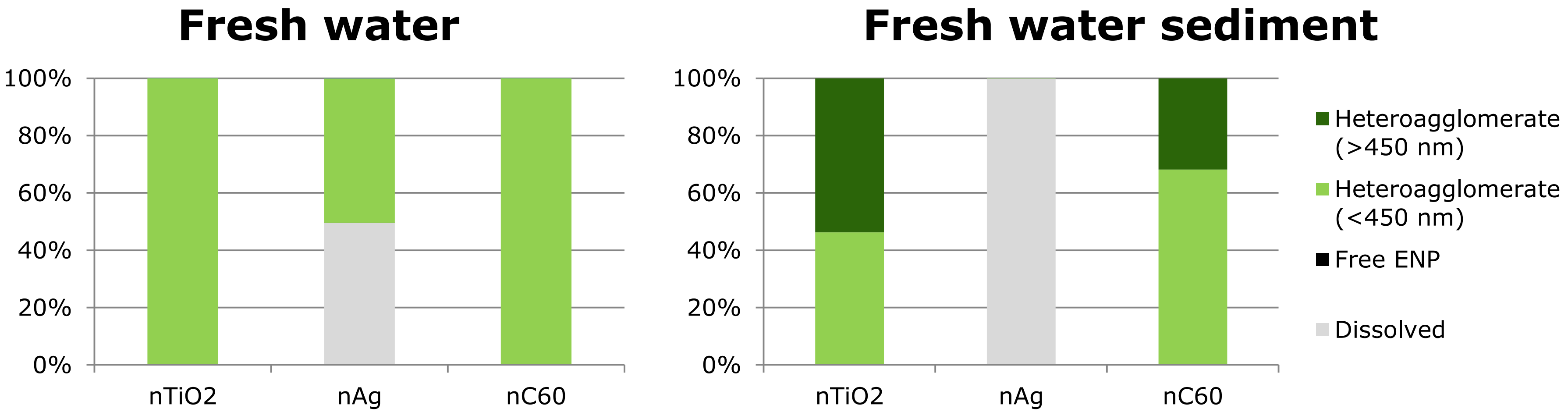
- Highest concentration for $nTiO_2$ compared to nC_{60} and nAg
  - Explained by difference in **production volume**:

    42000, 90, 90 t/y of $nTiO_2$, nC_{60} & nAg, respectively
- Concentration nAg lower than nC60 with similar PV, mainly due to **dissolution** process



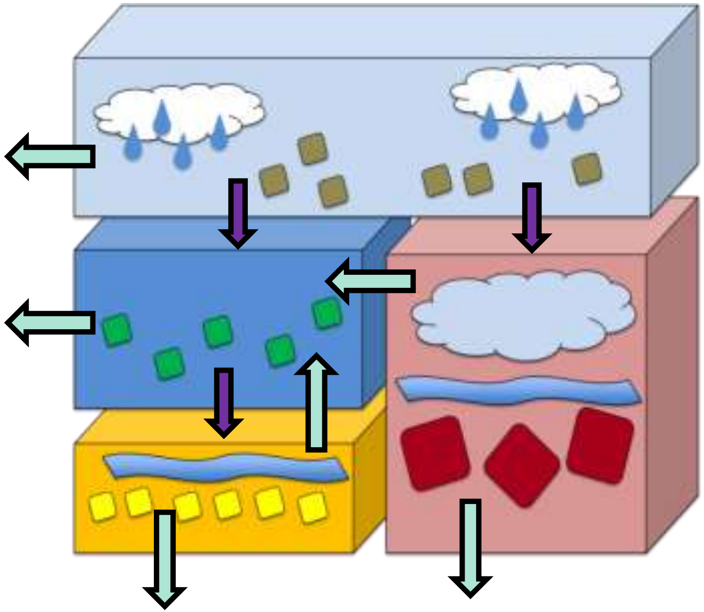
Results - speciation

- $nTiO_2$ and nC_{60} heteroagglomerates (<450 nm) dominate freshwater dissolved split with heteroagglomerates (<450 nm) for nAg
- Also $nTiO_2$ and nC_{60} heteroagglomerates (>450 nm) in sediment



Conclusion

- Required adaptations for nanomaterials included
- SimpleBox4.0-nano operational
- Dissolution, attachment efficiency and size most important input
- Environmental modeling of nanomaterials is feasible



Outlook

- Further work on SimpleBox4nano:
  - Improve usability
  - Extend database of parameters

- Nanomaterial specific information requirements
  - Anticipated to go into effect in 2020

- 4-5 june 2018, ECHA workshop on EUSES update: https://echa.europa.eu/nl/-/workshop-on-euses-update-needs

Free to use

Download here

Further inquiries:
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NanoFASE Fate and Exposure models for you - www.nanofase.eu

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Litterature

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