NanoFASE models and exposure assessment: overview, lessons learned and future developments







### Outline

- Overall Aims and Objectives, project structure
- Environmental Exposure Assessment
  - Tiered approach to assessment conceptual
- Fate/Exposure models in NanoFASE
  - SimpleBox4Nano; LOTOS-EUROS; NanoFASE WSO model
- NanoFASE WSO model: achievements
- Exposure Assessment Framework: achievements
- The future: regulatory uptake (EUSES), risk governance/Safe by Design



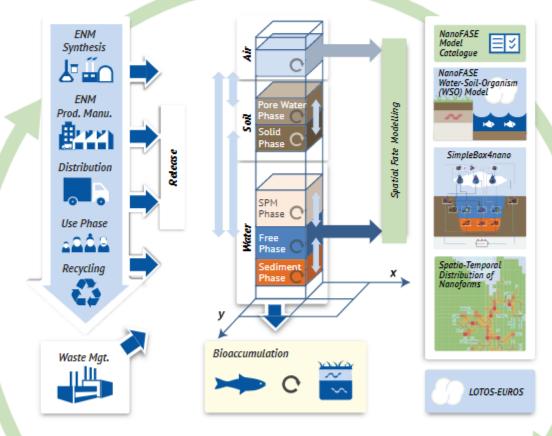


Aims and Objectives

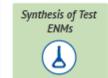
www.nanofase.eu



ENM Enabled Product Value Chains and Release Pathways Environmental Reactors and ENM Fate & Transformations Dynamic Fate and Exposure Modelling for ENM Forms Entering the Environment



NanoFASE ENMs Experimental Toolbox



Dispersion & Exposure



Characterisation



Knowledge Base



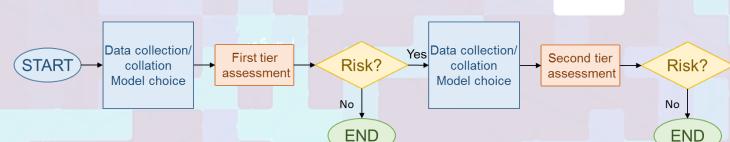
Protocols



Step 2 Step 3

#### REGULATORY RELEVANCE

Nano WG April 2020



Increasing complexity

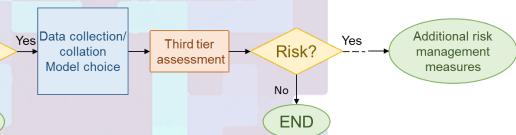
Increasing realism

Decreasing conservatism

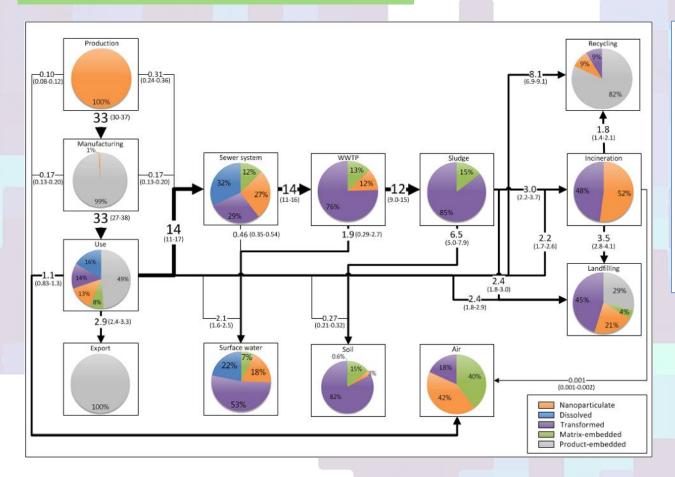
Increasing data demands and "expertise" required to run



## Tiered exposure assessment







## Emissions modelling

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.

