Exposure Assessment and Modelling, NanoFASE– Intentions, Achievements and Outcomes

Claus Svendsen & 65 others

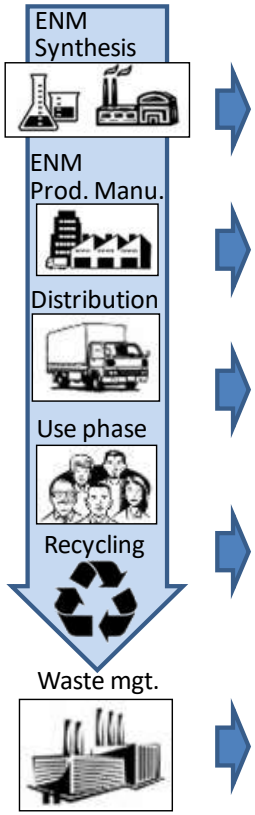
UKRI-CEH, Wallingford, United Kingdom

NOTA BENE – *Some slides highlight scientists who presented related papers at ICEEN. Collaborators are recognized! Visit our online library.*

Exposure assessment in the environment:

How much is released and where does it go?

1) ENM enabled Product value chains & release pathways



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Chapter R.16: Environmental exposure assessment

Version 3.0 – February 2016

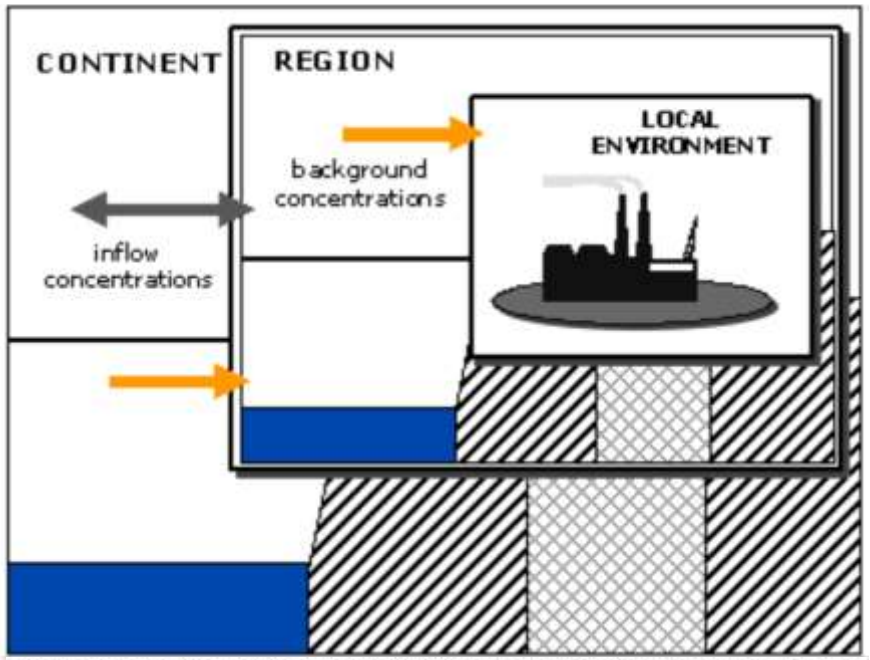

Figure R.16-7: The relationship between the continental, regional, and local scales

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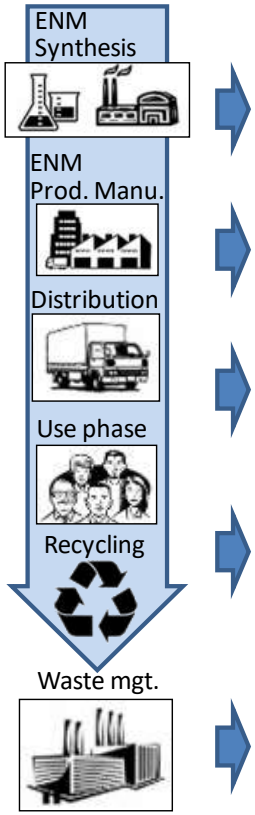

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Chapter R.16: Environmental exposure assessment

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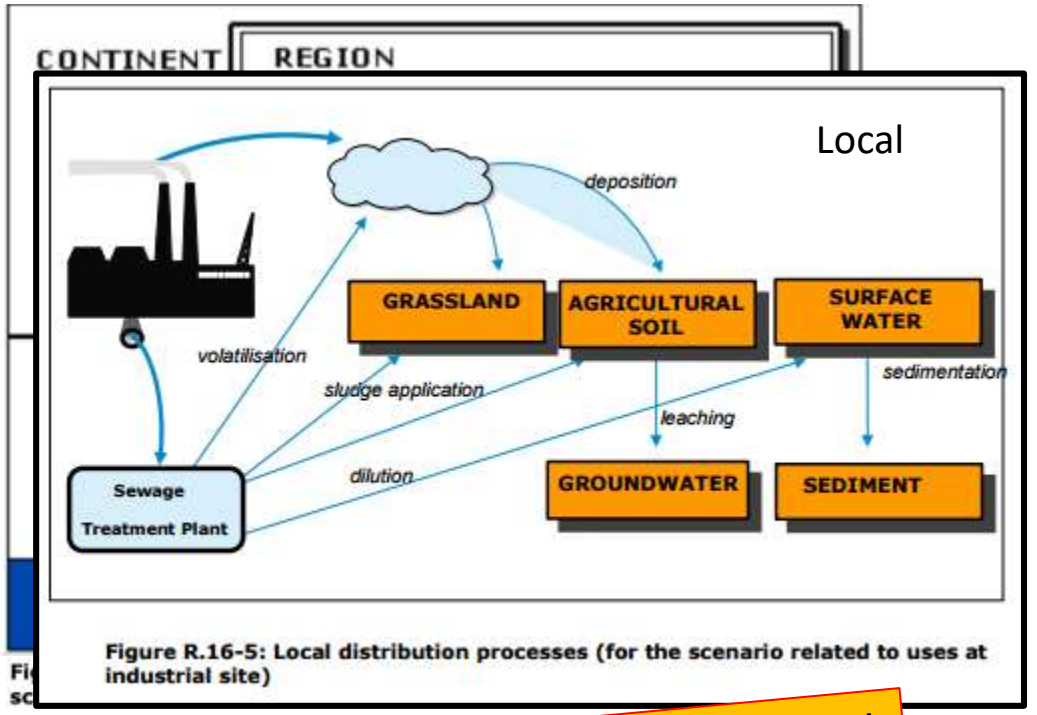

Figure R.16-5: Local distribution processes (for the scenario related to uses at industrial site)

REMEMBER – THIS IS THE GOAL!

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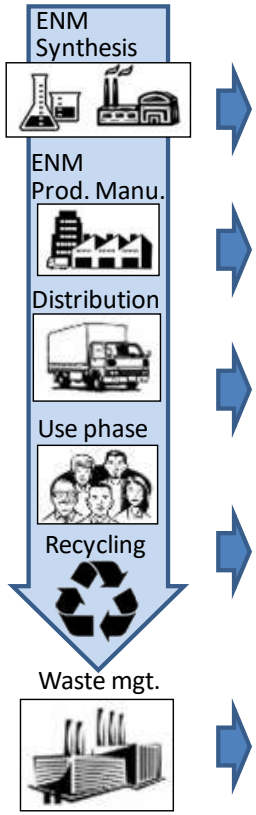
1) ENM enabled Product value chains & release pathways



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Chapter R.16: Environmental exposure assessment

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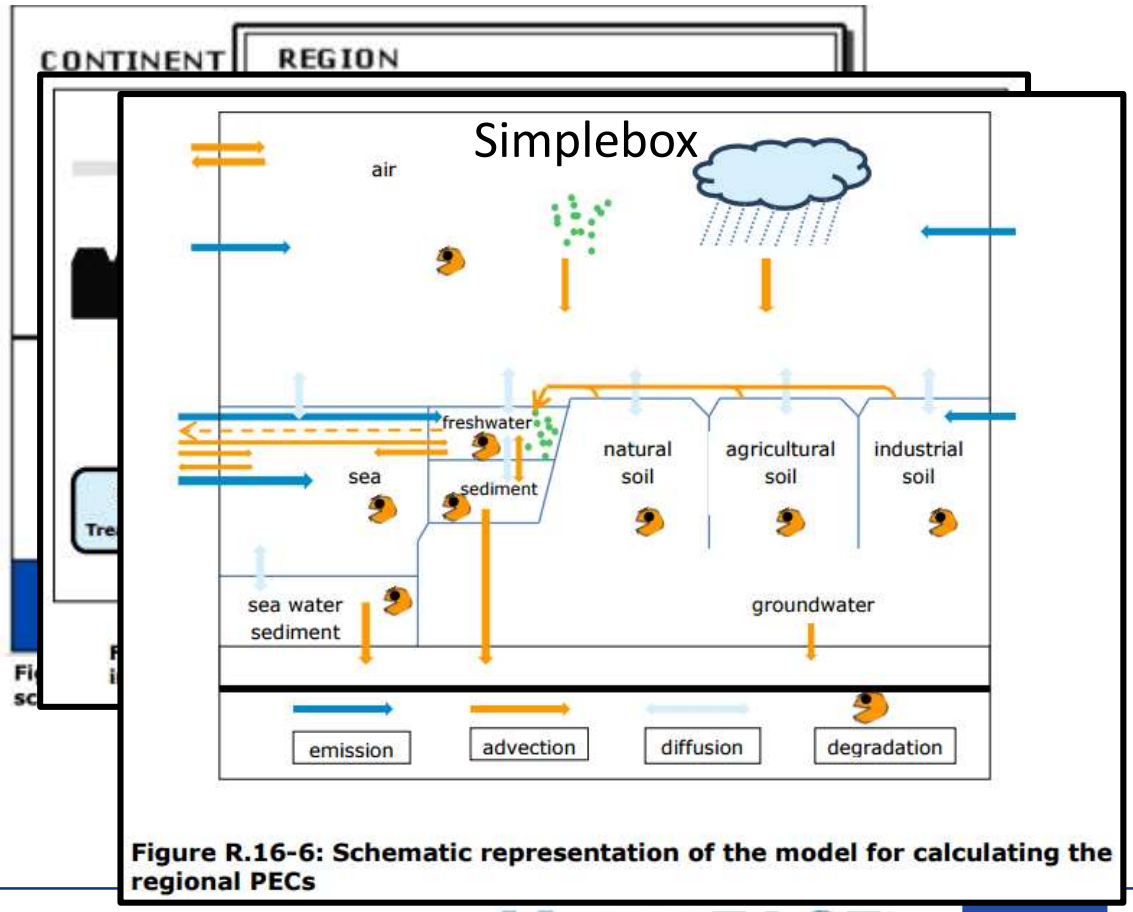

Figure R.16-6: Schematic representation of the model for calculating the regional PECs

Exposure assessment in the environment:

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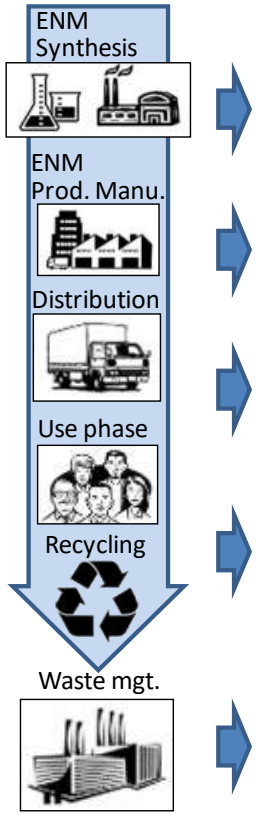

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Chapter R.16: Environmental exposure assessment

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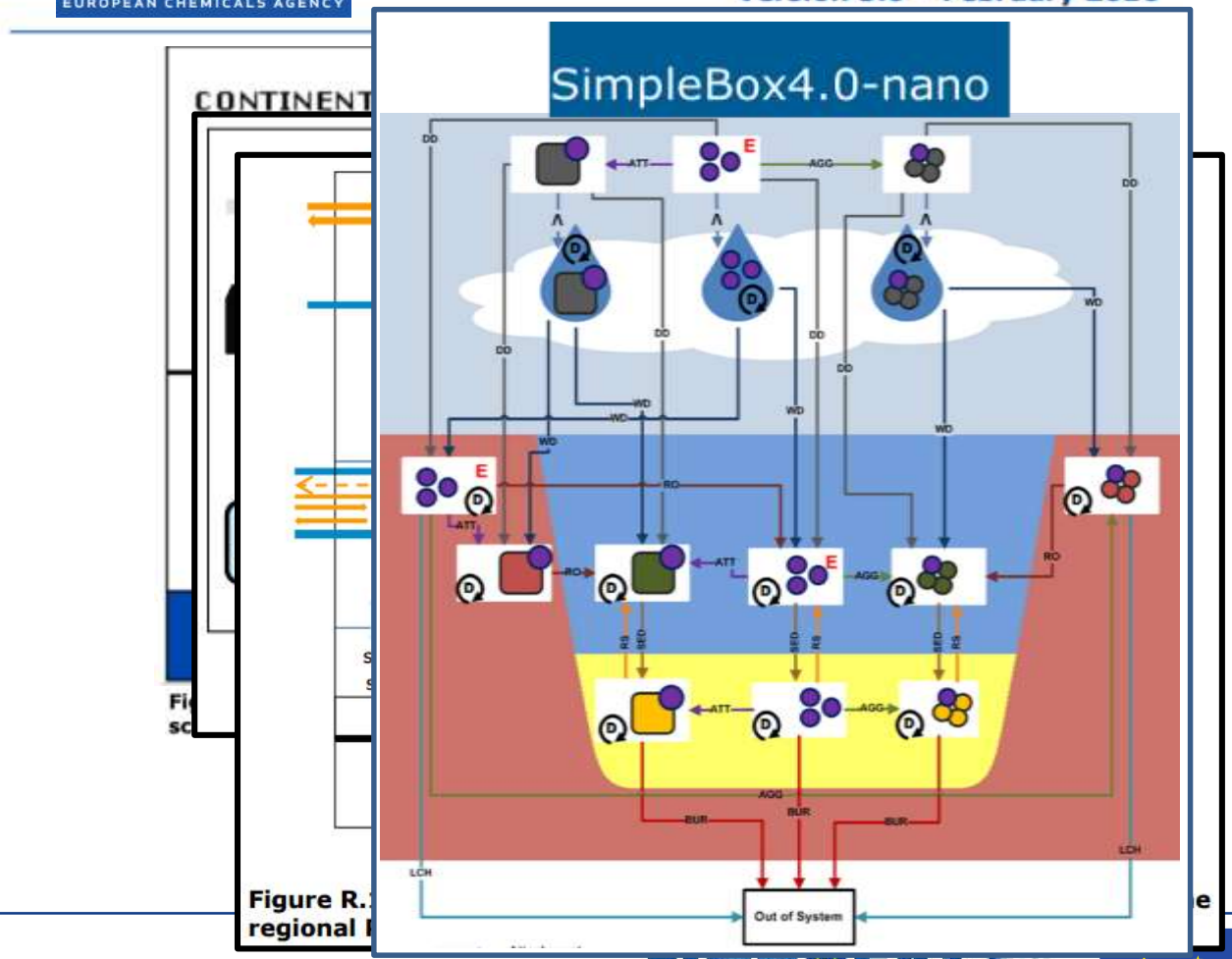
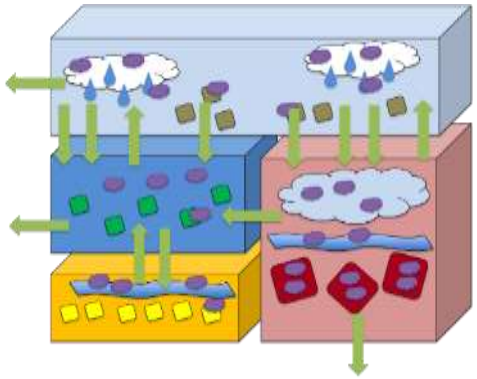


Putting the models together and comparing

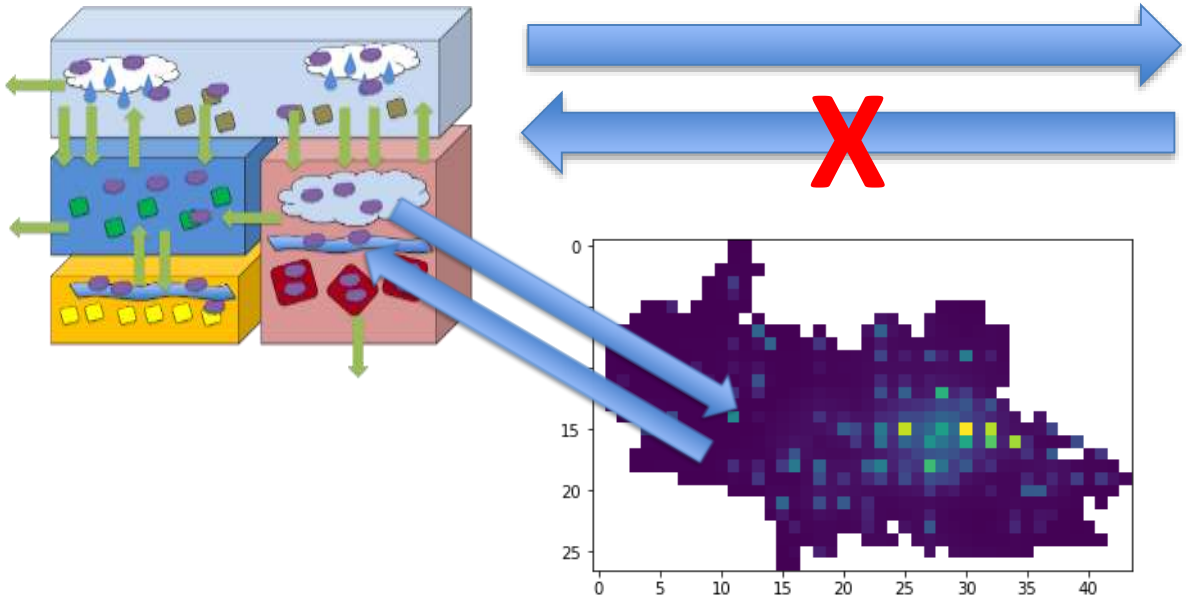
Towards validating nanomaterial PECs from SimpleBox4nano using the NanoFASE-WSO spatiotemporal multimedia fate model



SimpleBox4nano
Screening level
Steady state conditions
Regional to continental scale
Background, regional concentrations

Putting the models together and comparing

Towards validating nanomaterial PECs from SimpleBox4nano using the NanoFASE-WSO spatiotemporal multimedia fate model



SimpleBox4nano	NanoFASE Water-Soil-Organism
Screening level	Higher tier
Steady state conditions	Time explicit
Regional to continental scale	Gridded: 5x5 km
Background, regional concentrations	Local concentrations

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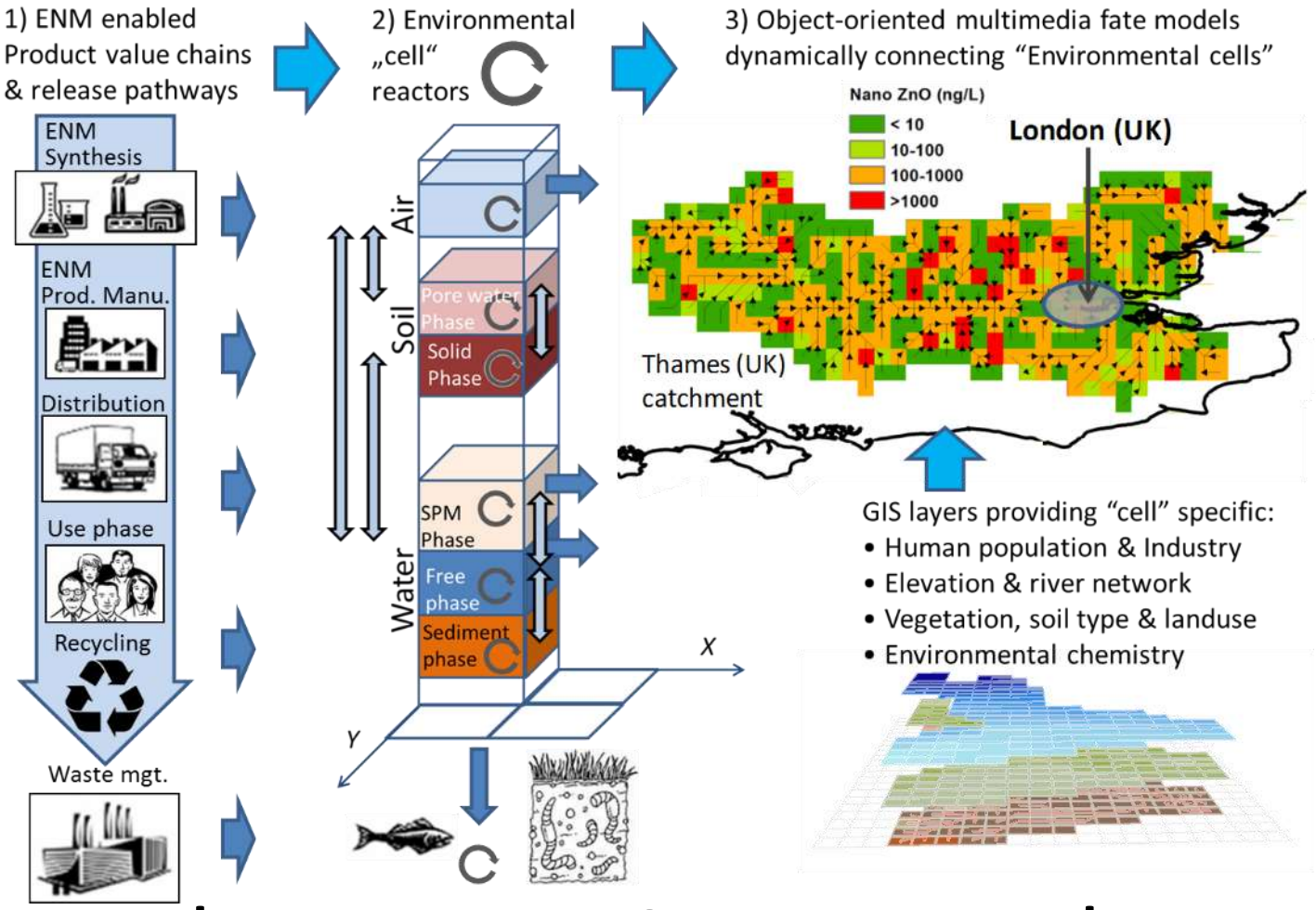