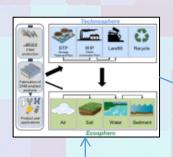
Adams, V et al 2018 Environmental Pollution, 243, pp 17-27





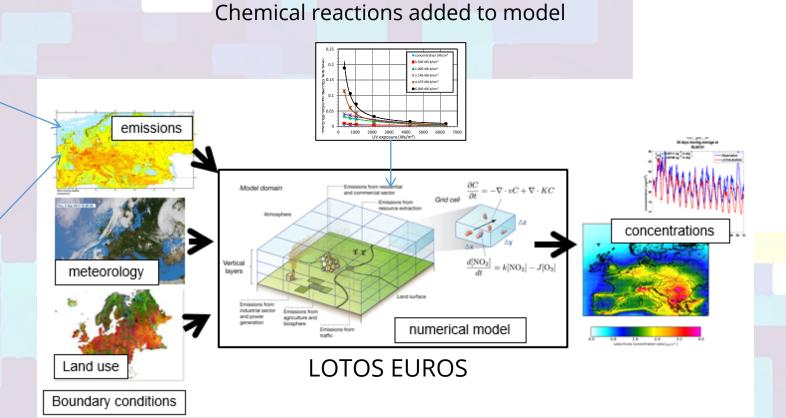
## LOTOS-EUROS

Emission inventory





Measured ENM emissions used as input data







- A screening level exposure model
- Nano-capable version of SimpleBox
- SimpleBox is the basis of EUSES, the environmental exposure modelling tool used in REACH

## SimpleBox4Nano

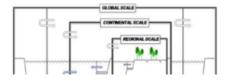
#### SimpleBox4nano

<u>SimpleBox4nano</u> is a regulatory-relevant multimedia fate model that is specifically fit for use with nanomaterials. The tool predicts background concentrations of nanomaterials in air, water, sediment and soil. For this reason, it is the perfect <u>second-tier (screening)</u> tool as part of the NanoFASE Exposure Assessment Framework, which also includes <u>third-tier (higher realism)</u> assessment tools.

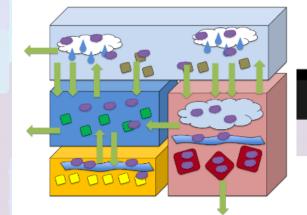
The EU's <u>REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals</u>) regulations require that environmental exposure assessmen of chemicals be predicted by modelling. This is done by following the approach and methodology set out in the <u>European Union System for the Evaluation of Substances (FUSES)</u>. FUSES is a decision-support tool for predicting environmental exposure in the assessment of chemicals. Part of

#### http://nanofase.eu/show/simplebox4nano\_1299

a series of well-finded boxes of all, water, sediment and soli of regional, well-finded and global scales. Simplebox is a mistry-finding into account both physical and chemical substance properties and characteristics of the environment modelled. It takes user-specified release rates of the chemical into the environment as input, and produces exposure concentrations in the different compartments of the environment as output. This type of model is known as a 'Mackay model', after its inventor, Donald Mackay.





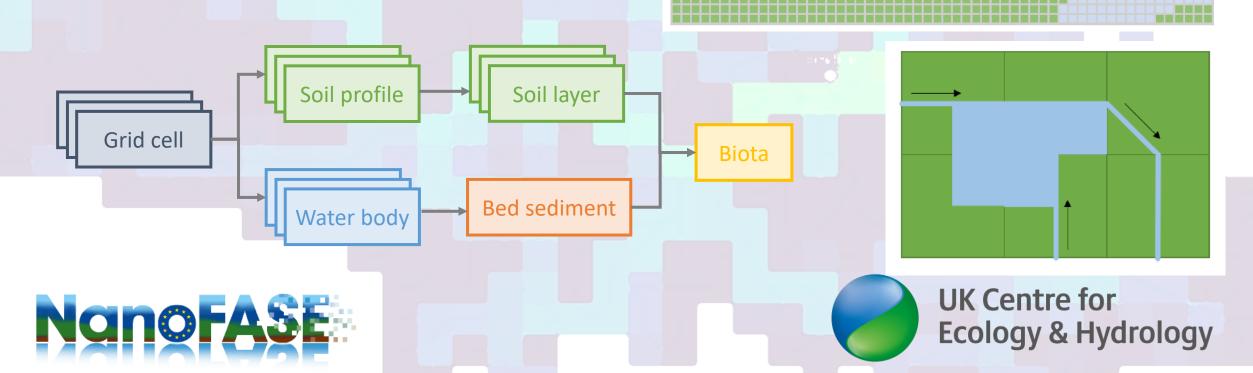




#### NANOFASE MODEL

# The NanoFASE water-soil-organism model

Spatiotemporal model of nanomaterial fate, speciation and bio-uptake in the environment