The NanoFASE Approach

Centre for Ecology & Hydrology
NATURAL ENVIRONMENT RESEARCH COUNCIL

NanoFASE

Exposure assessment (of Nano) in the environment:

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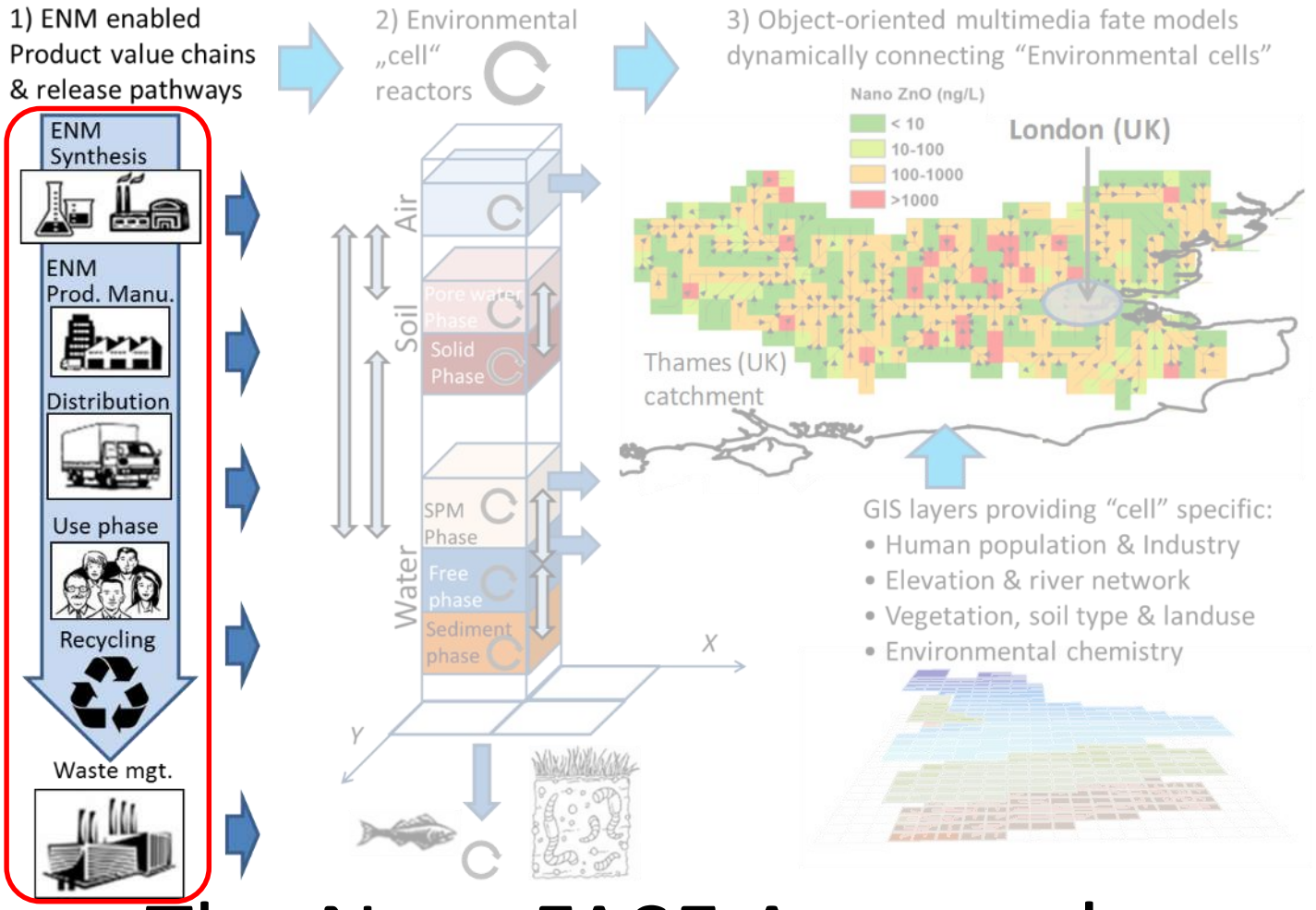


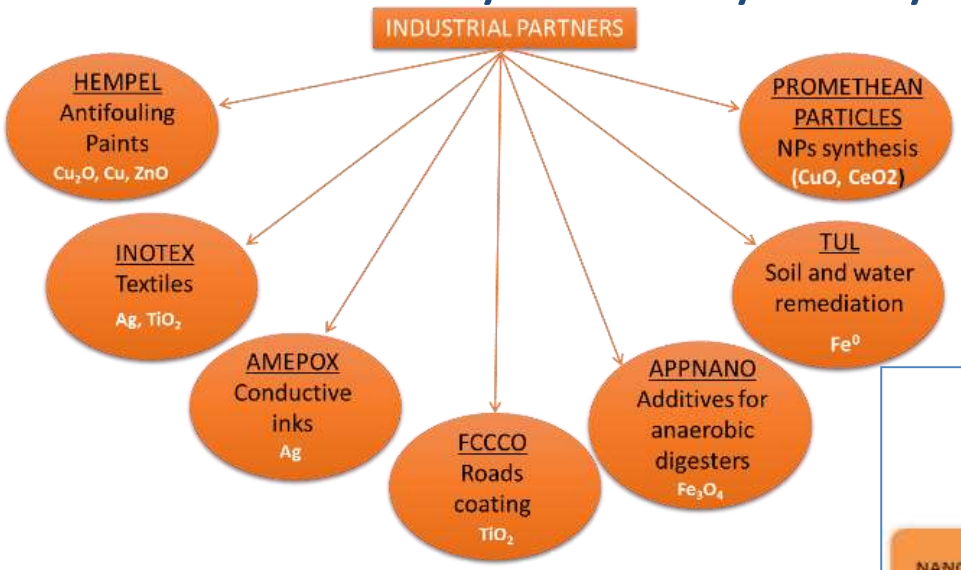
The NanoFASE Approach

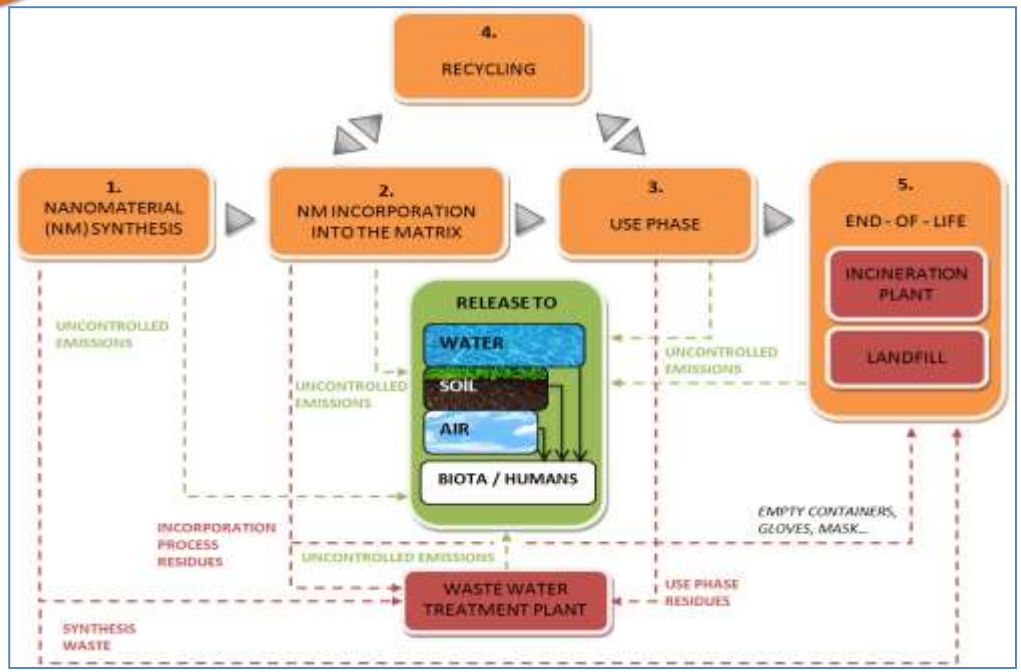
Centre for Ecology & Hydrology
NATURAL ENVIRONMENT RESEARCH COUNCIL

NanoFASE

Charting nano releases and forms from products

- Case Study Pathway Analysis to guide experiments





Nano Product value chain and release paths (WP4)

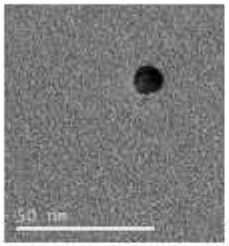
SILVER TEXTILES

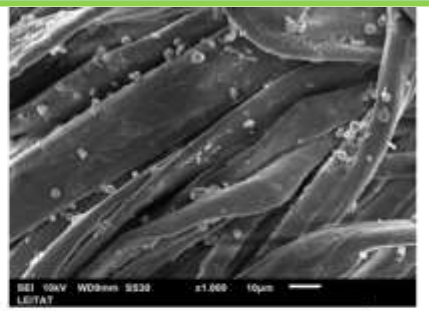
4. RECYCLING

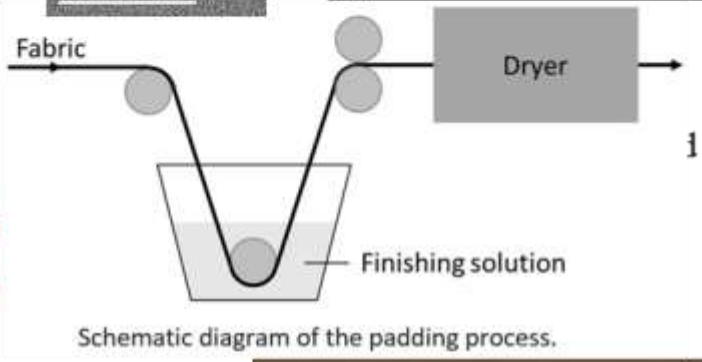
1. Ag NPs WET SYNTHESIS

2. 2.1 NPs INCORPORATION INTO DISPERSION
2.2 COATING PROCESS

3. USE PHASE







Schematic diagram of the padding process.

RELEASE DURING USE PHASE WILL MAINLY E UP IN WATER DUE TO HOUSEHOLD WASHIN

UNCONTROLLED EMISSIONS

UNCONTROLLED EMISSIONS

RELEASE TO THE ENVIRONMENT
- WATER WP8
- SOIL WP7
- AIR WP6
- BIOTA WP9

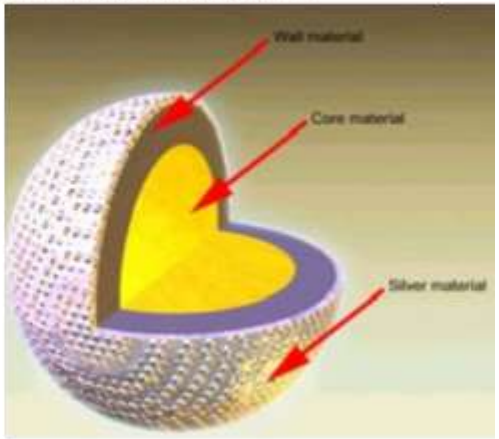
INCORPORATION PROCESS RESIDUES

SYNTHESIS WASTE

WASTE WATER TREATMENT PLANT WP5

EMPTY CONTAINER S, PPE…

5. END - OF - LIFE
- INCINERATION PLANT WP5
- LANDFILL WP5



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GUIDEnano

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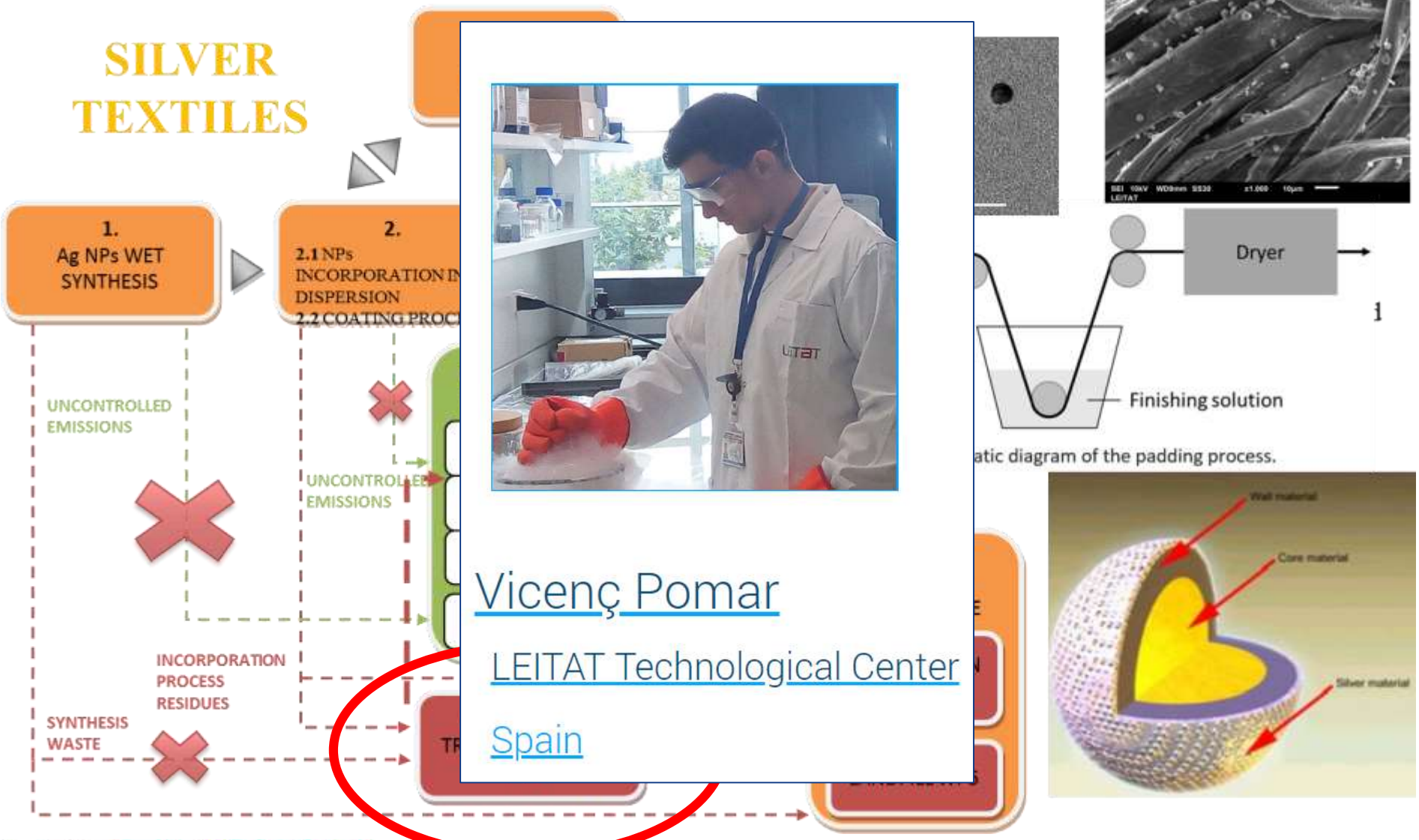
Nano Product value chain and release paths (WP4)



Vicenç Pomar

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Spain

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GUIDE nano

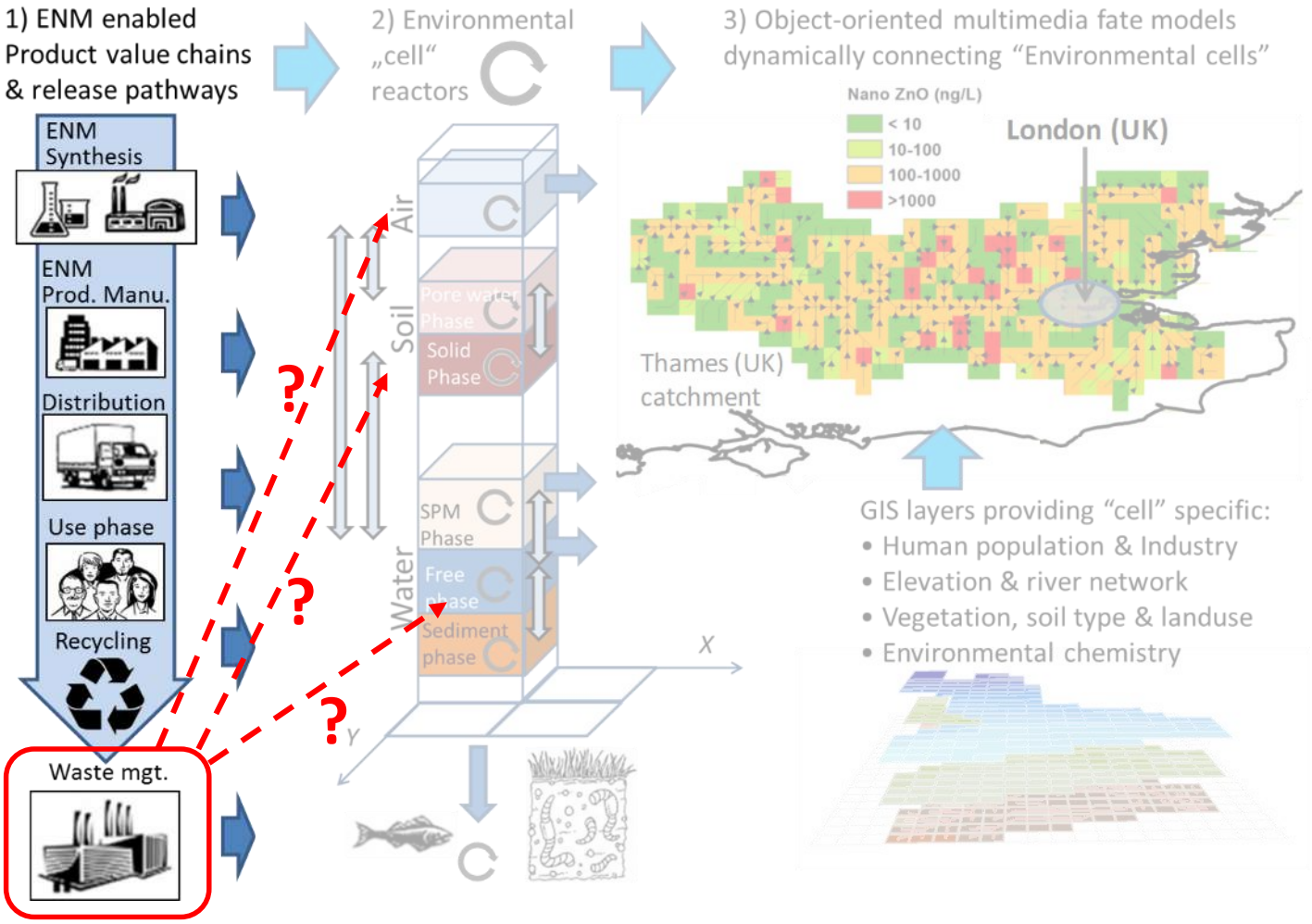
NanoFASE

Nano Product value chain and release paths (WP4)

Ag CONDUCTIVE INKS - TO INFINITY AND BEYOND:
"The Golden Fleece" smart sail concept to support space exploration missions. NanoFASE partner AMEPOX's nano silver products used in printed control circuits and application of metallic coatings.

Exposure assessment (of Nano) in the environment:

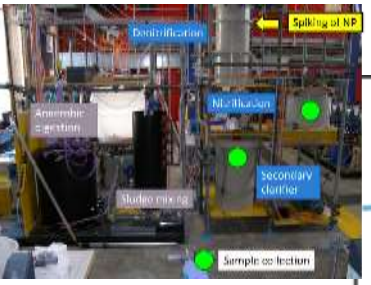
How much is released, and where does what go?