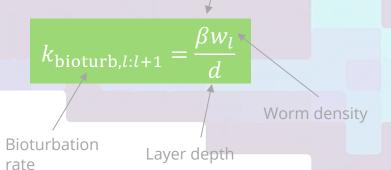
#### NANOFASE MODEL

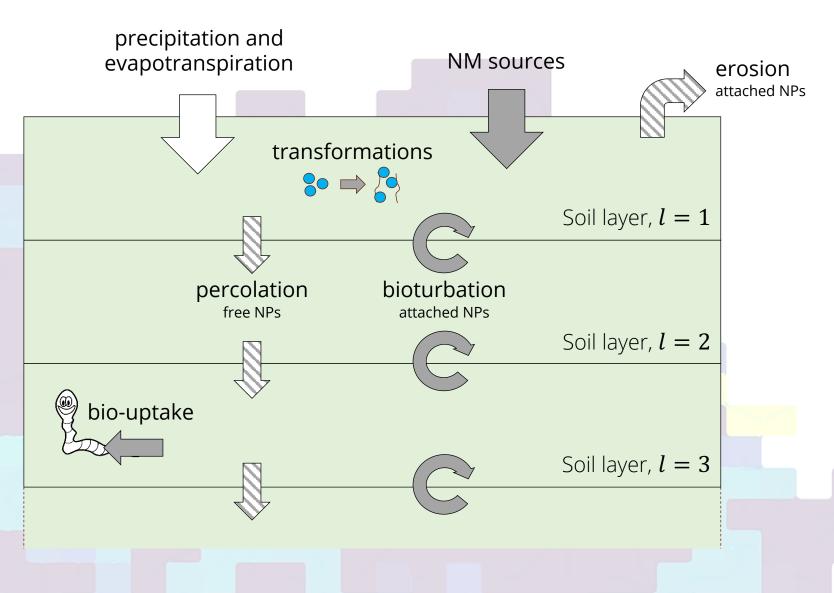
## Soil profile

Transformations: e.g. attachment to soil matrix

Bioturbation rate is function of earthworm density:

Empirical bioturbation parameter









UK Centre for Ecology & Hydrology

#### NANOFASE MODEL

## Rivers and estuaries

Transformations: e.g. **heteroaggregation** to SPM

Attachment efficiency

Collision frequency

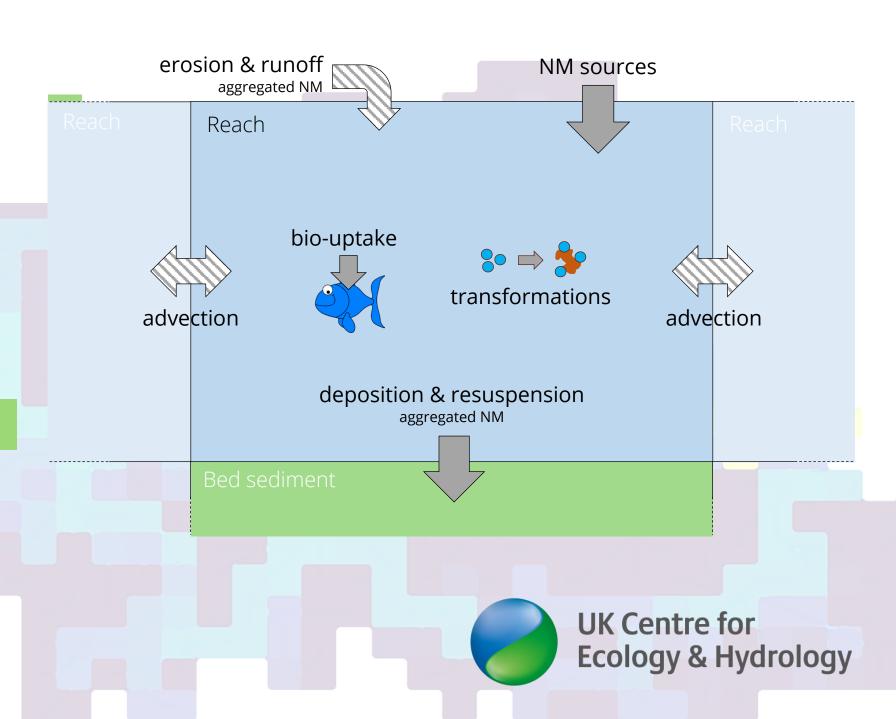
 $k_{\text{hetero}} = \alpha_{\text{hetero}} k_{\text{coll}} C_{\text{spm}}$ 