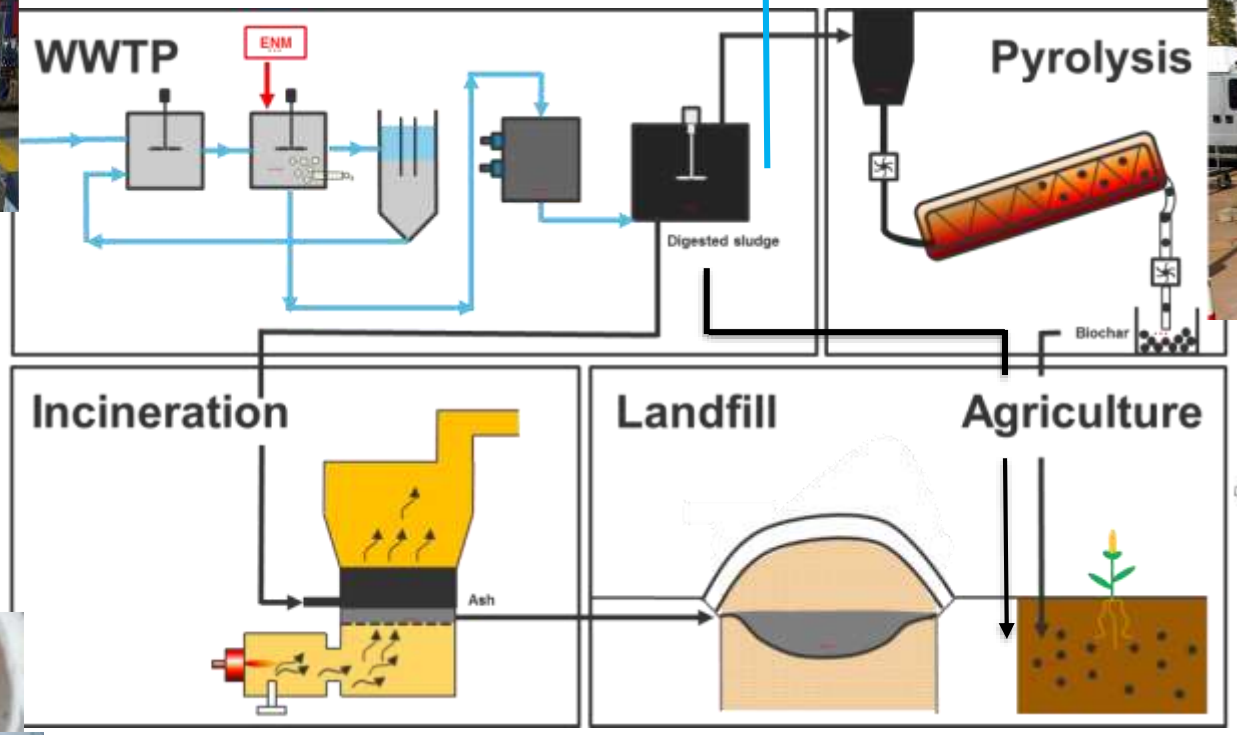


Waste Water Management

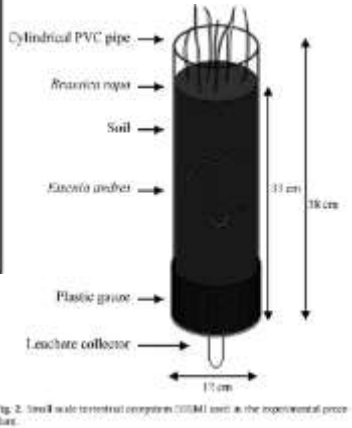
Investigating forms leaving end of life stage (WP5)

Investigate fate and transformation of ENM in major managed waste facilities:





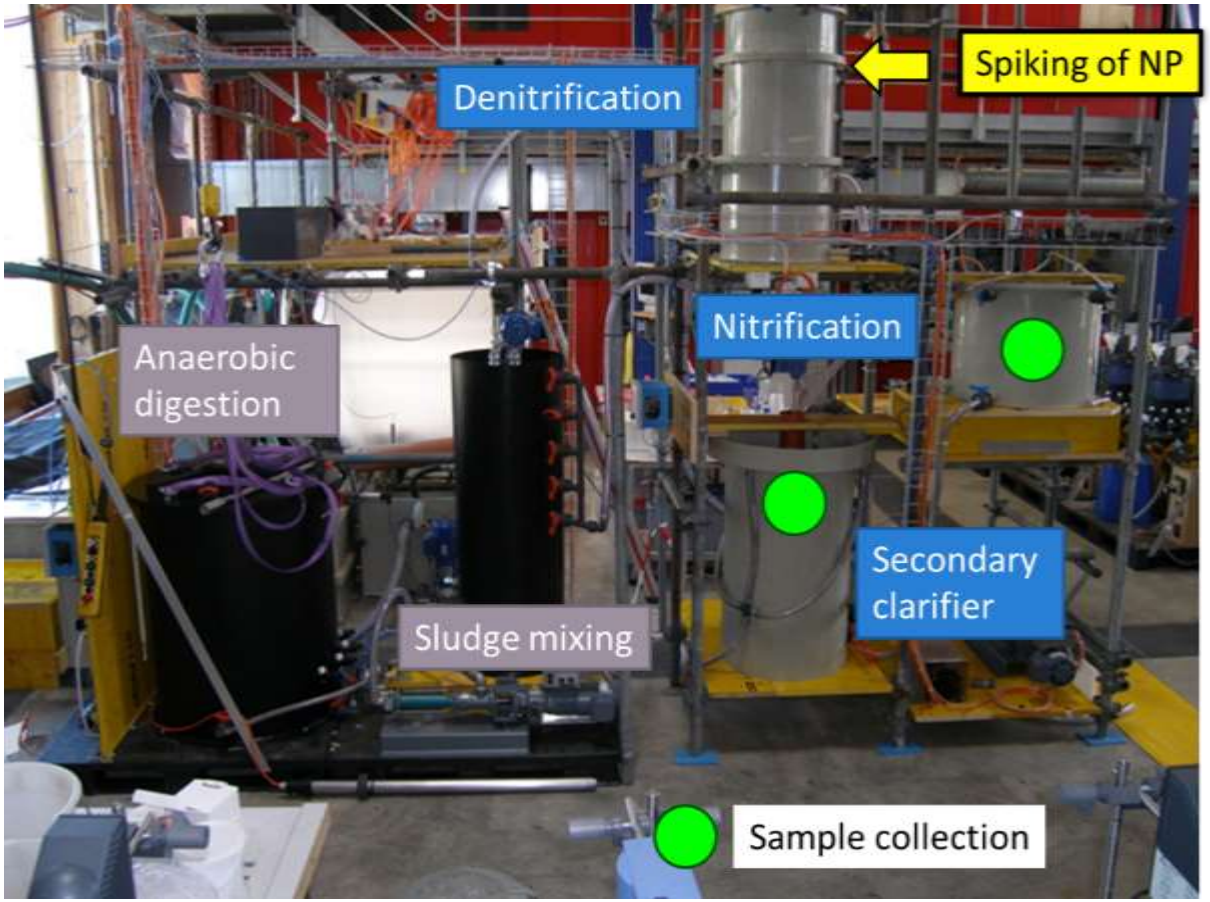
Sewage sludge incineration



Exposure assessment (of Nano) in the environment:

How much is released, and where does what go?

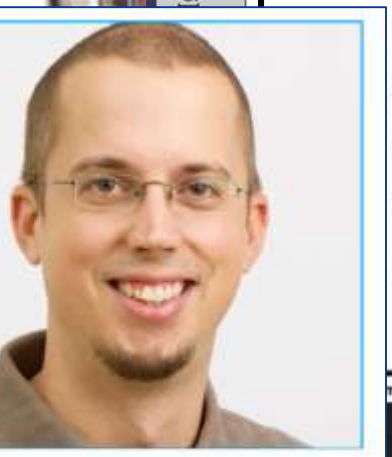
Waste Water Treatment Plant



Exposure assessment (of Nano) in the environment:

How much is released, and where does what go?

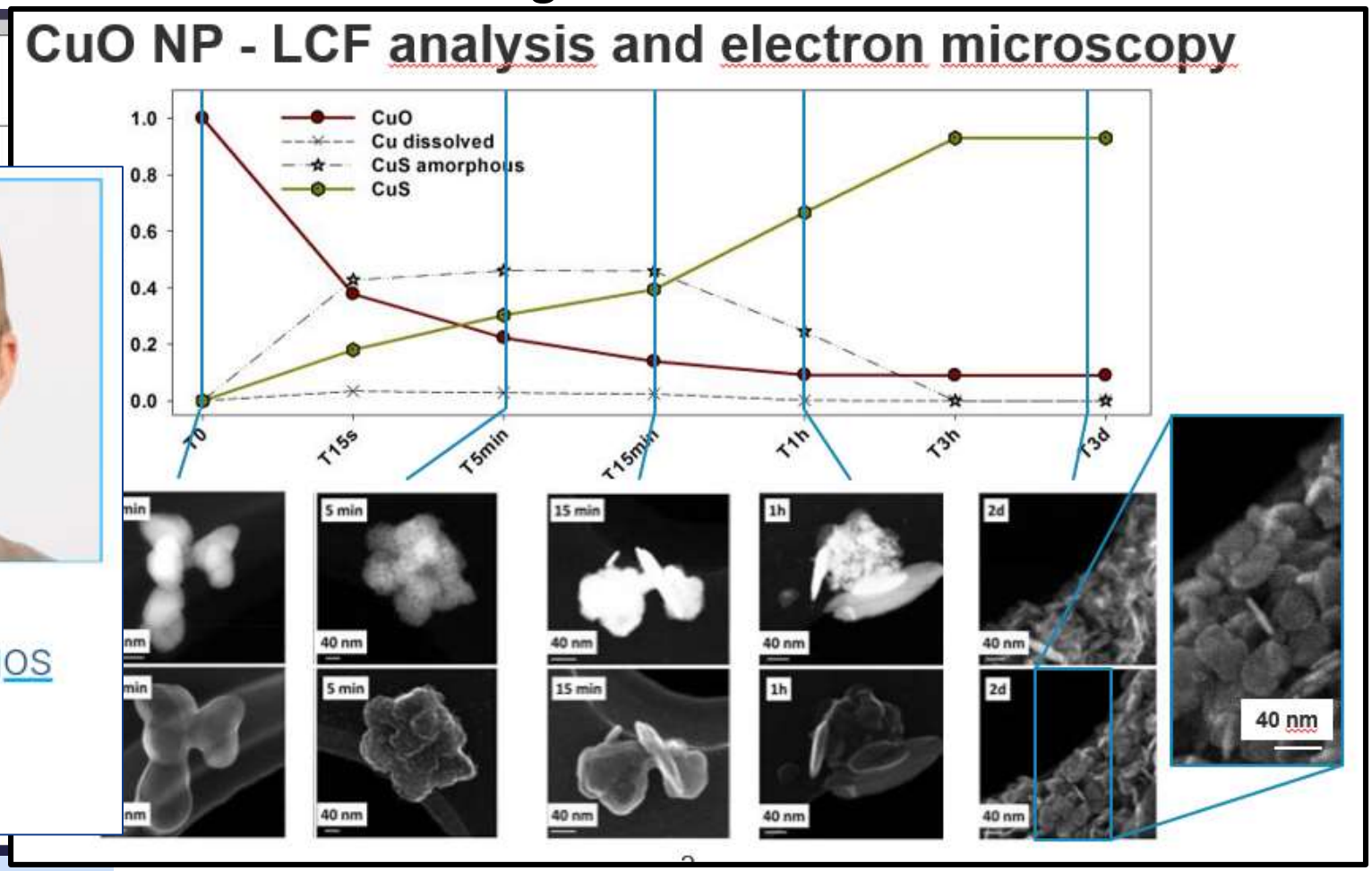
Waste Water Treatment Plant – Ag and CuO NPs



Alexander Gogos

EAWAG

Switzerland



eawag aquatic research

Gogos, A et al (2017) ES:nano

NanoFASE

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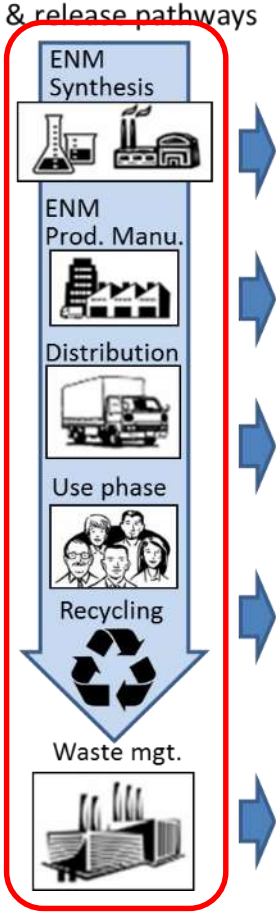

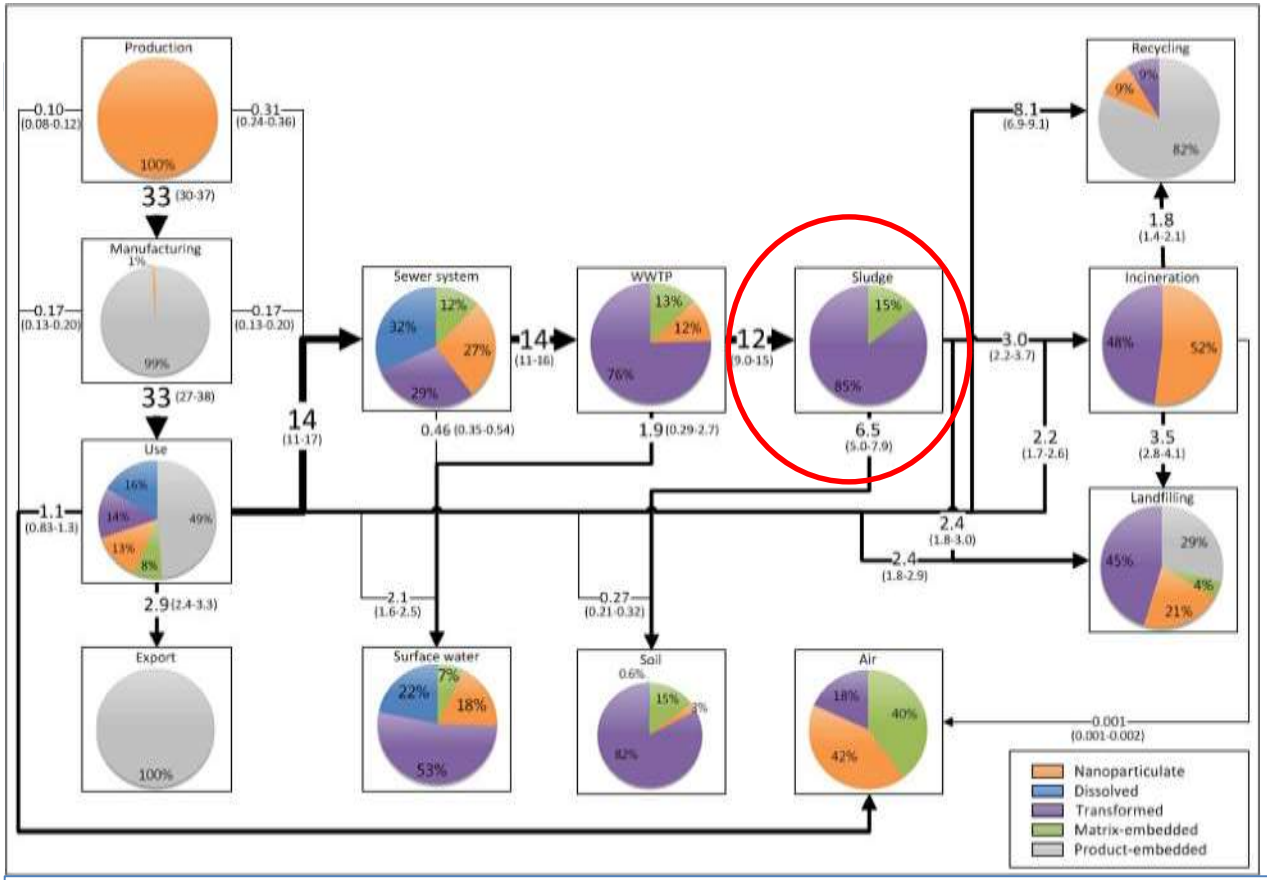

Flows of nano-Ag and distributions among the forms released during its life cycle. All flows are described in tons/year in the European Union with the means of the probability distributions.

Adams, V et al 2018 Environmental Pollution, 243, pp 17-27

Exposure assessment (of Nano) in the environment:

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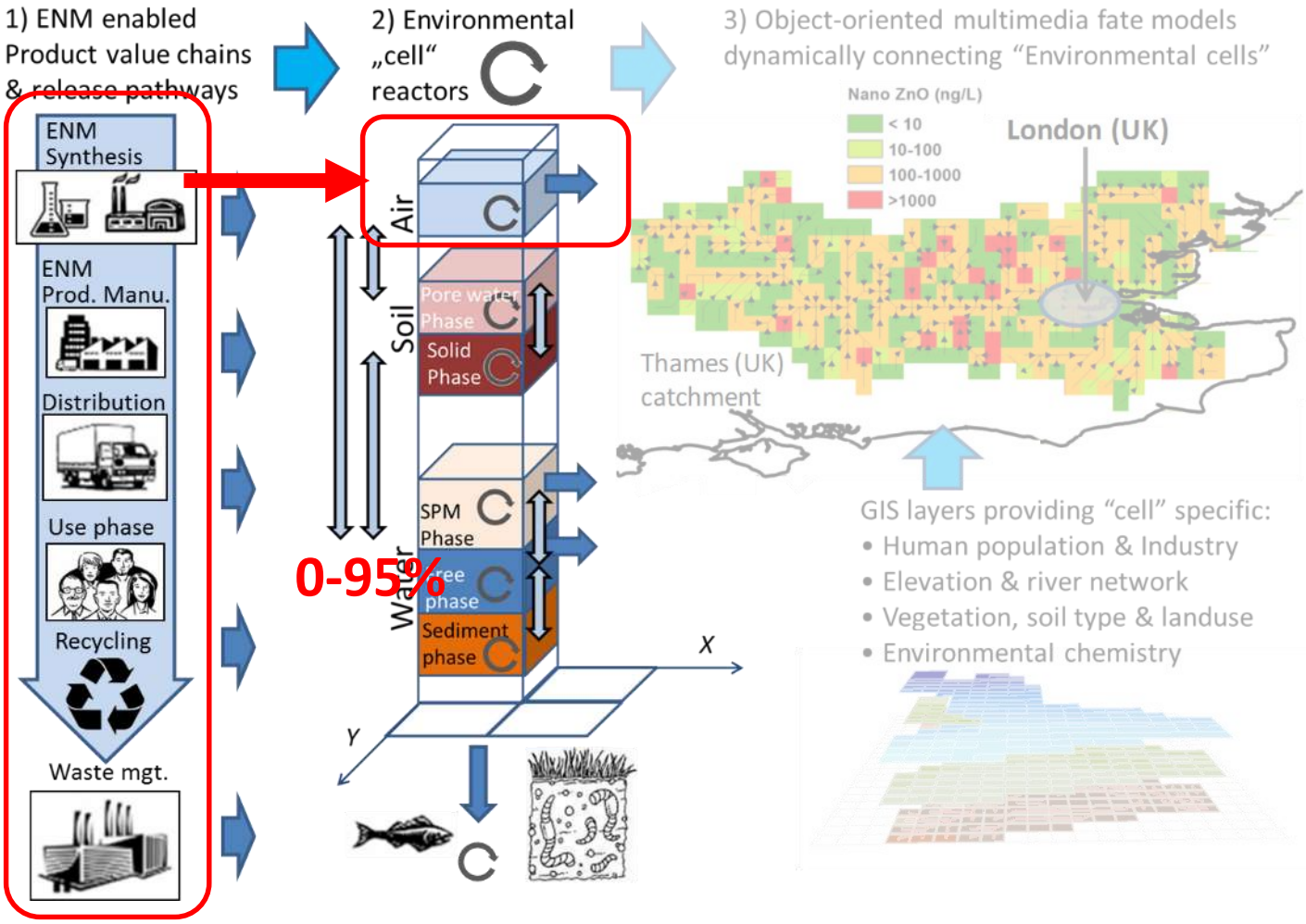
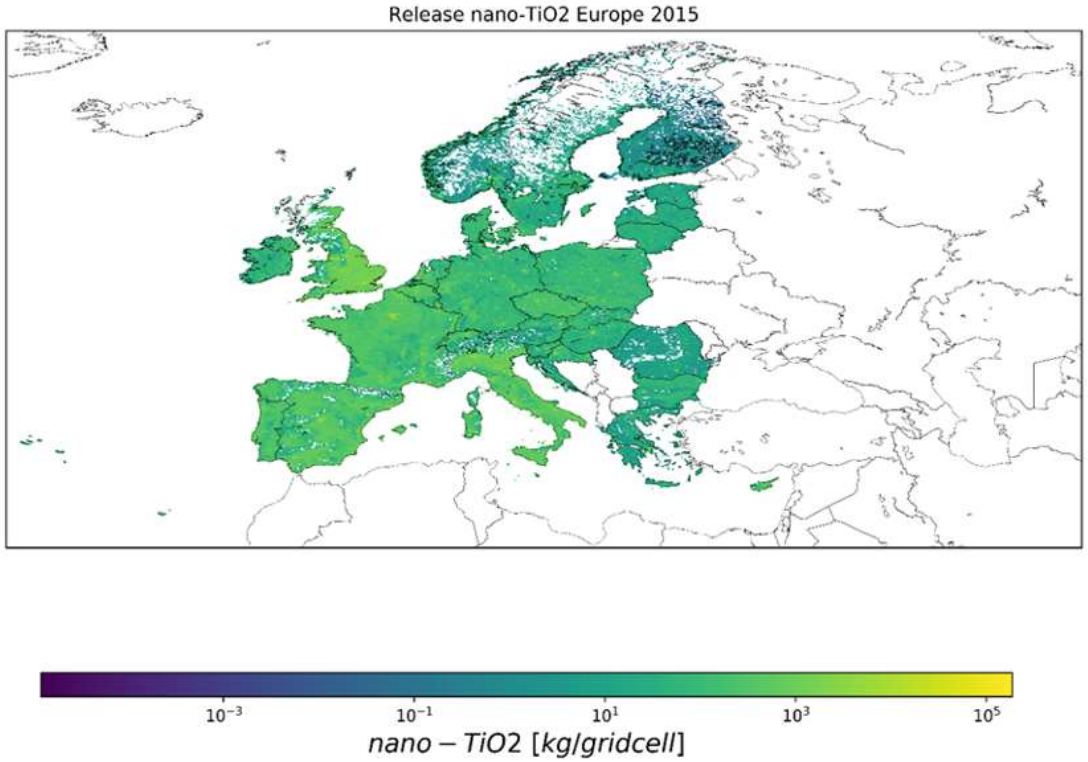


Exposure assessment (of Nano) in the environment:

Modelling air phase distributions?