Heteroaggregation rate

SPM particle concentration

 $\alpha_{hetero} = 0.01$  freshwater 0.1 estuarine

NanoFASE



## How it all fits together

NM emissions data<sup>1</sup>

Meteorological data

Other data Geography Soil properties Land use Atmospheric deposition model (LOTOS-EUROS¹)

Hydrological model (HMF<sup>2</sup>)

NanoFASE watersoil-organism model Spatiotemporal NM fate, speciation and bio-uptake

[1] doi:10.1016/j.envpol.2018.07.108 [2] doi:10.5194/gmd-10-4145-2017 [3] doi:10.3390/hydrology1010063



UK Centre for Ecology & Hydrology

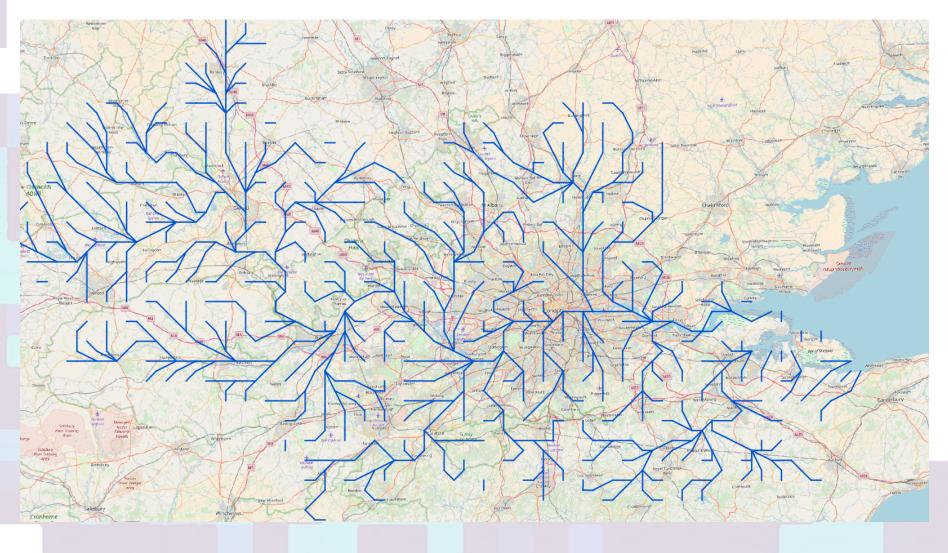


to the Thames catchment

Resolution: 5x5 km

Years: 2000-2020

Materials: TiO<sub>2</sub>







## Where do NMs end up?

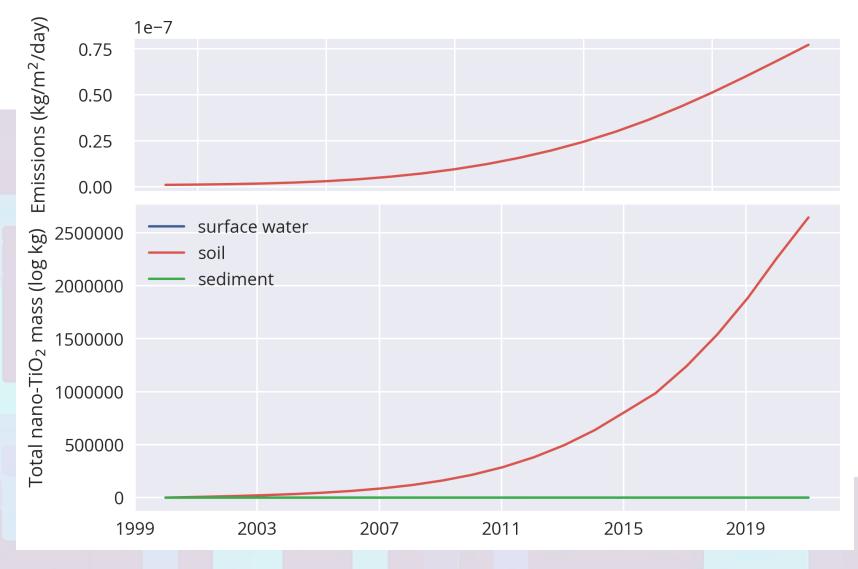
Total mass of nano-TiO<sub>2</sub> in the entire catchment, split by environmental compartment.



Soil acts as a sink



Main driver to long-term dynamics 2 exponentially increasing emissions







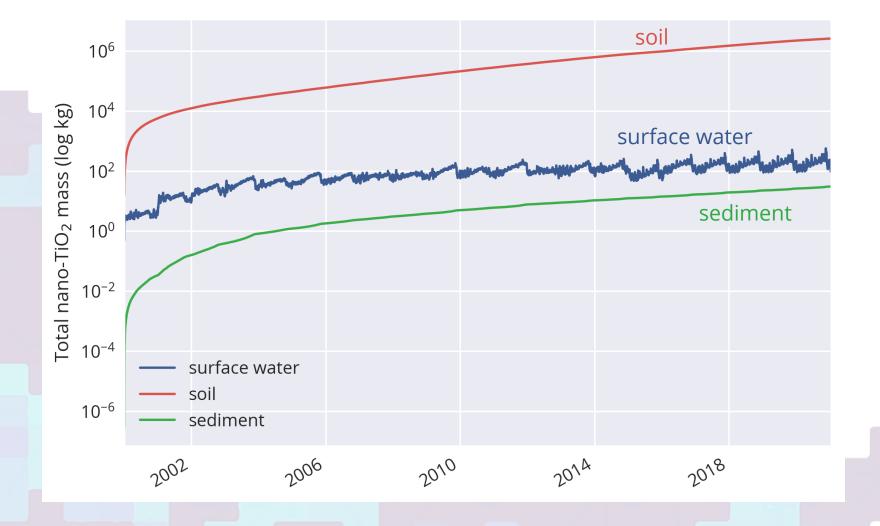
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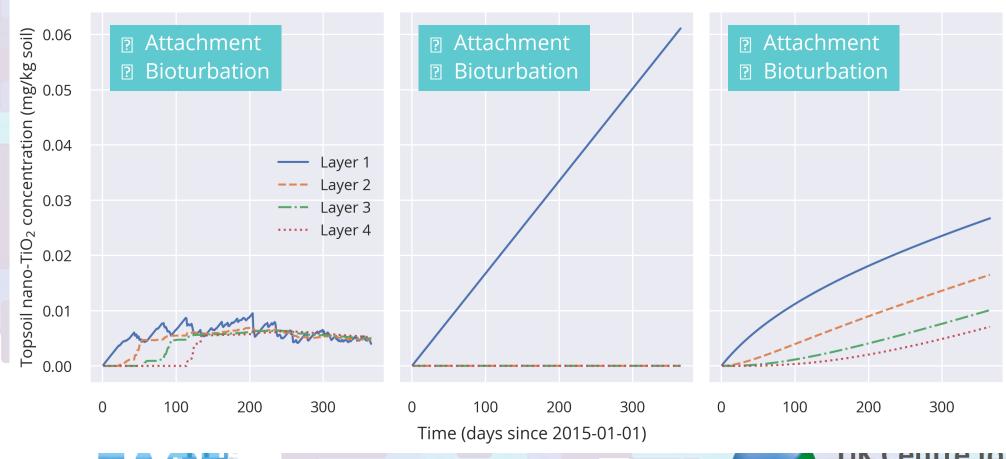
Main driver to long-term dynamics exponentially increasing emissions