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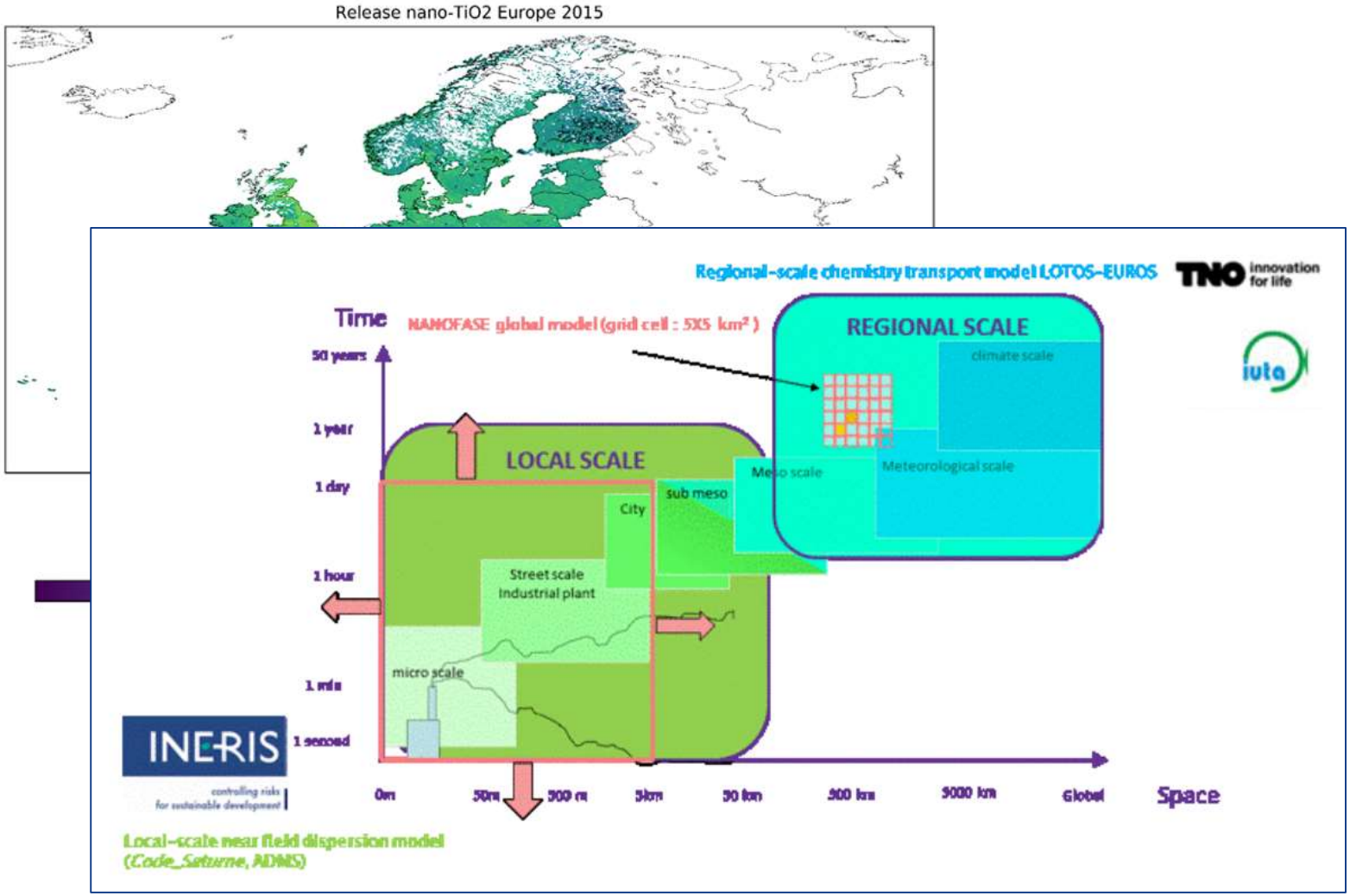

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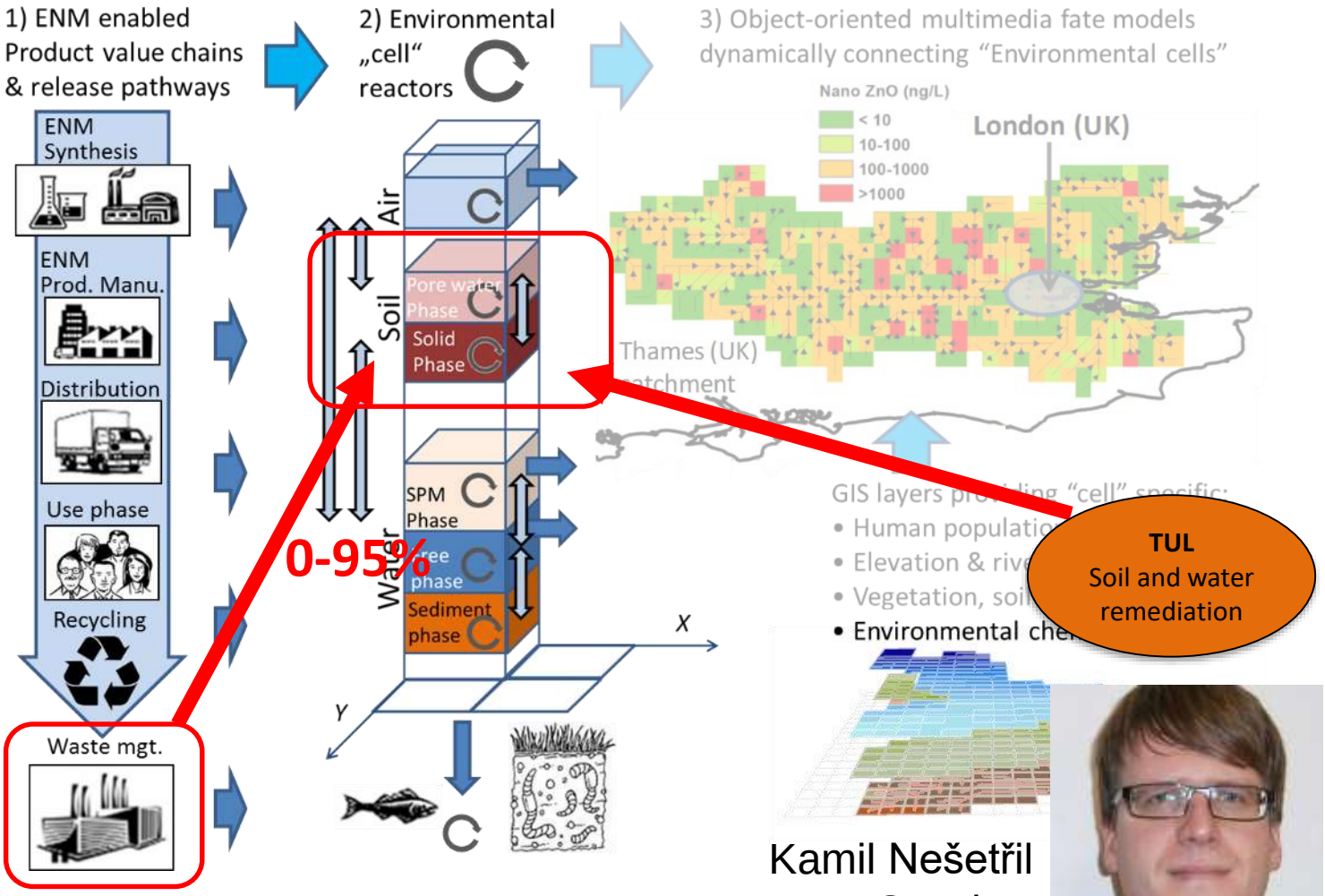
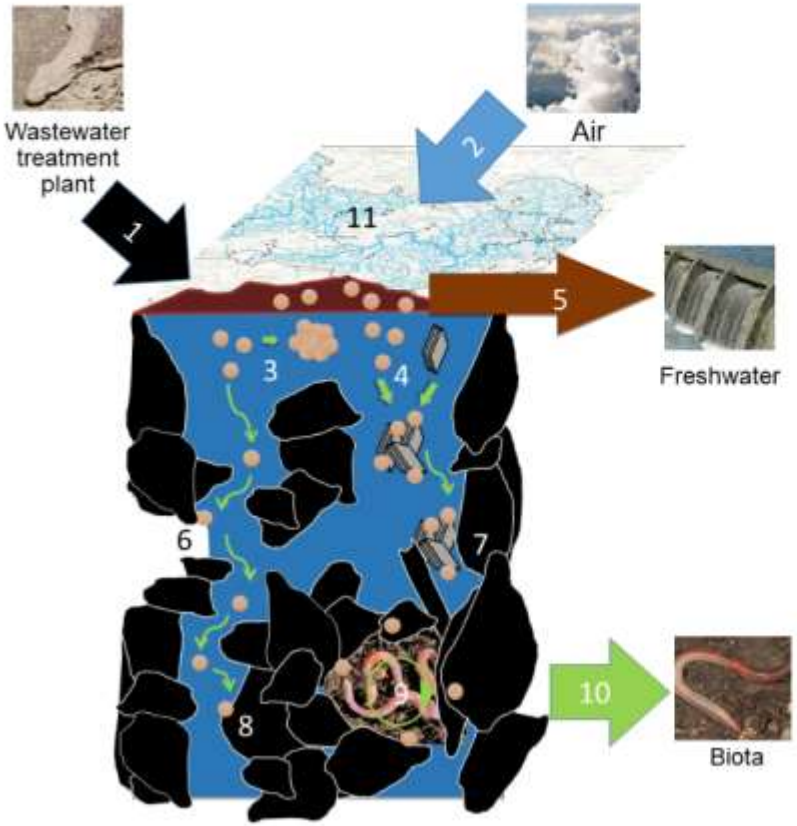


Kamil Nešetřil
TUL, Czech
Republic

NanoFASE Soil modelling module

Environmental Fate of ENMs: Soil Compartment

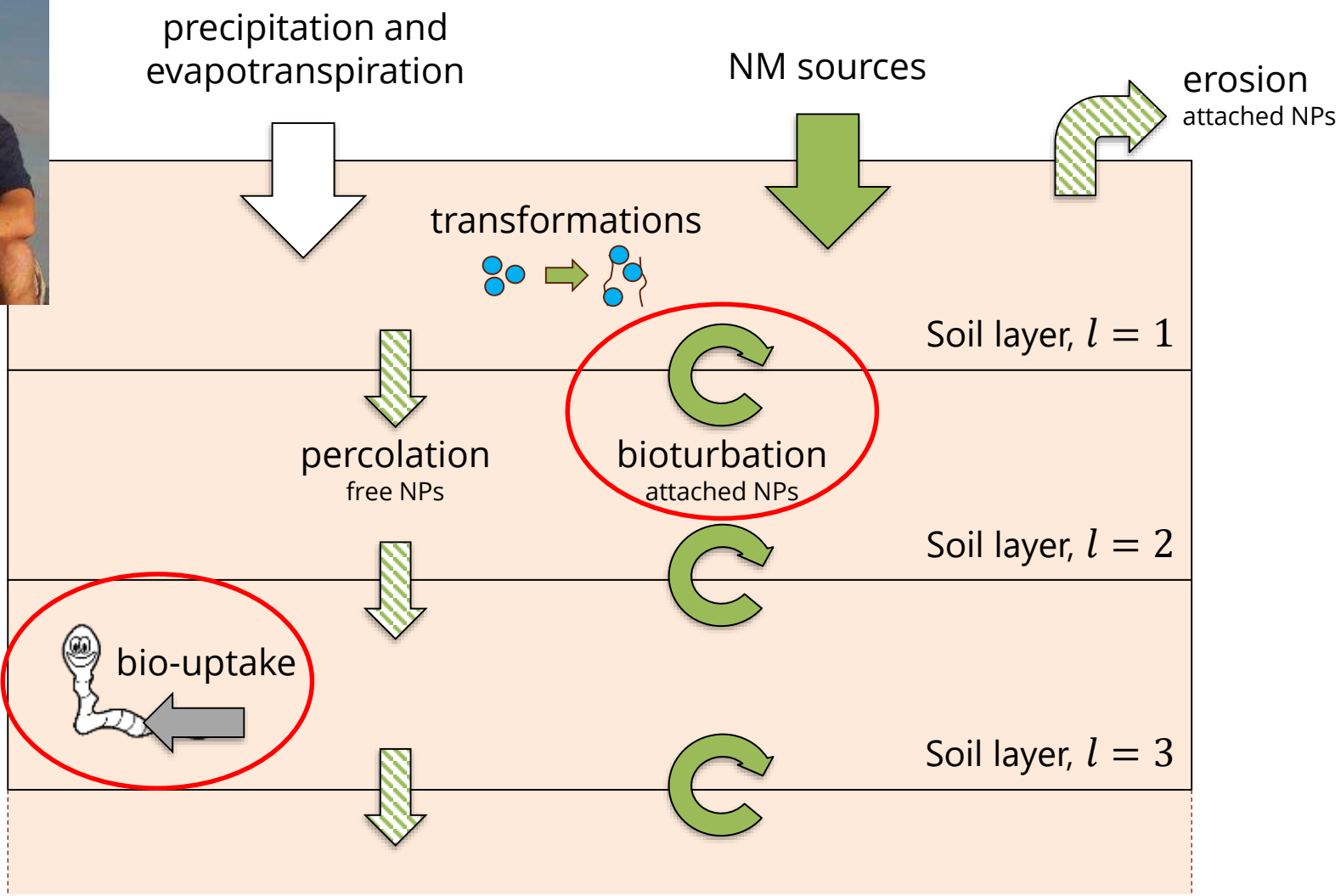
Soils are exposed to ENMs mostly through deposition of sludge on agricultural land. A range of organisms can be exposed and possibly be affected, including food crops, also giving an entry into the human food chains. ENMs are also applied deliberately to soils, e.g. as zerovalent iron to remediate contaminated soils, as nanofertilizers or as nanopesticides.



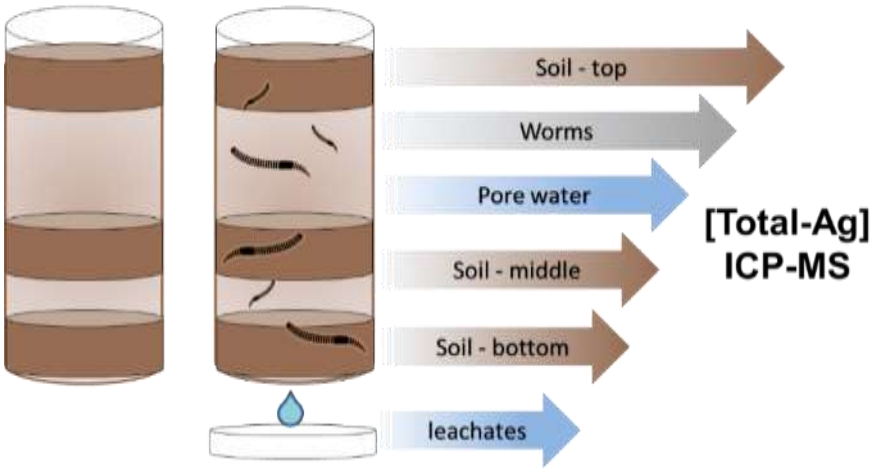
1. Sludge deposition
2. Atmospheric dry deposition
3. Homoaggregation
4. Heteroaggregation
5. Surface runoff
6. Air-water interaction
7. Straining
8. Attachment
9. Bioturbation
10. Bio-uptake
11. Spatial distribution
12. Mass transfer

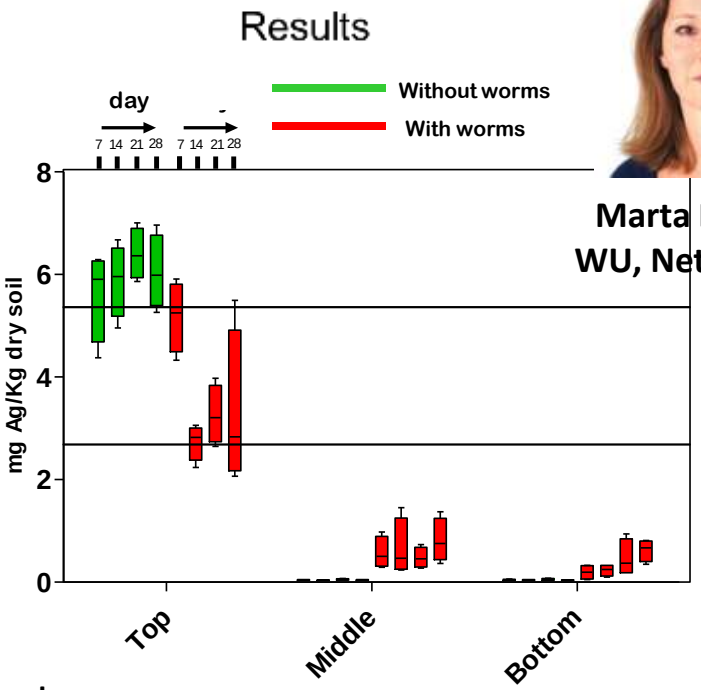
NanoFASE Soil modelling module

Sam Harrison
UKRI-CEH, UK



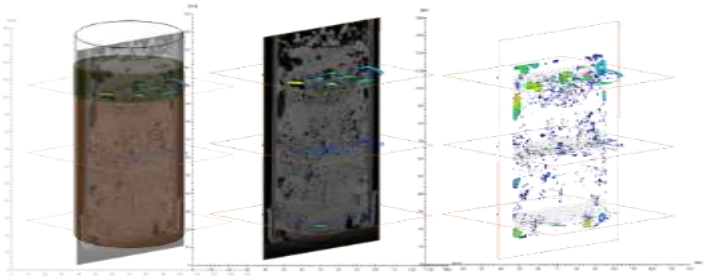
NP mobility in Soil vs Earthworm driven bioturbation





Marta Baccaro
WU, Netherlands

x ray computed tomography

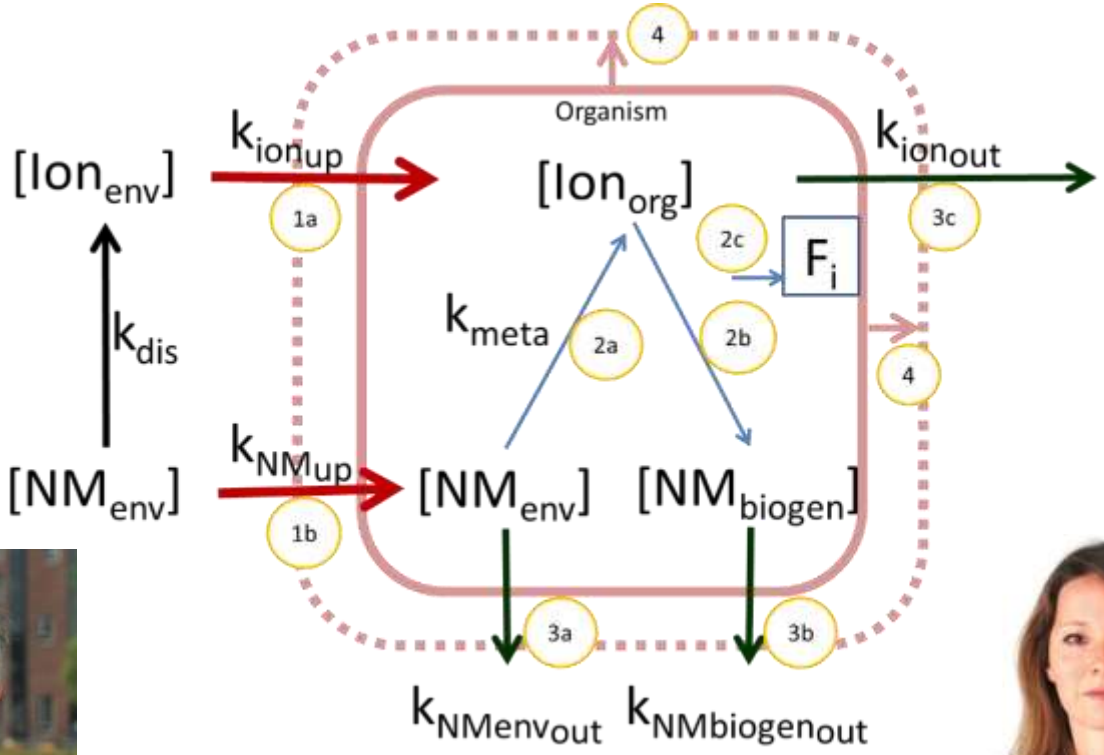


Consequences for leaching and for run-off

Baccaro, M. et al, Environmental Pollution, 2019

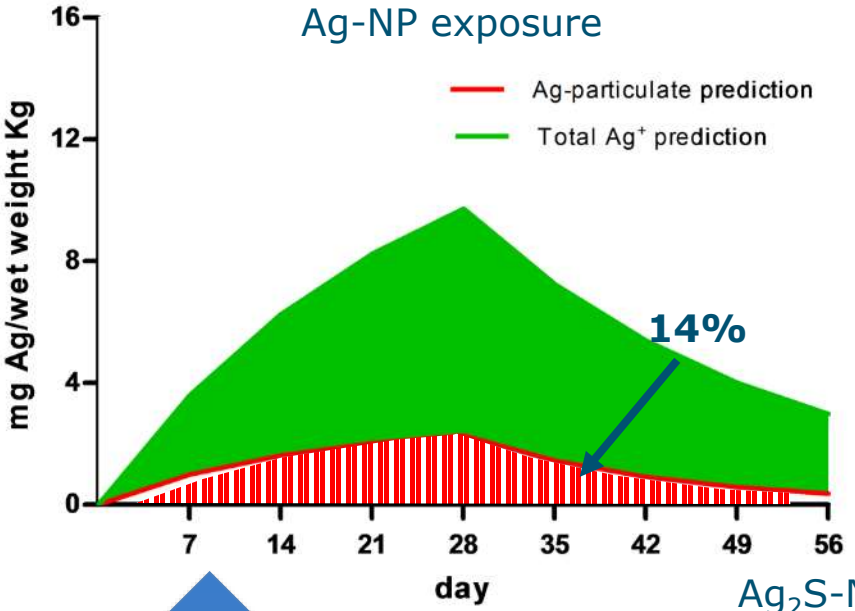
Accumulation kinetics in different biota

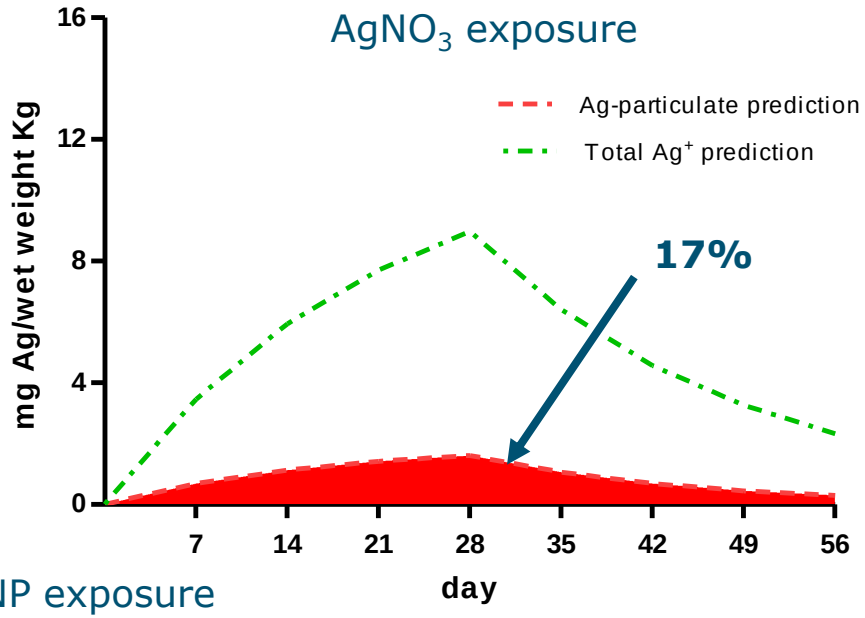
Conceptual model



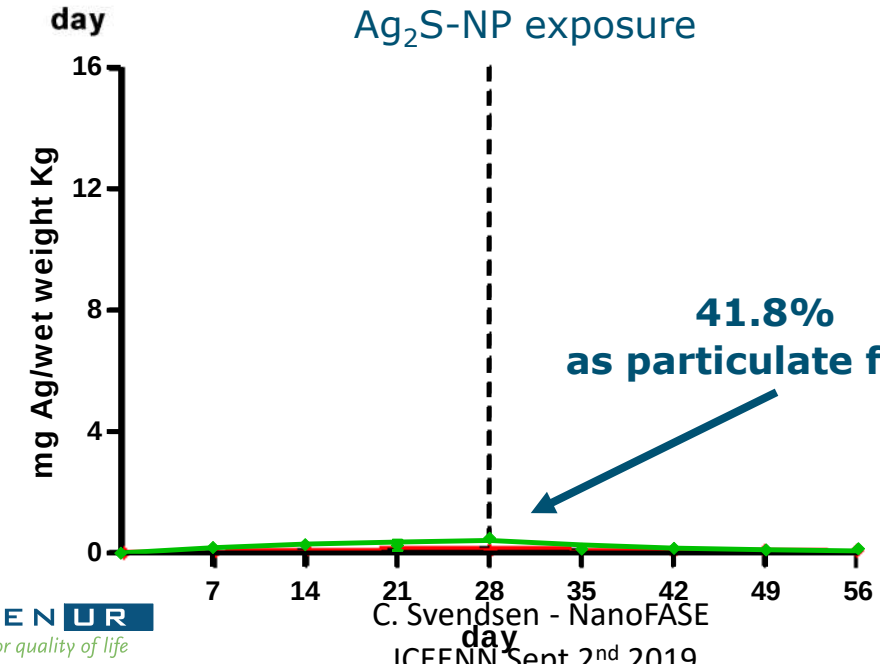
Nico van den Brink, and Marta Baccaro, WU, Netherlands