### Attachment and bioturbation in soils



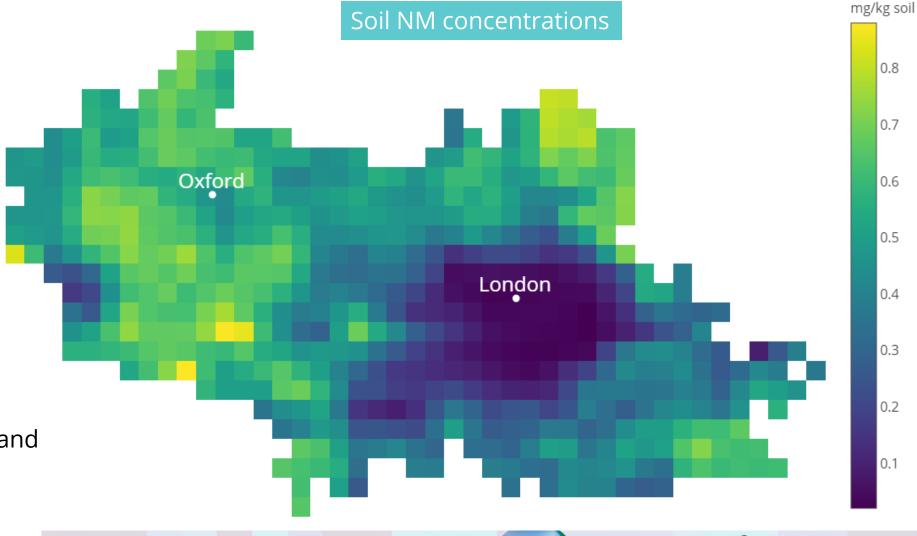




the hotspots?

Nano-TiO<sub>2</sub> predicted environmental concentrations (PEC) in soil at the end of 2020.

Main determinant of spatial distribution land use



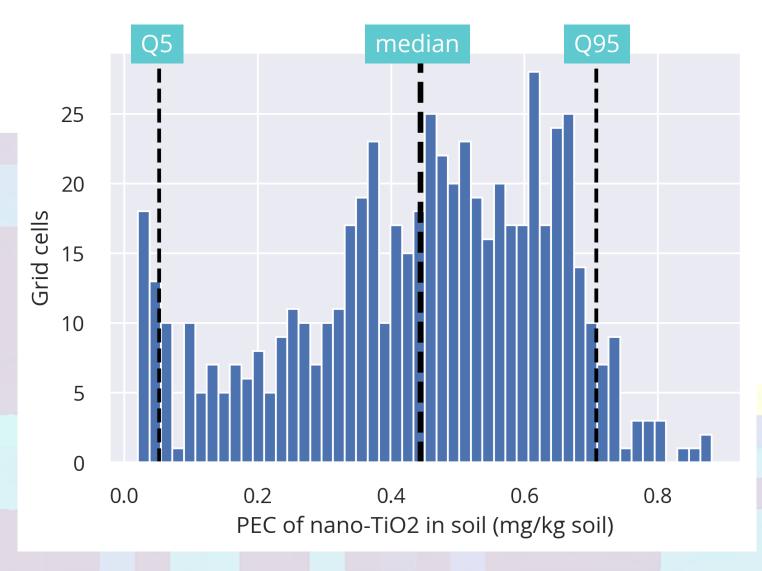




What is the spatial distribution?

Nano-TiO<sub>2</sub> predicted environmental concentrations (PEC) in soil at the end of 2020.

Q5 0.05 mg/kg soil Median 0.44 mg/kg soil Q95 0.71 mg/kg soil







# What are the dynamics?

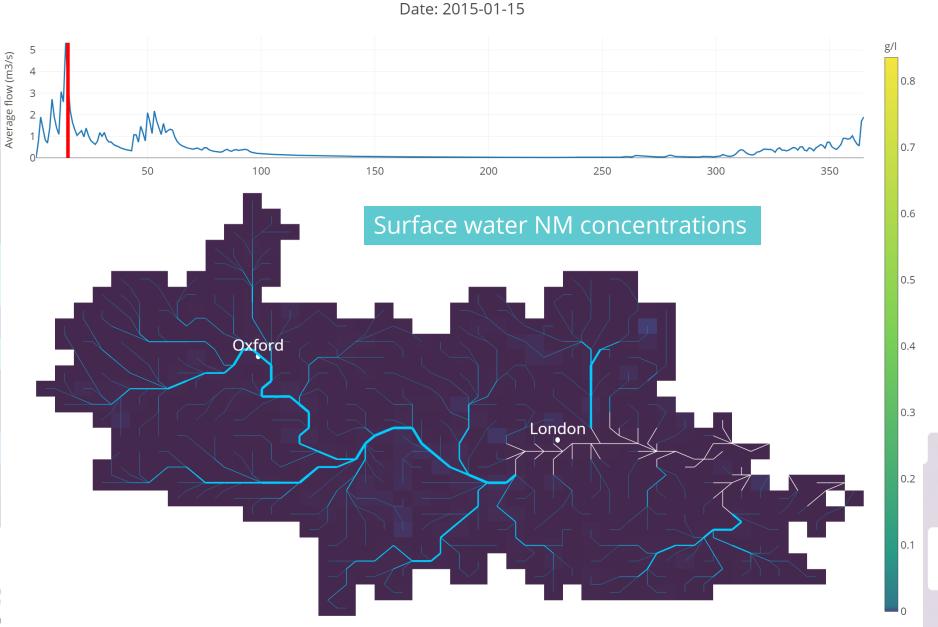
Influence of dynamic variables, e.g. hydrological flows, over time.