Earthworm uptake (ions vs particulate)





10x less when aged



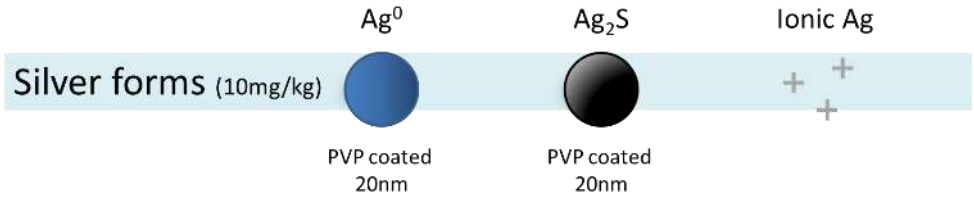
Marta Baccaro
WU, Netherlands

WAGENINGEN UR
For quality of life

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

Tracking Uptake In Organisms (Pristine Vs Aged NM)

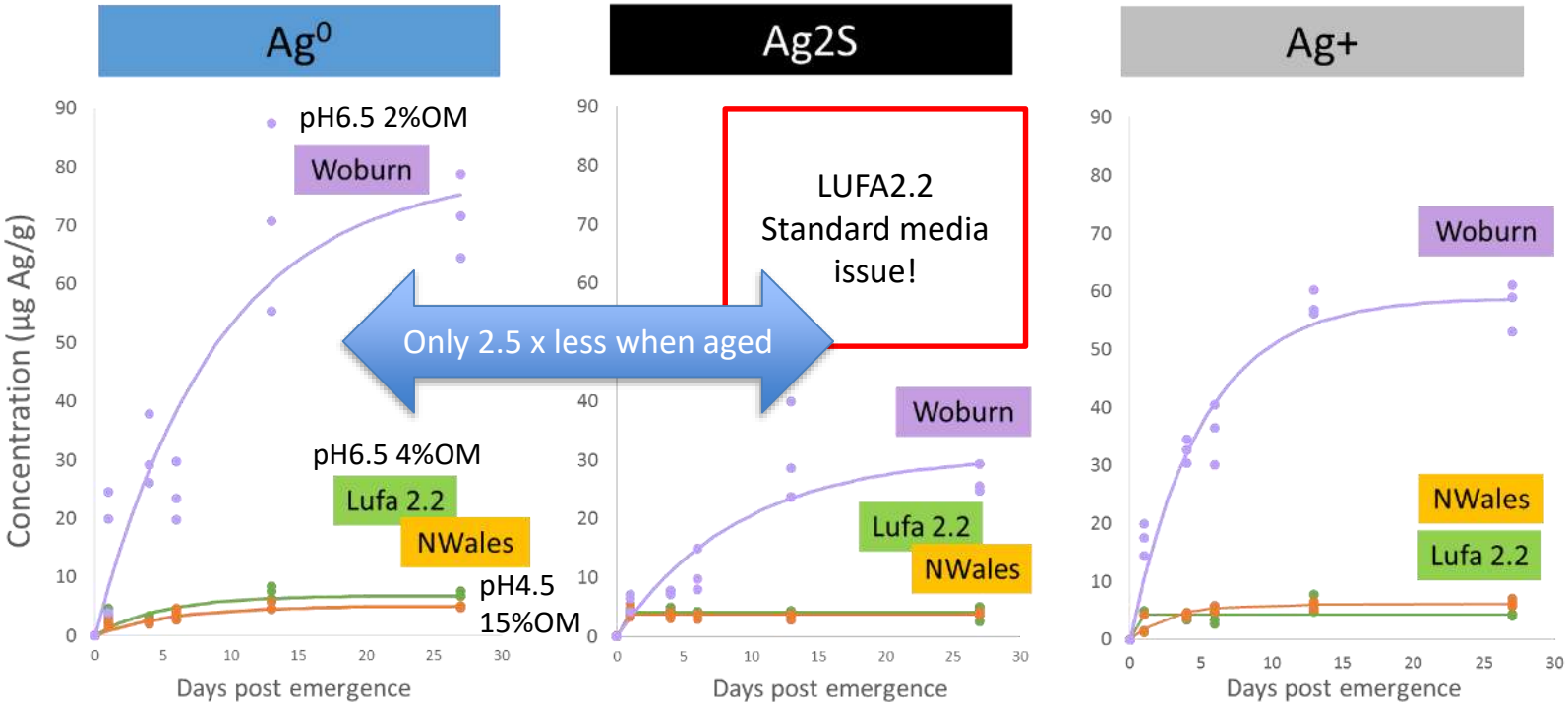
Kinetics of uptake of Ag and Ag_2S-NPs by wheat in different soils



Amaia Etxabe Green

Elma Lahive

UKRI-CEH, UK



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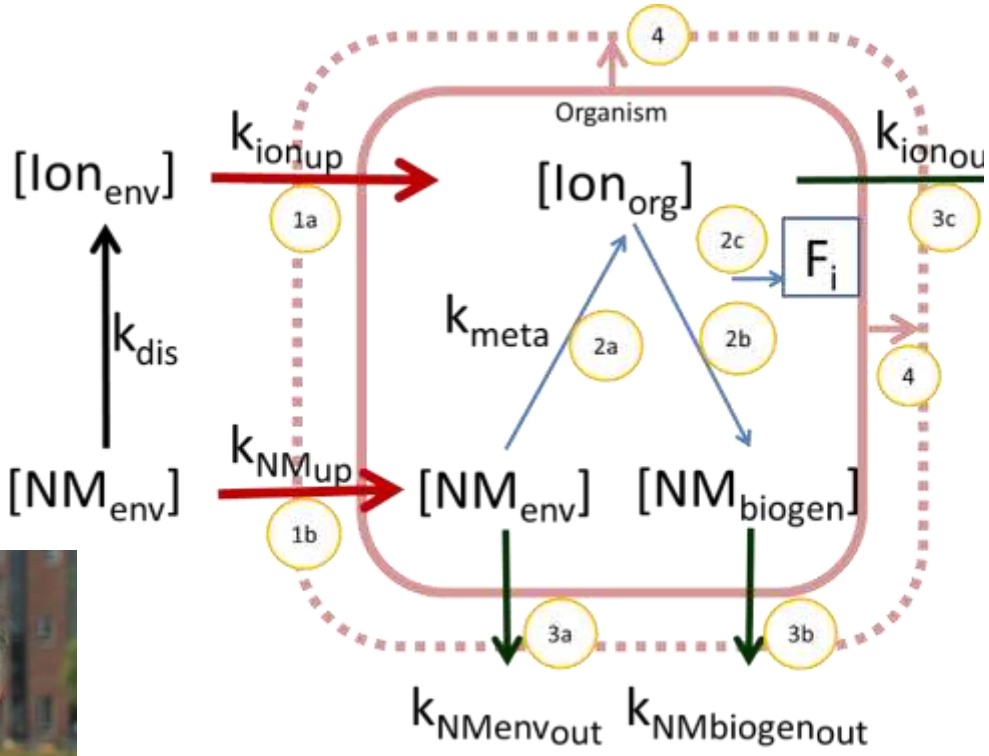

Nico van den Brink, WU, Netherlands

Detailed study of:

Snails;

Patricia Silva
Uni. of Aveiro.
Portugal

Mealworms;

Zahra
Khodaparast
Uni. of Aveiro,
Portugal

Fish;

Nathanial Clark & Richard Handy
Uni. of Plymouth, UK

Exposure assessment (of Nano) in the environment:

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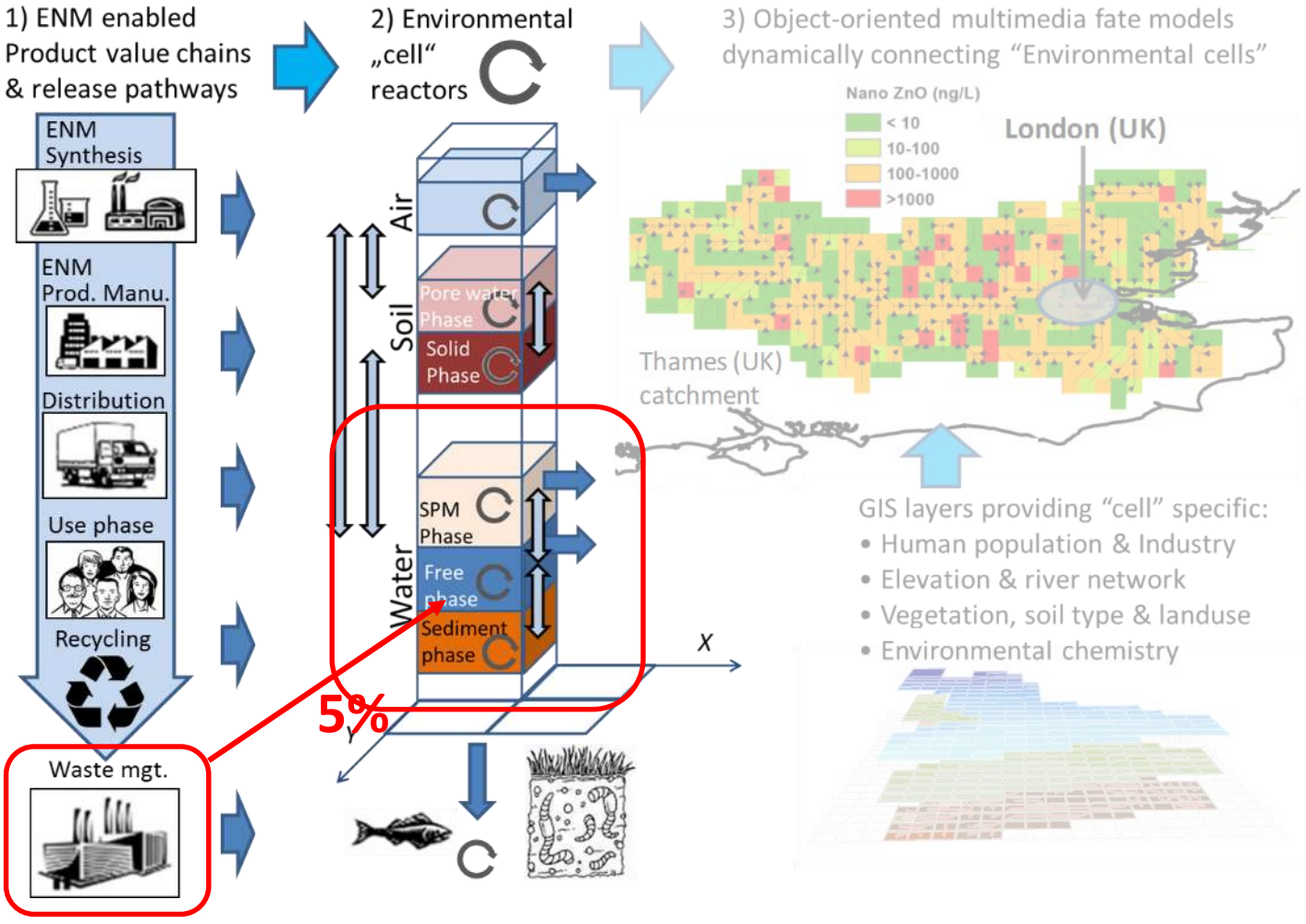
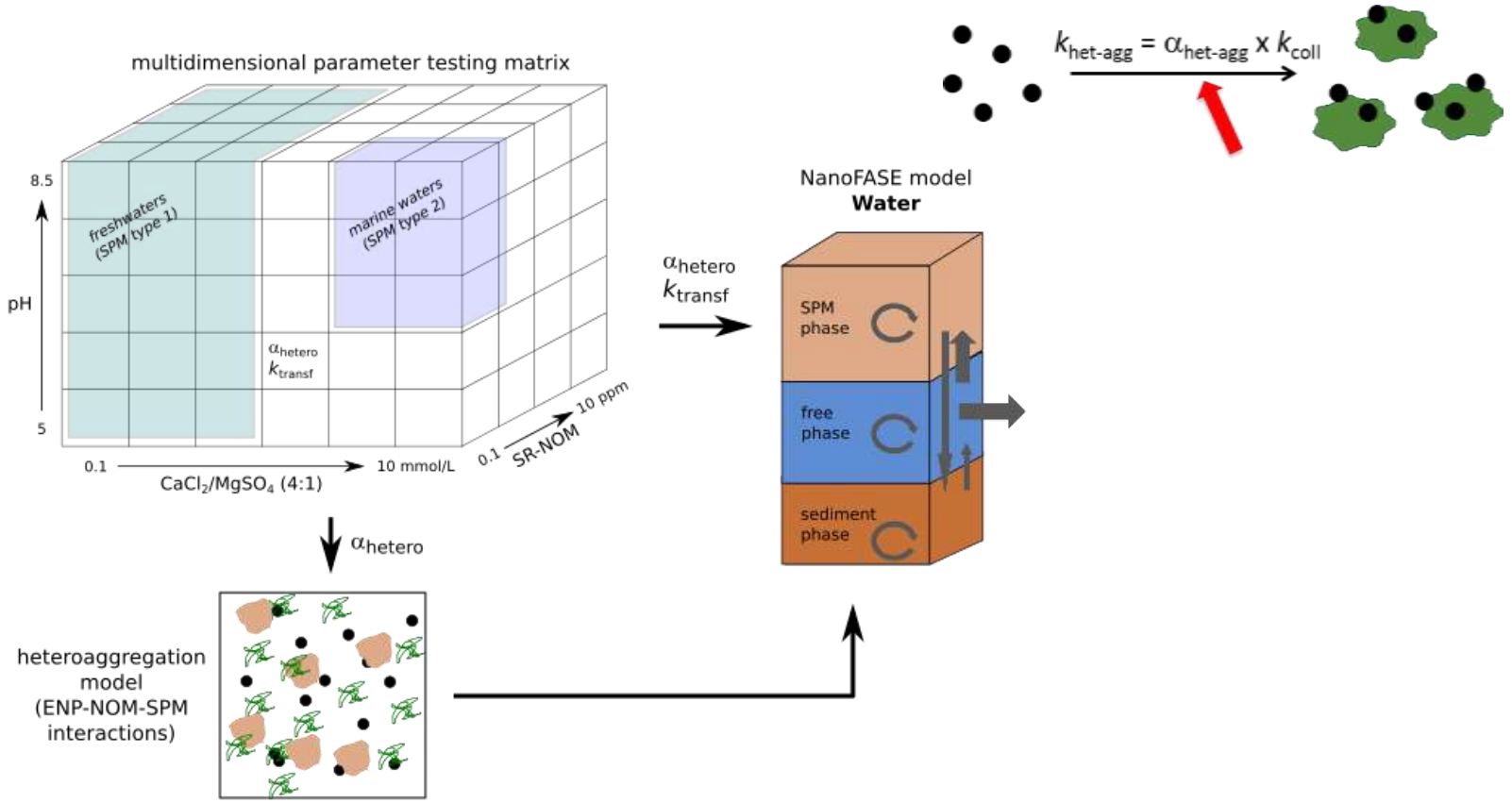


Waste Water
95% Sludge
5% Effluent

Waste Water Treatment Plant

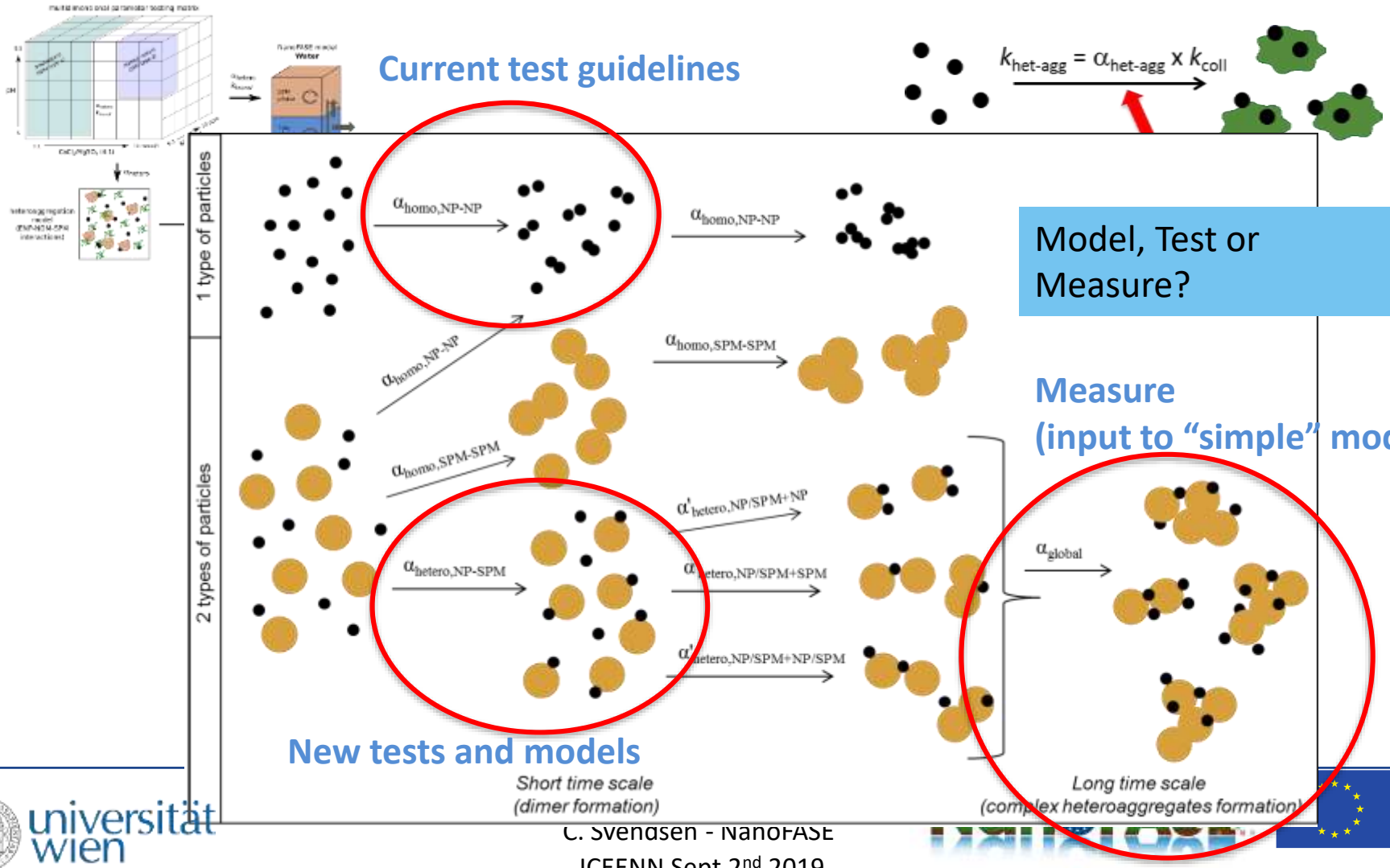
Assessing NM behaviour in Surface Waters and Sediments

Cover fate in realistic natural water chemistries



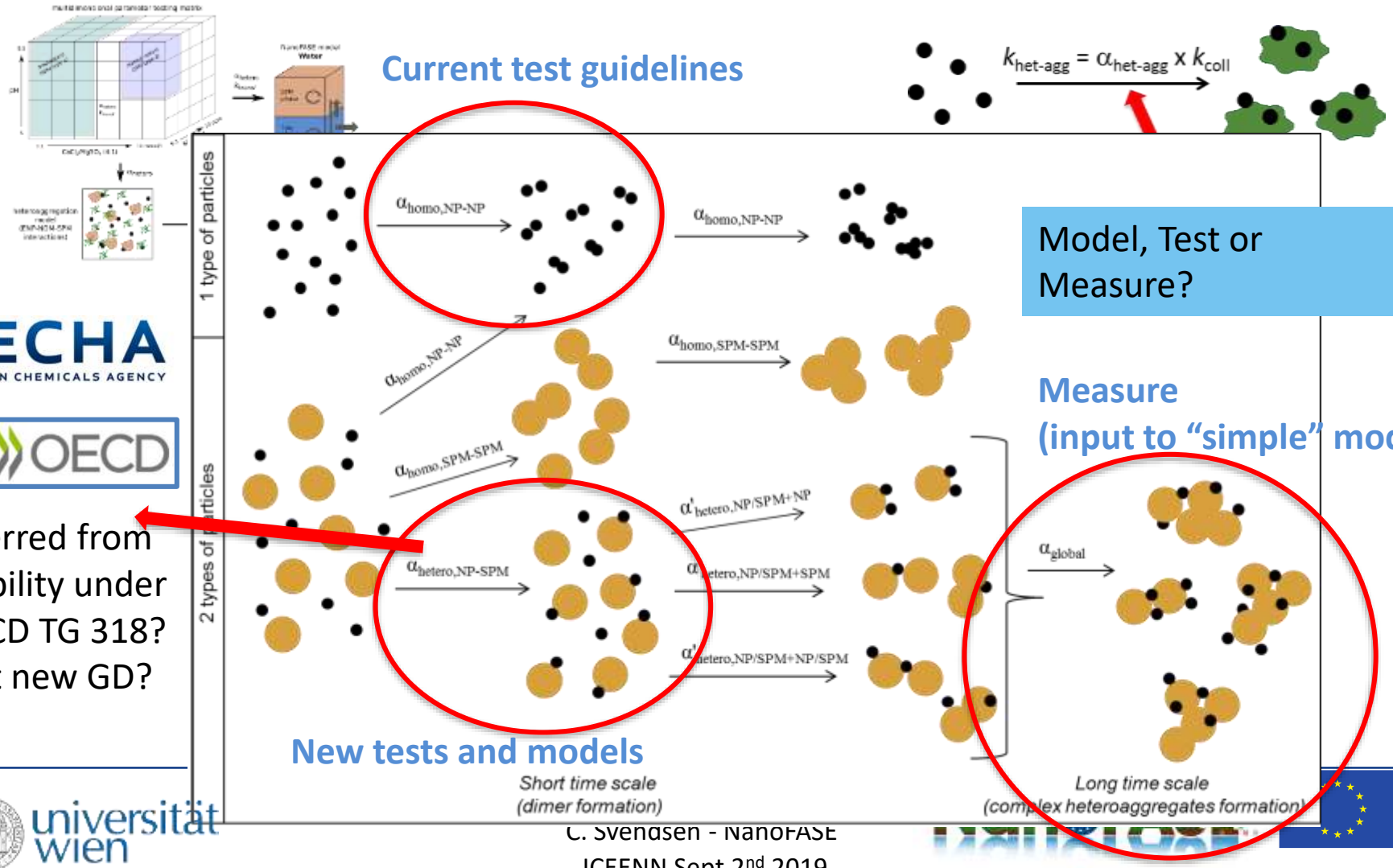
Assessing NM behaviour in Surface Waters and Sediments

Cover fate in realistic natural water chemistries



Assessing NM behaviour in Surface Waters and Sediments

Cover fate in realistic natural water chemistries



ECHA EUROPEAN CHEMICALS AGENCY

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Assessing NM behaviour in Surface Waters and Sediments

Cover fate in realistic na…s

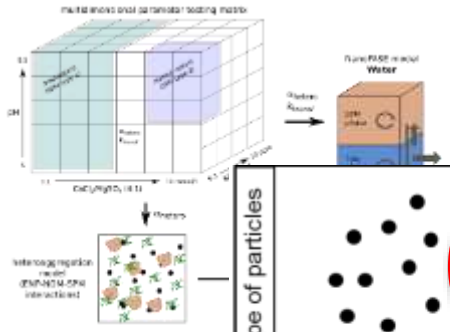
Helene Walch, Uni of Vienna
Experimental work

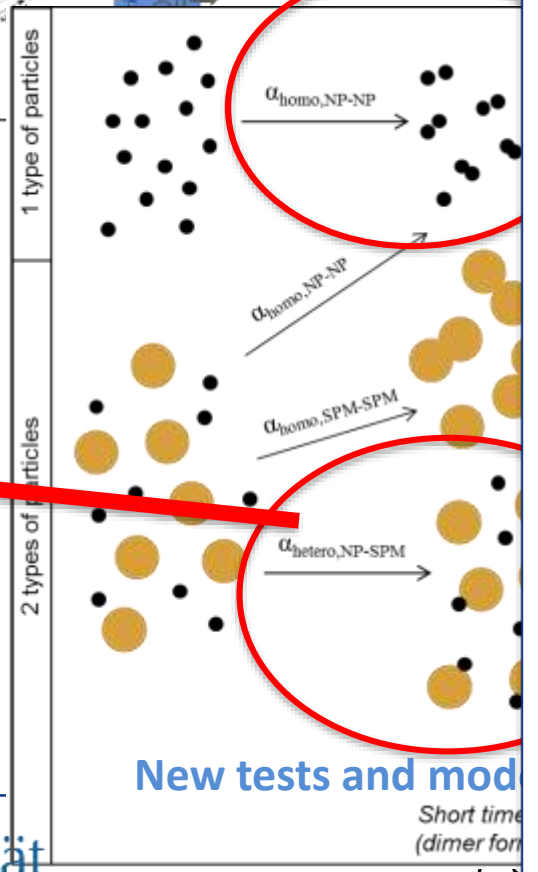
Modelling from:
Serge Stoll &

Group of Environmental Physico Chemistry
UNIVERSITÉ DE GENÈVE

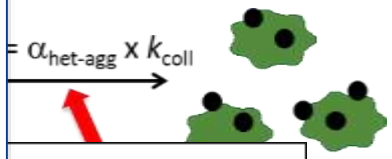
Marianne Seijo

Current test g…



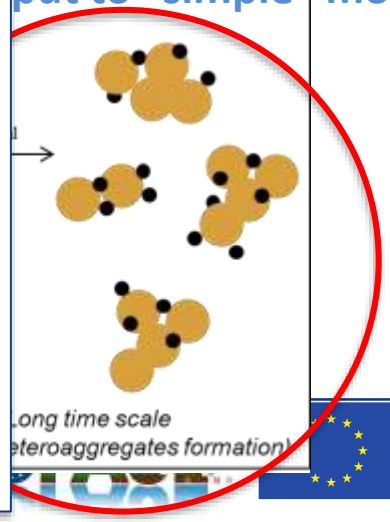


New tests and mod…
Short time…
(dimer for…



…odel, Test or
…easure?

…easure
…put to "simple" models)



Inferred from stability under OECD TG 318? Just new GD?

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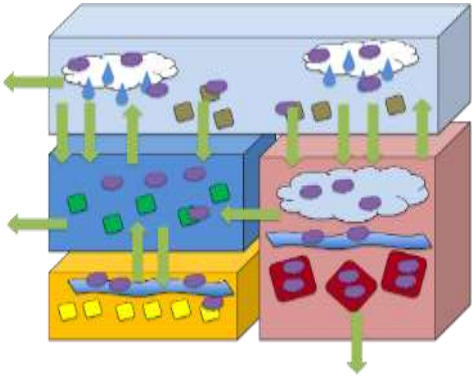
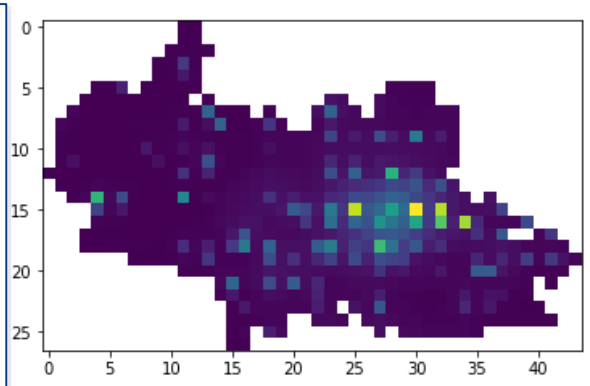
Putting the models together and comparing

Towards validating nanomaterial PECs from SimpleBox4nano using the NanoFASE-WSO spatiotemporal multimedia fate model



Steve Lofts, UKRI-CEH, UK



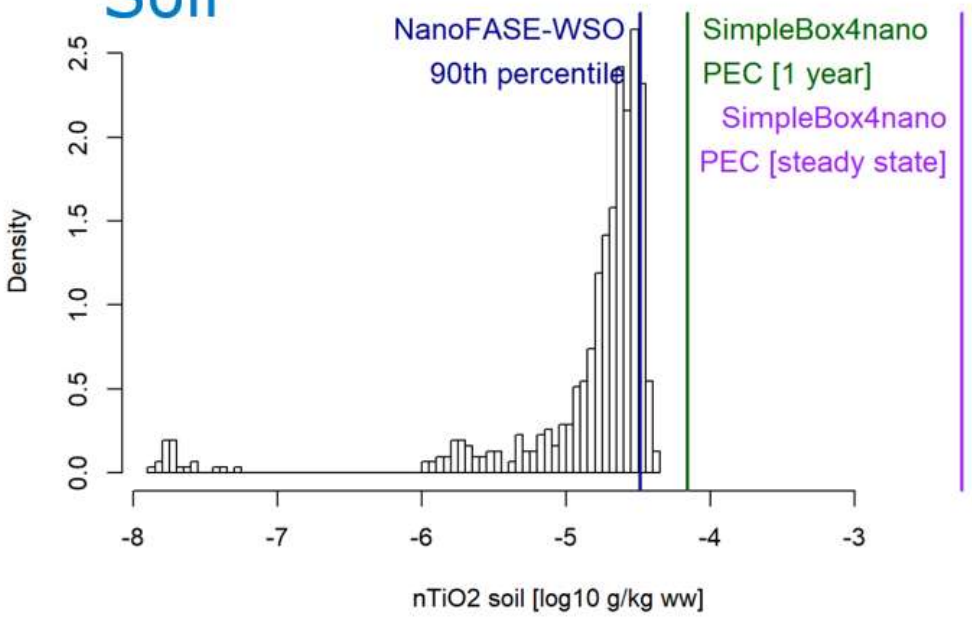
SimpleBox4nano	SE Water-Soil-Organism
Screening level	er
Steady state conditions	Time explicit
Regional to continental scale	Gridded: 5x5 km
Background, regional concentrations	Local concentrations

Putting the model together and comparing

Scenario

- TiO_2 in the Thames catchment
- Concentrations from NF-WSO is after 1 year.

Soil



Putting the model together and comparing

Scenario

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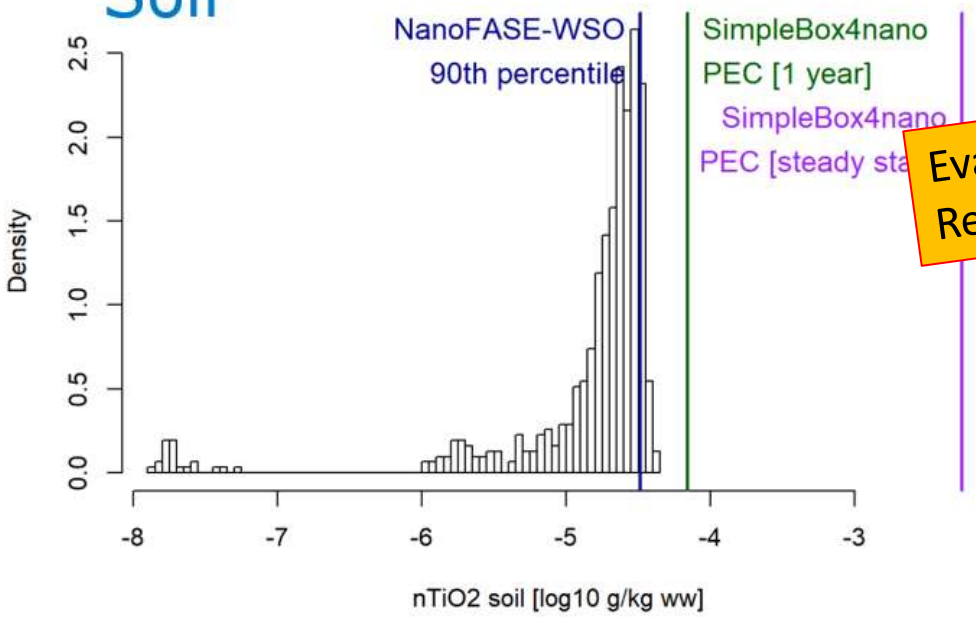
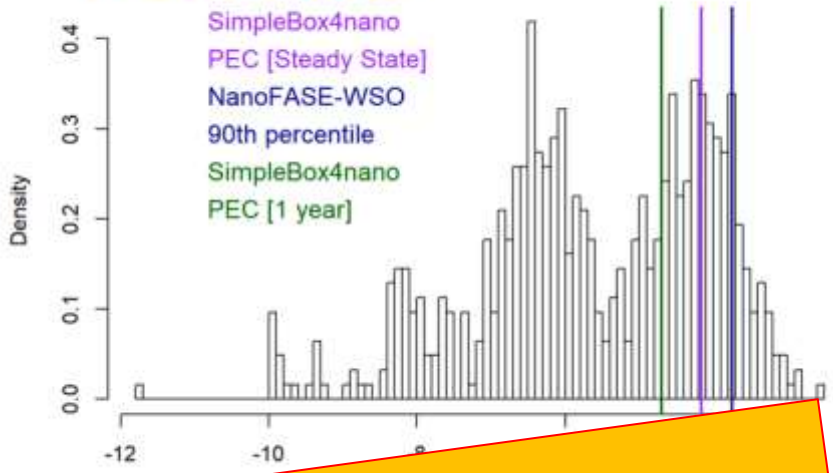
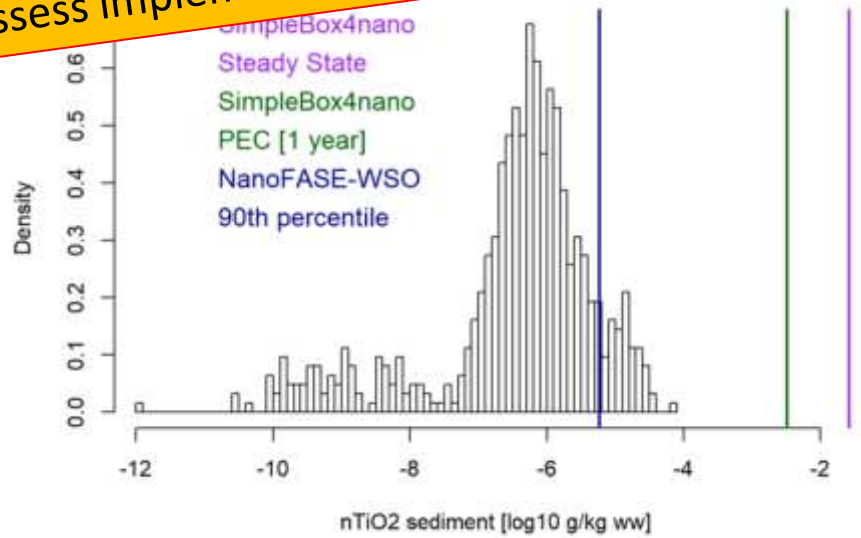


Fresh Water



Evaluation suggests:
Reassess implementation of resuspension rate



Putting the model together and comparing

Sensitivity

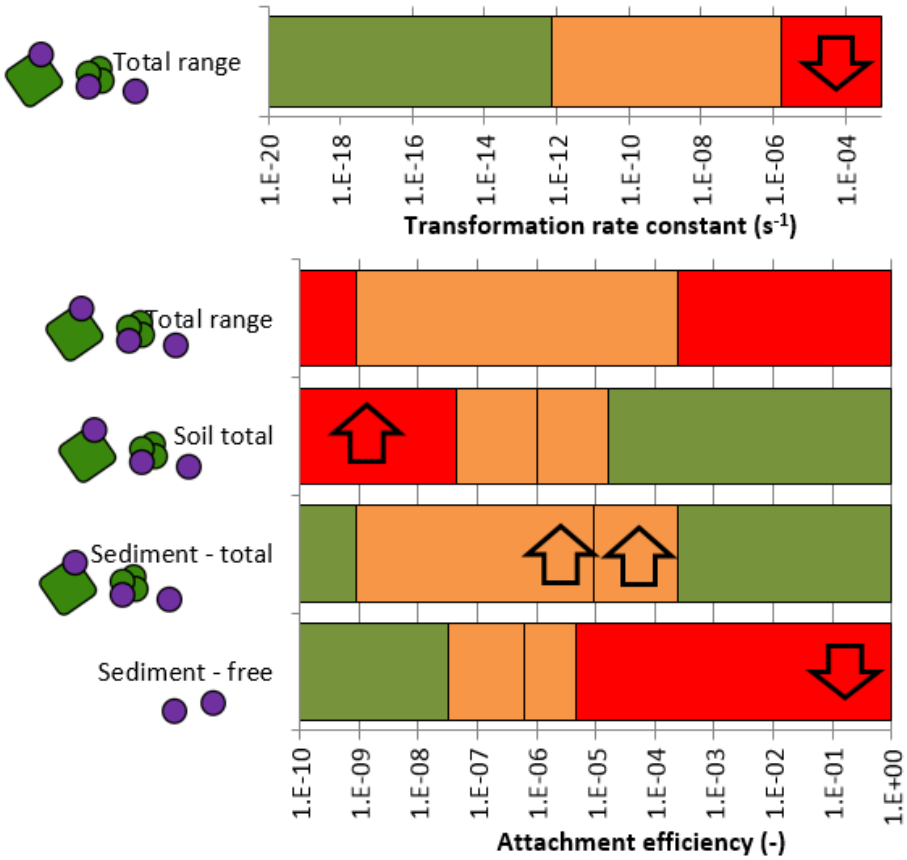
PEC insensitive

Critical range
2.5-97.5th percentile

PEC sensitive

- PEC sensitive to transformation rates above approx. 10^{-12} s^{-1}
- PEC sensitive to attachment efficiency for heteroaggregation
  - Varied sensitivity between compartments.

Critical ranges of parameters that need quantification/measurement.



Meesters, J.A.J. 2019. "A Model Sensitivity Analysis to Determine the Most Important Physicochemical Properties Driving Environmental Fate and Exposure of Engineered Nanoparticles." ES nano 10.1039/C9EN00117D

Implications for ERA considerations, approaches and tools

Environmental fate

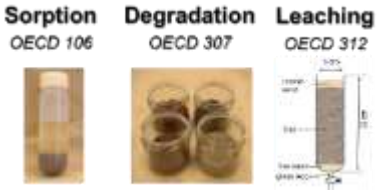
- Very different - rules if and where there may be possible Nano Exposures
  => should inform what Nano-form(s) are “exposure relevant”
- Long time scales => Current standard hazard tests may not be “worst case”
  => Pre-aging of test media?

Biodegradation/ accumulation/ biomagnification

- Tested exposure forms must be the exposure relevant ones
- Form (size and speciation) of internalised material ideally identified

Technical / Analytical needs + Test Guidance (match question with precision)

- New analytical and testing techniques needed (kept simple and repeatable)
- Move from “Solute based” to “kinetic” tests



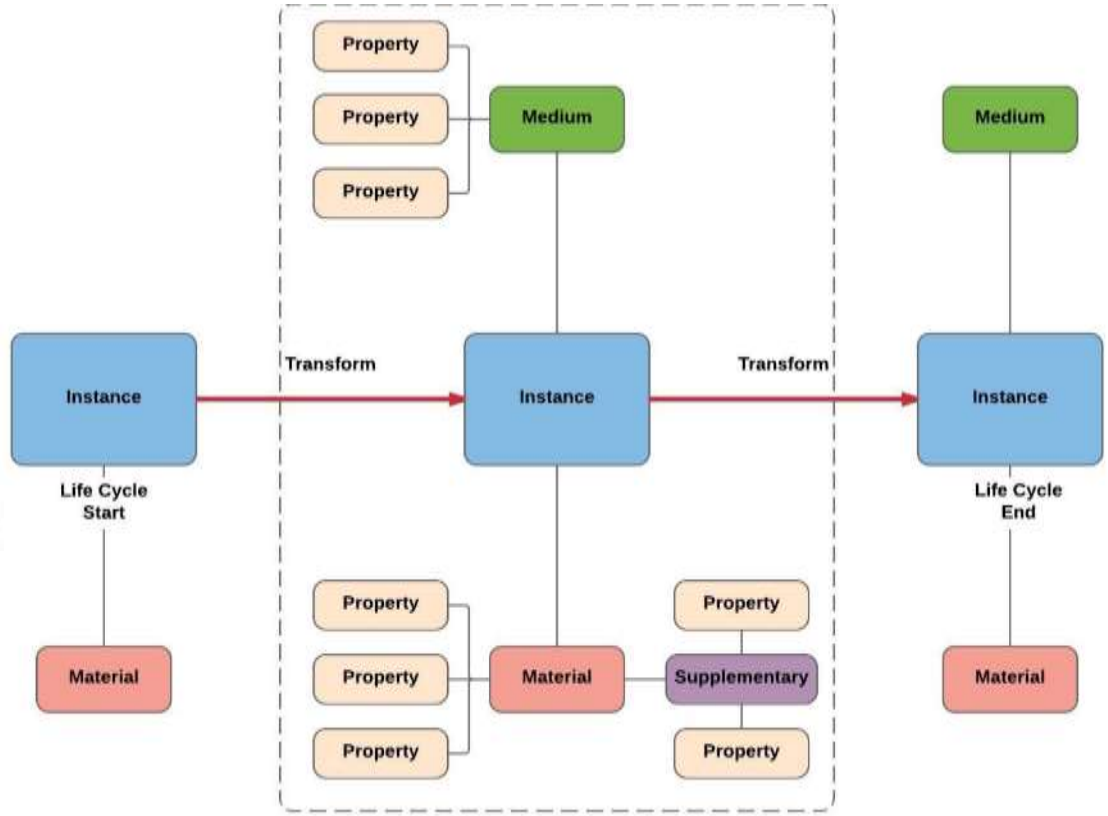
ICPMS to spICPMS

New analytics for organic NMs

X-ray based for speciation

Exposure - Nanomaterial fate in the environment:

How are we are handling, storing, and sharing the data?