Low flows 12 high concentrations



Estuary is big I low concentration





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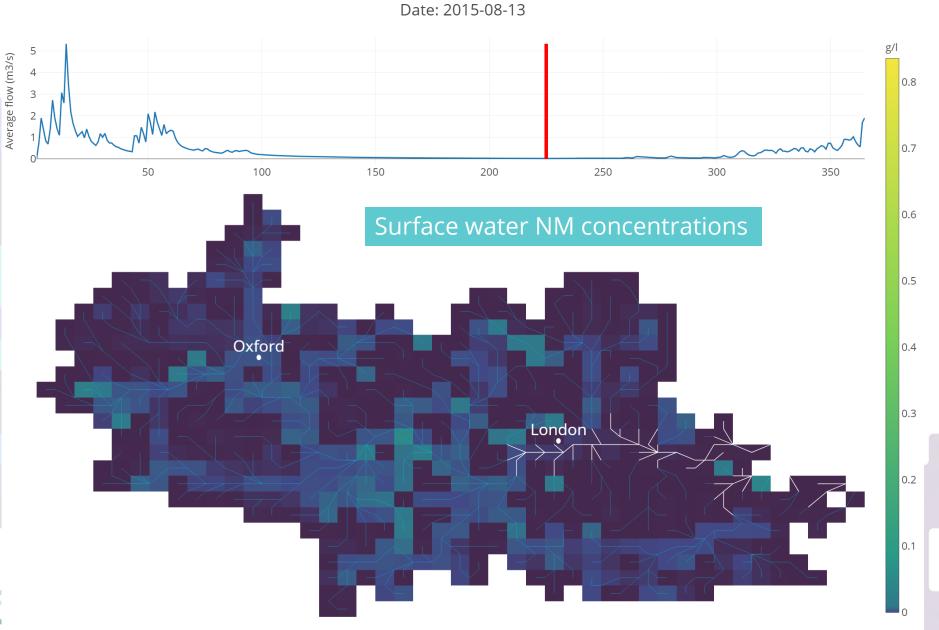
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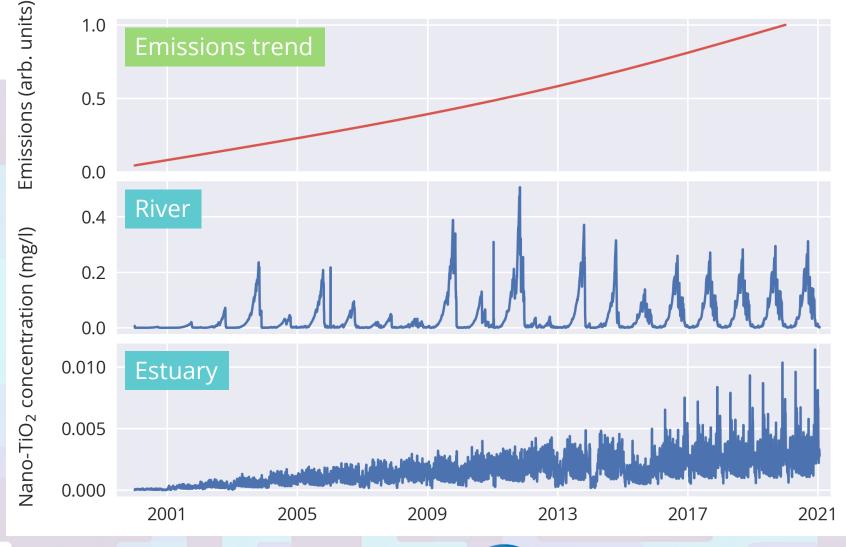




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Influence of dynamic variables, e.g. hydrological flows, over time.