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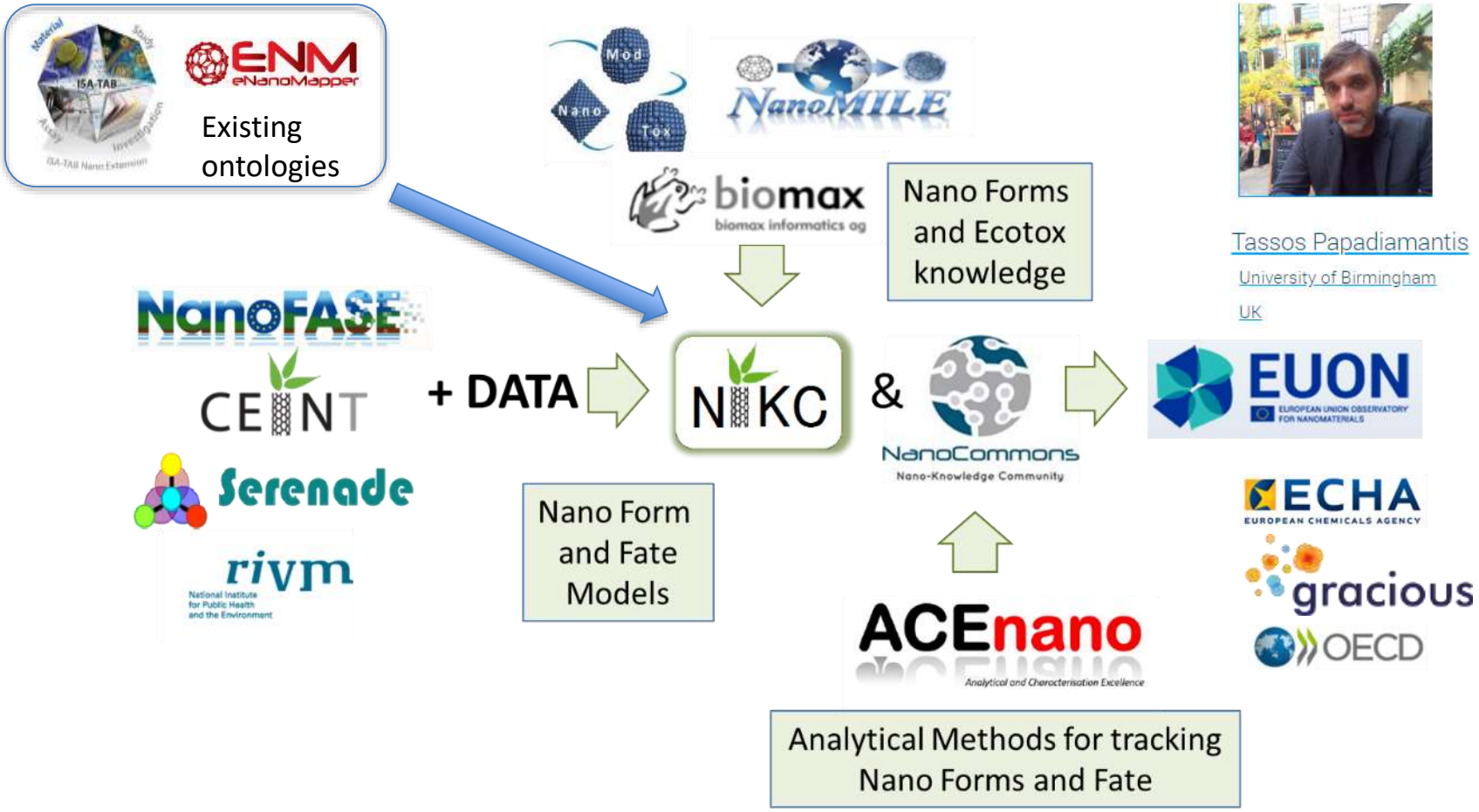

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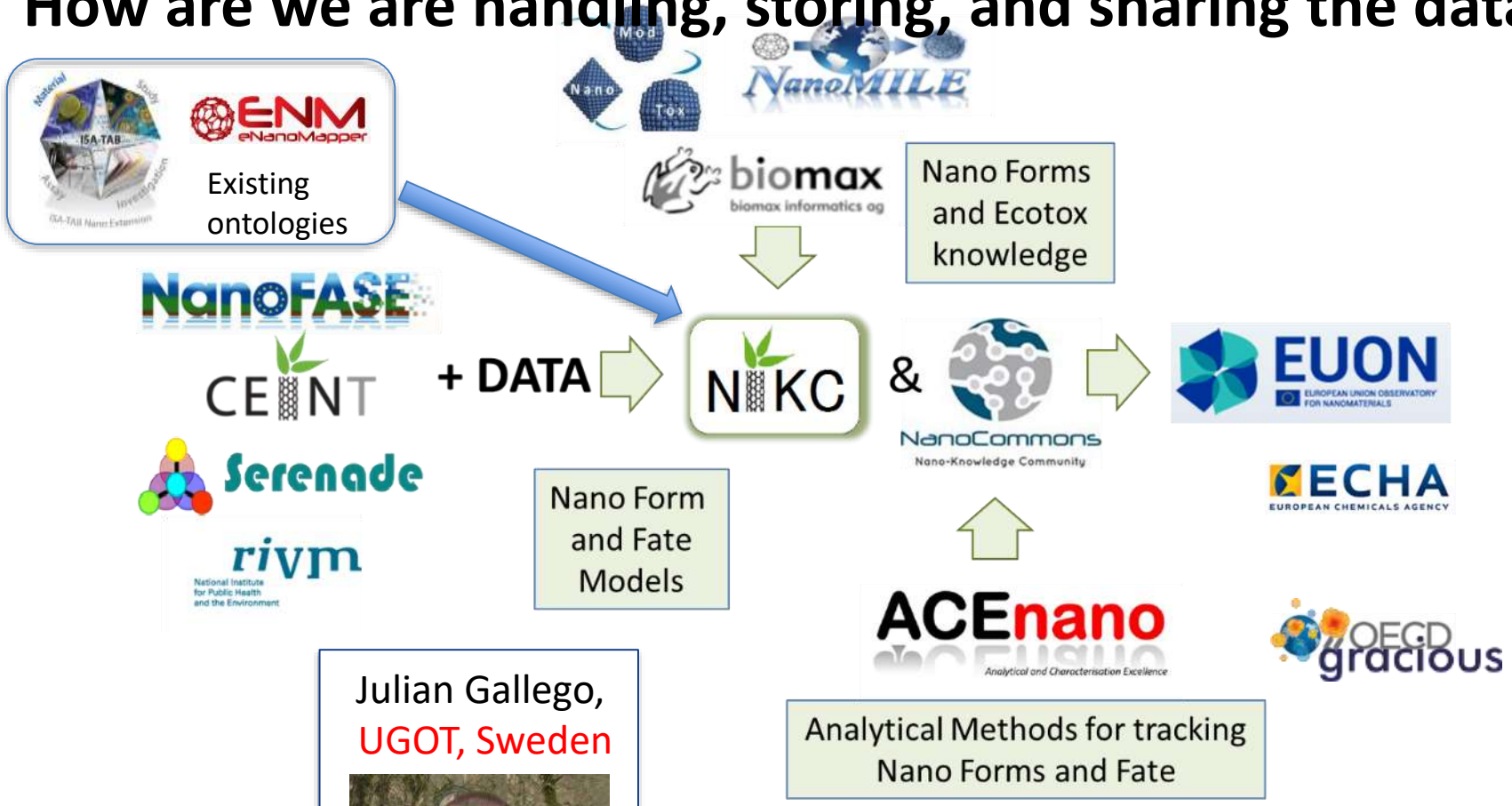


Julian Gallego,
UGOT, Sweden

Exposure - Nanomaterial fate in the environment:

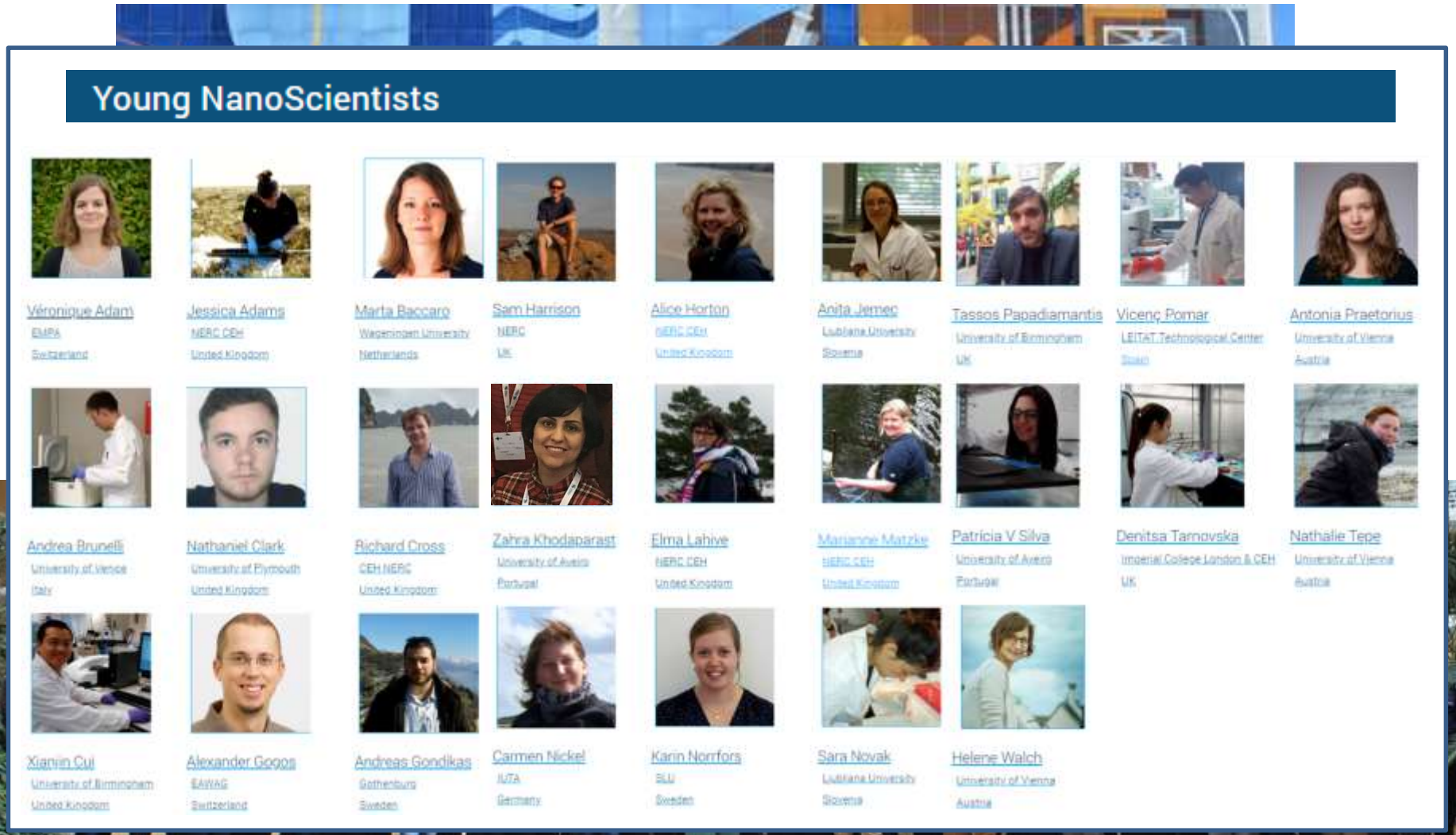
In what format will we deliver it to you all?

NanoFASE

www.NanoFASE.eu (EU H2020 Proj. 646002)

Exposure - Nanomaterial fate in the environment:

In what format will we deliver it to you all?



How will we deliver it to you all?

1. **The new knowledge in Papers and Presentations:**
   http://www.nanofase.eu/documents

2. **Accessible Online resources and tiered Exposure Assessment Framework:**

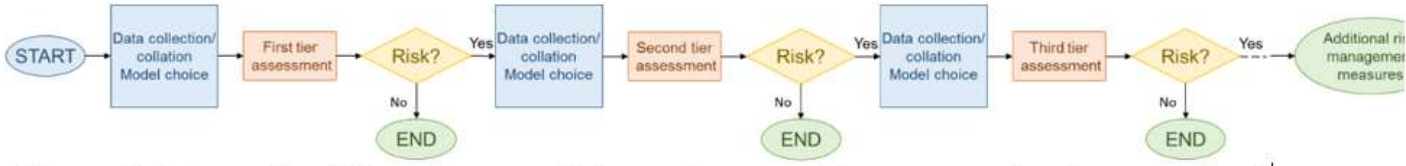


Figure 2: Schematic of tiered approach to environmental assessment using models of increasing complexity.

3. **Fantastically well trained people: The (NanoFASE) "Young Nano Scientists"**

4. **Efforts made to translate our New Knowledge into International Standards:**

ICPMS to spICPMS

New analytics for organic NMs

X-ray based for speciation

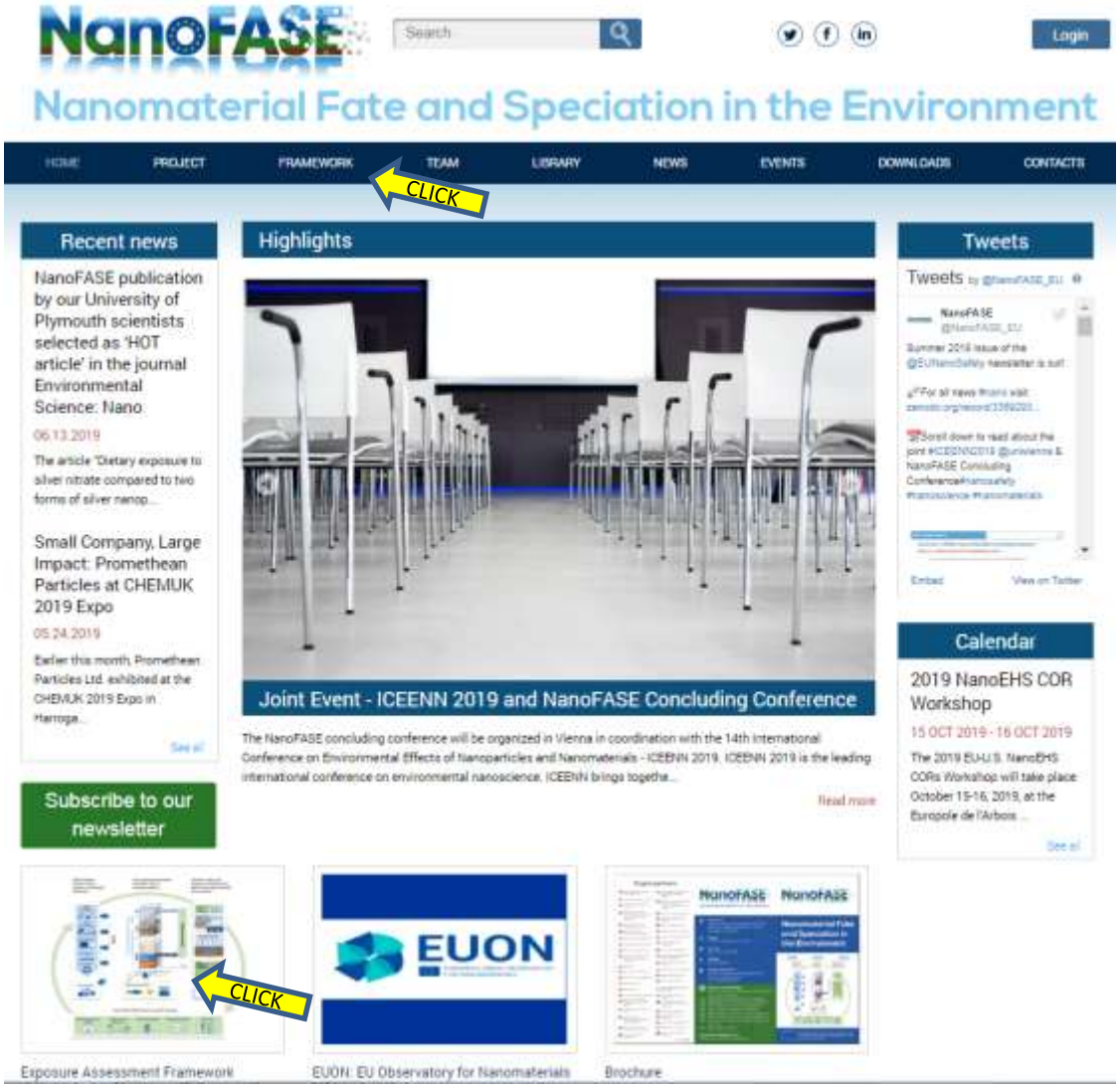
Exposure - Nanomaterial fate in the environment:

In what format will we deliver it to you all?

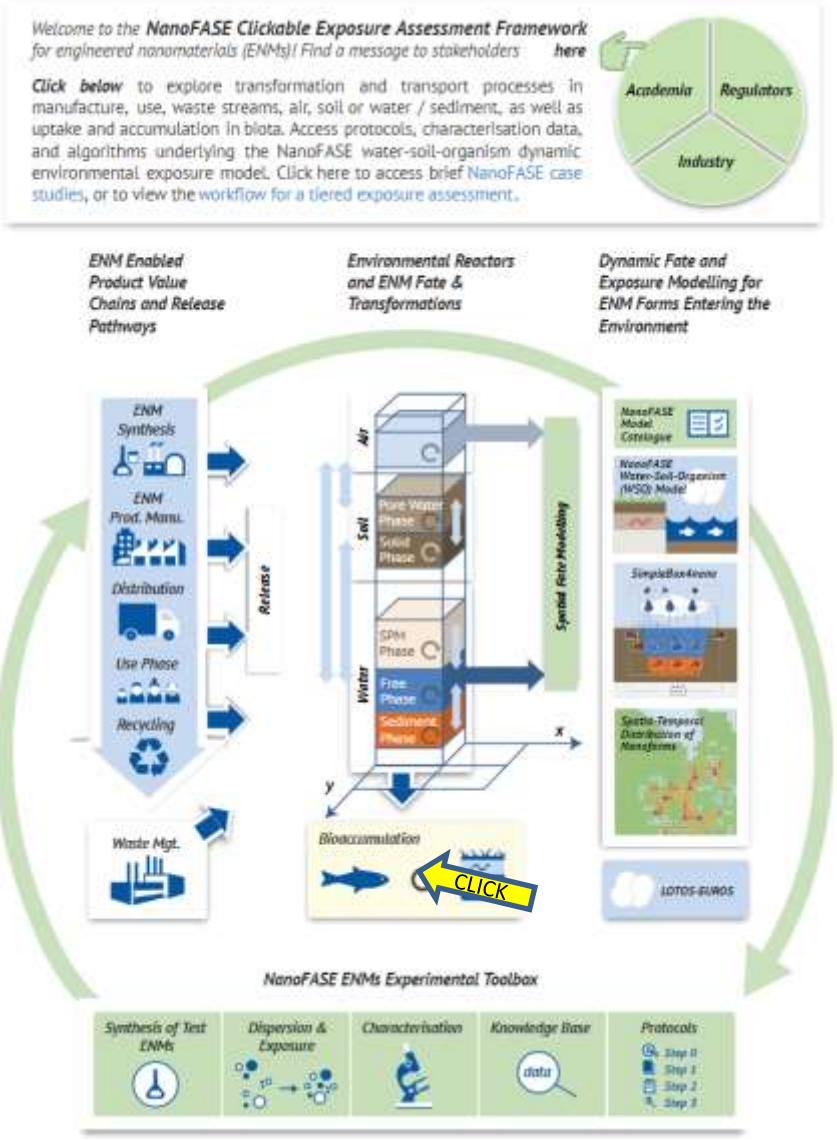
NanoFASE

www.NanoFASE.eu (EU H2020 Proj. 646002)

NanoFASE "Clickable Framework" modules



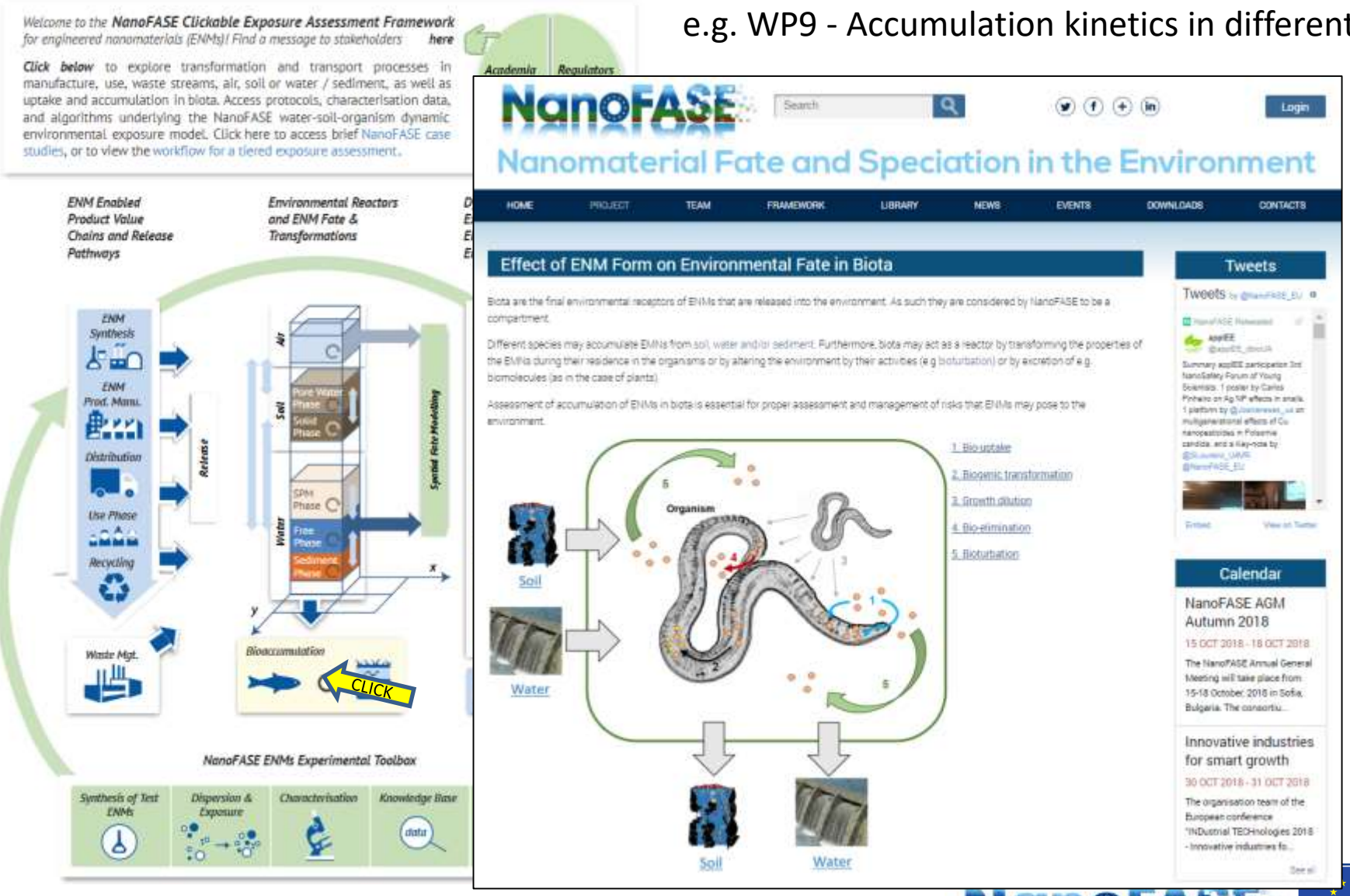
NanoFASE Exposure Assessment Framework



e.g. WP9 - Accumulation kinetics in different biota

NanoFASE Exposure Assessment Framework

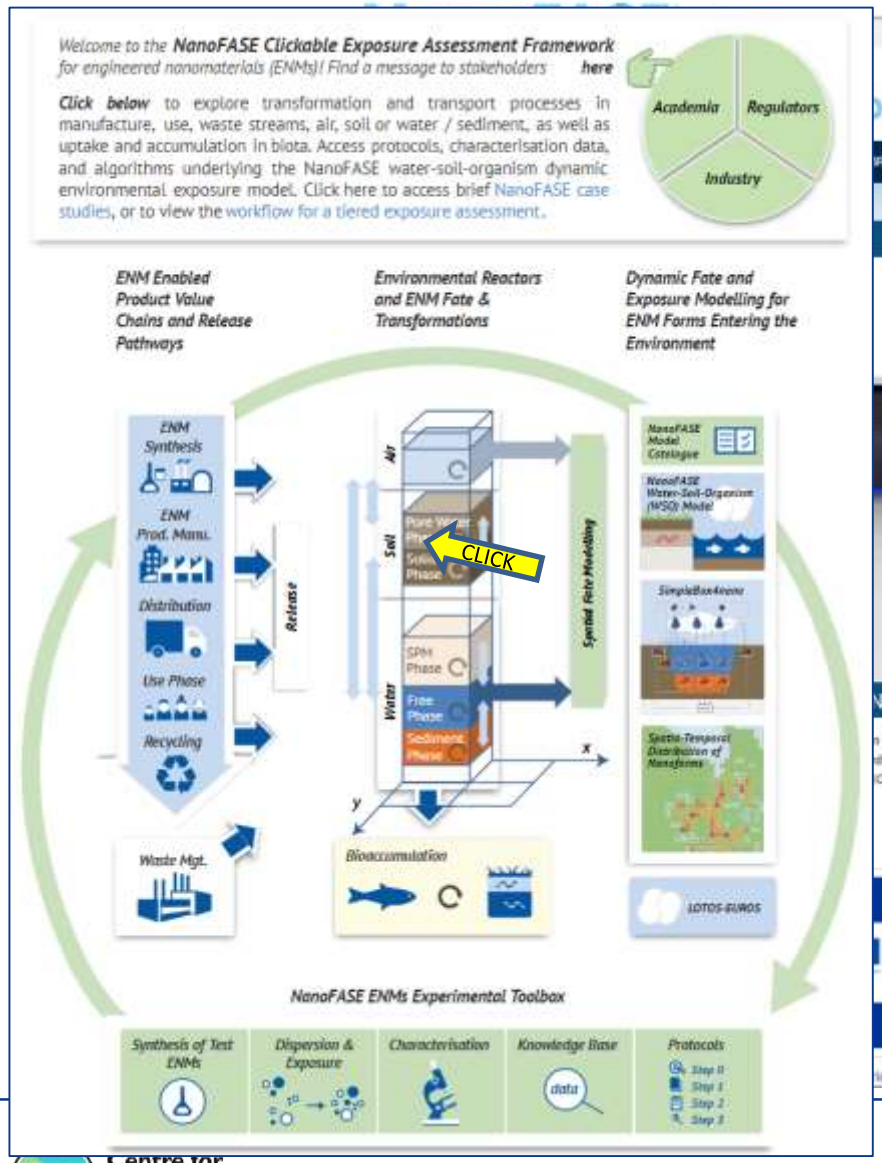
e.g. WP9 - Accumulation kinetics in different biota

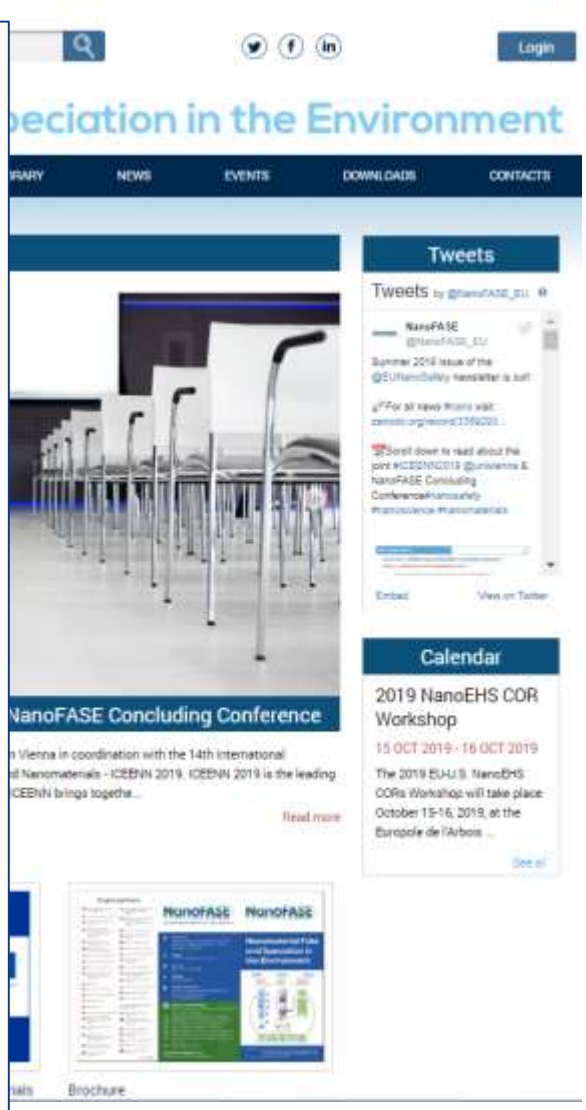


NERC SCIENCE OF THE ENVIRONMENT

NanoFASE

NanoFASE Soil modelling module





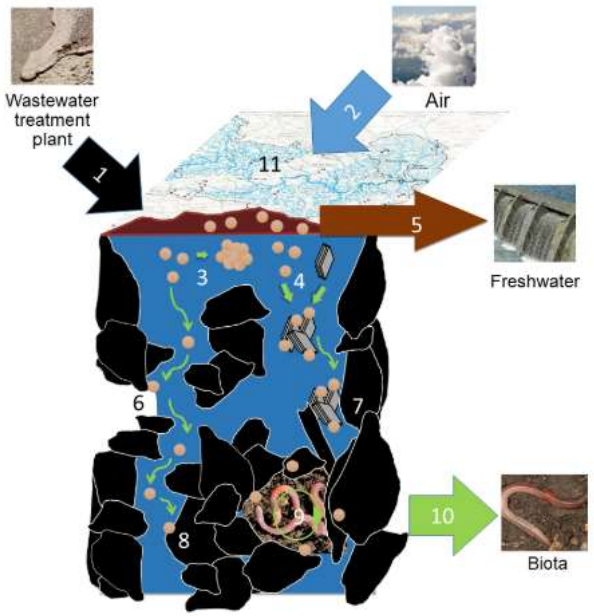
NanoFASE Soil modelling module

Welcome to the **NanoFASE Clickable Exposure Assessment Framework** for engineered nanomaterials (ENMs)! Find a message to stakeholders here

HOME | PROJECT | TEAM | FRAMEWORK | LIBRARY | NEWS | EVENTS | DOW

Environmental Fate of ENMs: Soil Compartment

Soils are exposed to ENMs mostly through deposition of sludge on agricultural land. A range of organisms can be exposed and possibly be affected, including food crops, also giving an entry into the human food chains. ENMs are also applied deliberately to soils, e.g. as zerovalent iron to remediate contaminated soils, as nanofertilizers or as nanopesticides.



1. Sludge deposition
2. Deposition
3. Homoaggregation
4. Hete[illegible]gation
5. Surface run-off
6. Air-water interaction
7. Straining
8. Attachment
9. Bioturbation
10. Bio-uptake
11. Spatial distribution

CLICK

Case studies

- Zerovalent iron
- Nanopesticides

Read also

Cornelis G, et al. (2014) Fate and Bioavailability of Engineered Nanoparticles in Soils: A Review. Crit. Rev. Environ. Sci. Technol. 44: 2720–2764. https://doi.org/10.1080/10643389.2013.829767

Login

Environment

DOWNLOADS | CONTACTS

Tweets

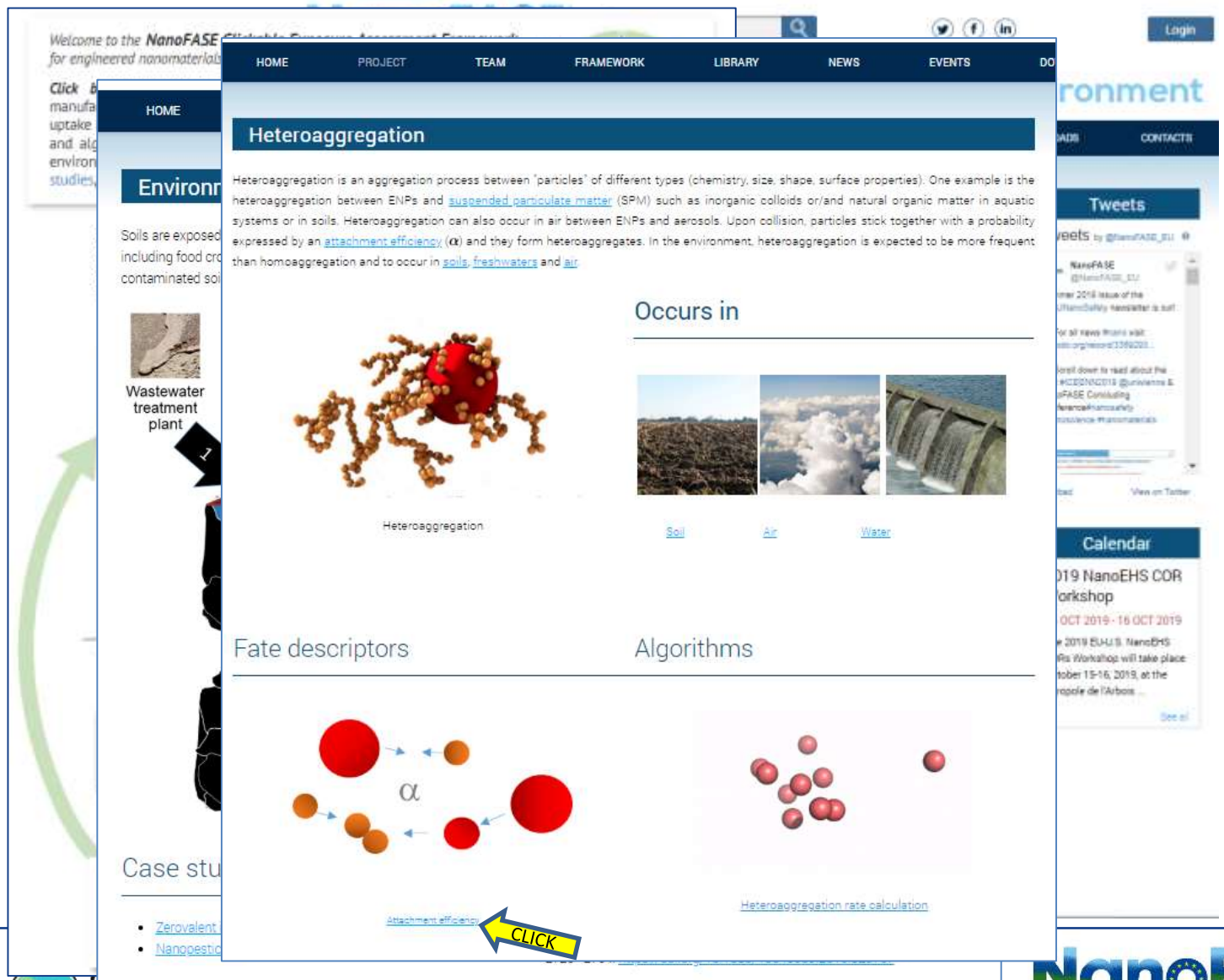
Calendar

2019 NanoEHS COR Workshop

15 OCT 2019 - 16 OCT 2019

The 2019 EU-U.S. NanoEHS CORs Workshop will take place October 15-16, 2019, at the Europole de l'Arbois ...

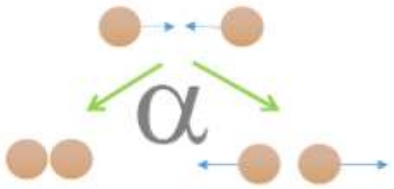
NanoFASE Soil modelling module



NanoFASE Soil modelling module

Attachment efficiency

Attachment efficiency (α) expresses the probability that upon collision of a particle with another surface or another particle, the two particles will stick to each other. In the case of favorable attachment, α equals 1, i.e. all collisions are successful. This is the case e.g. when the particles are oppositely charged or when the ionic strength is relatively high. In most cases, however, $\alpha < 1$, e.g. because of dissolved organic matter adsorption leading to steric hindrance or charges on the particle surfaces resulting in electrostatic repulsion. Attachment efficiency, together with hydrodynamics, determines the attachment rates in porous media such as soils or sediments as well as the homoaggregation and heteroaggregation rates in rivers and wastewater treatment plants.



Used for

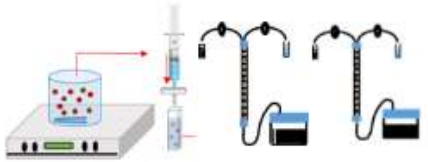
Attachment | Heteroaggreration | Homoaggregation

Algorithms

$$k_{att} = \alpha \frac{3(1-\theta)v}{2d_c}\eta_0 \qquad v = \alpha\beta n^2 \qquad v = \alpha\beta n_A n_B$$

Attachment rate calculation | Homoaggregation rate calculation | Heteroaggregation rate calculation

Protocols



Batch test | Saturated column test | Unsaturated column test

Read more

NanoFASE Report D7.2 Soil property - NM fate relationships

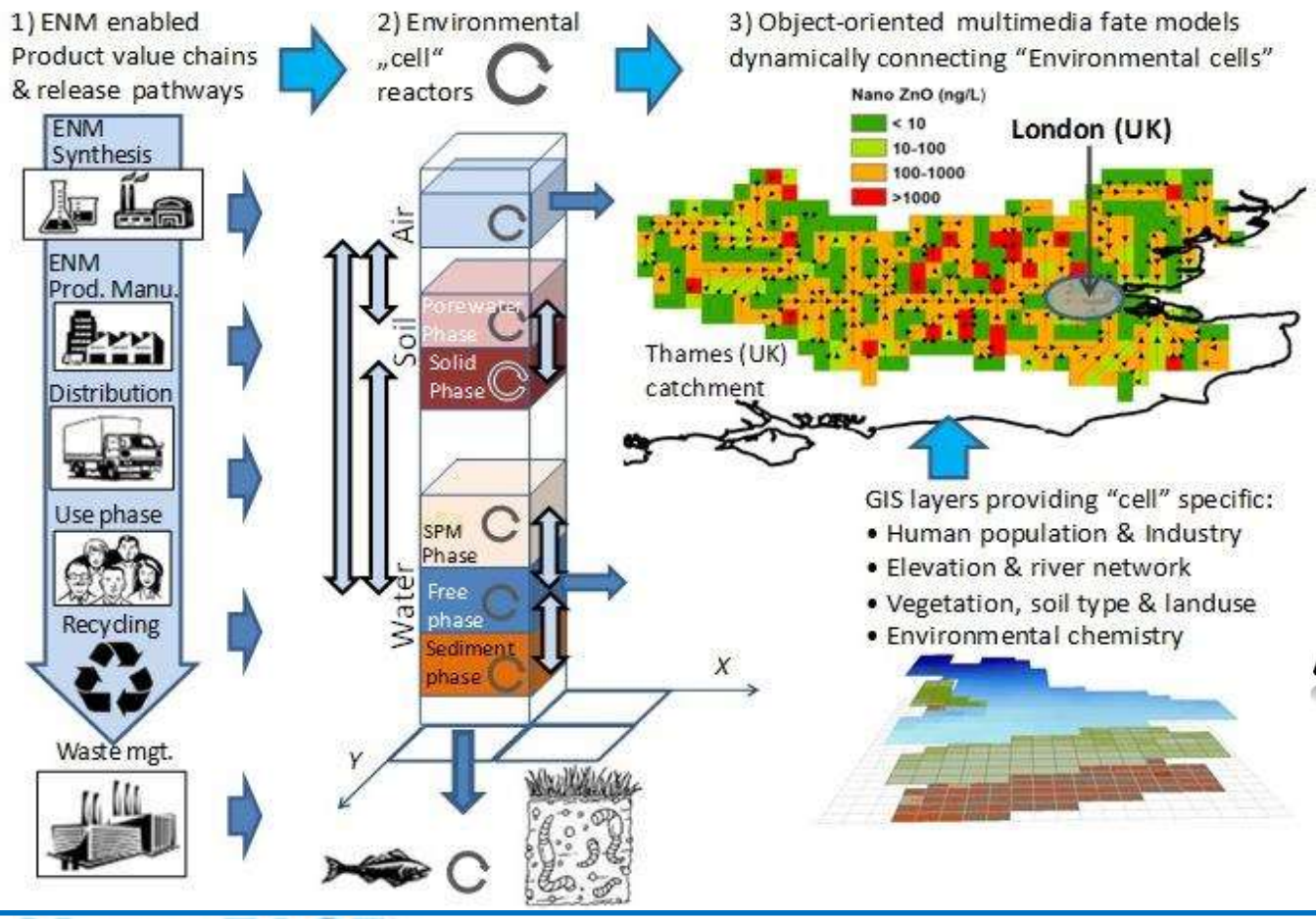
NanoFASE Report D8.1 Alignment between model requirements and experimental procedures

Read also

Petosa, A. R.; Jaisi, D. P.; Quevedo, I. R.; Elimelech, M.; Tufenkji, N. Aggregation and Deposition of Engineered Nanomaterials in Aquatic Environments: Role of Physicochemical Interactions. Environ. Sci. Tech. 2010, 44 (17), 6532-6549.

Exposure - Nanomaterial fate in the environment:

In what format will we deliver it to you all?



FOCUS ON:
“Reactors” and relevant ENMs (Focus on *relevant materials at each RA step*)

DELIVER:
Functional fate groups
a tool to understand *and reduce* complexity

gracious

Exposure assessment framework *catalogue* of models, parameters and methods

ACEnano OECD

Multimedia fate models
simplified to feed regulatory models (SimpleBox 4 Nano)

caLIBRAte nano risk governance ECHA EUROPEAN CHEMICALS AGENCY

NanoFASE CEINT **DATA +** NKC => NanoCommons Nano-Knowledge Community => EUON EUROPEAN UNION OBSERVATORY FOR NANOMATERIALS

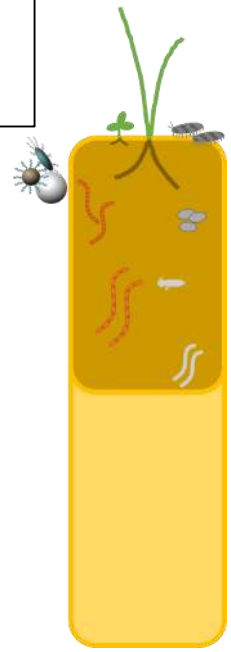
Putting it all together for exposure relevant NPs

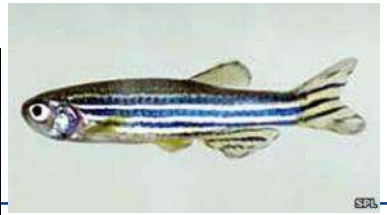
Mesocosm kinetic tests (Long term, Low dose, High complexity)

- Aquatic and terrestrial
- Include most species from earlier single species tests
- Performed in Aveiro (Portugal) Summer 2018
- Will validate the single species experiments
- Results to be expected early 2019.





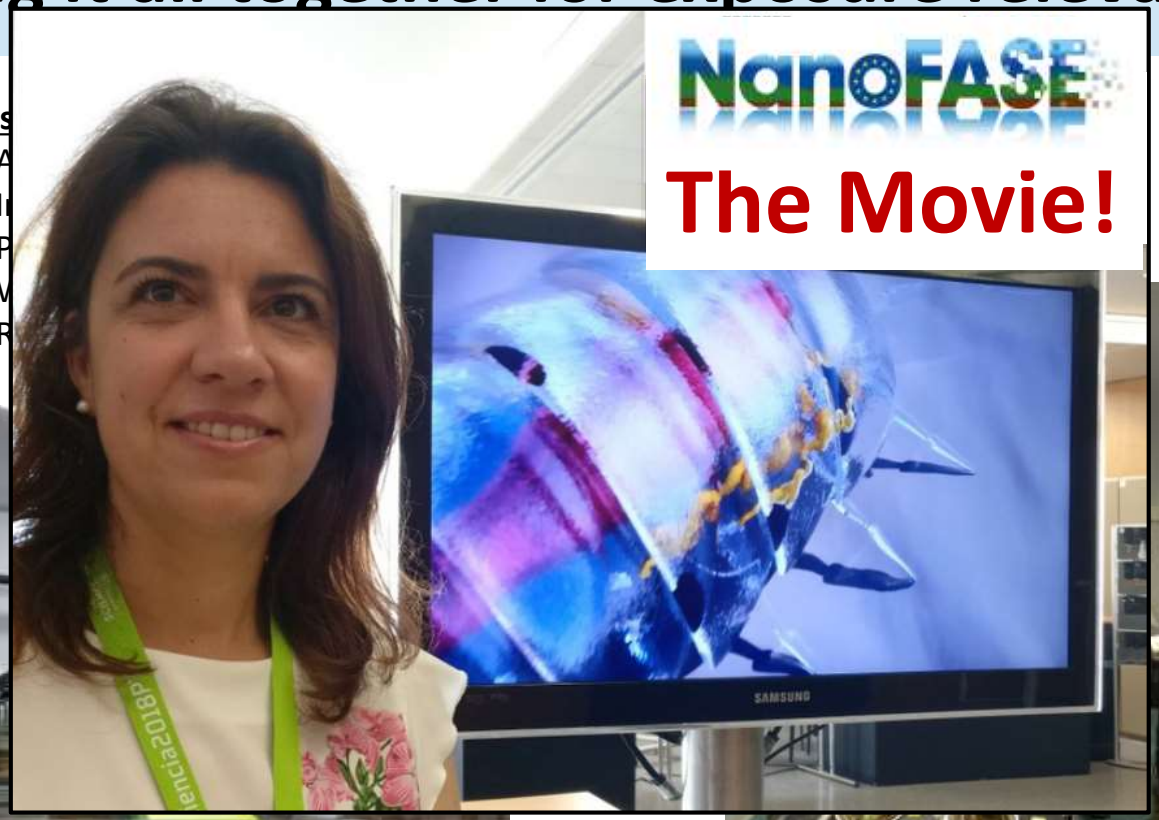


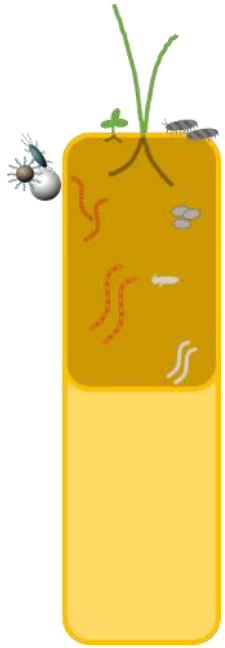





Putting it all together for exposure relevant NPs

Mes
- A
- I
- P
- V
- R





"***NanoFASE THE MOVIE!***" is out – search "NanoFASE and Mesocosm"

Exposure - Nanomaterial fate in the environment:

Thank you! Onwards and upwards!