Riverine temporal trend strongly influenced by hydrology

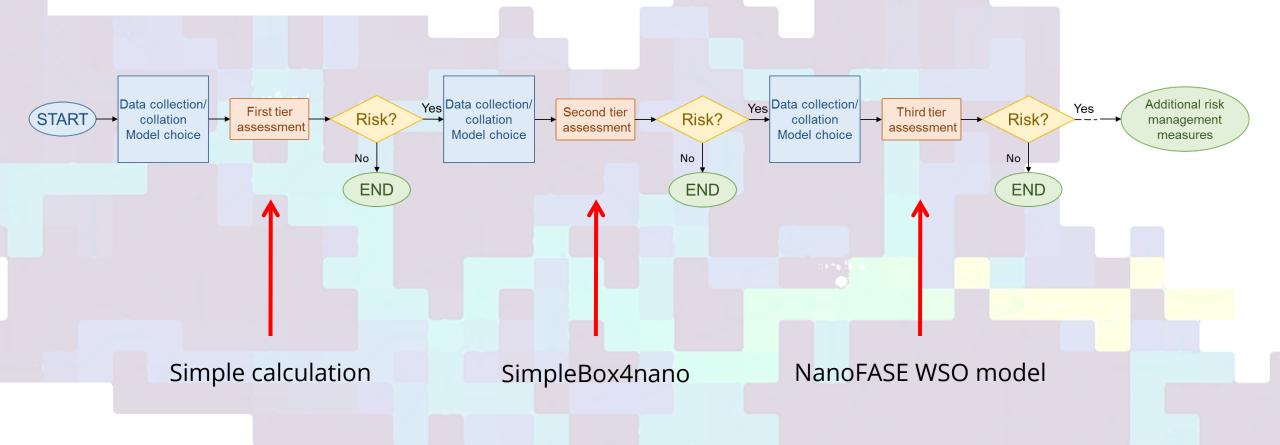






#### REGULATORY RELEVANCE

## Tiered exposure assessment







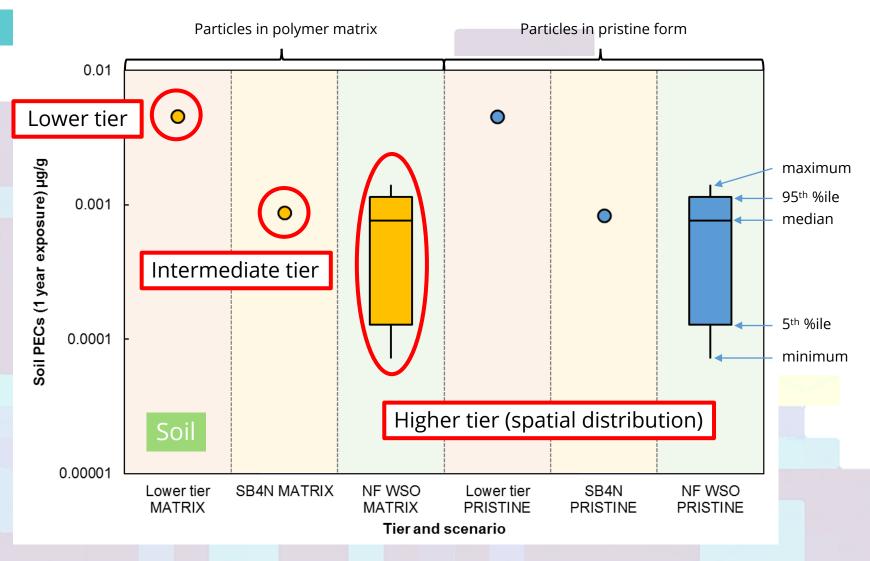
#### REGULATORY RELEVANCE

Tiered exposure assessment

Case study: TiO<sub>2</sub> applied as road coating in Thames catchment

High tiers = lower PEC

nanofase.eu/exposure\_ assessment\_framework







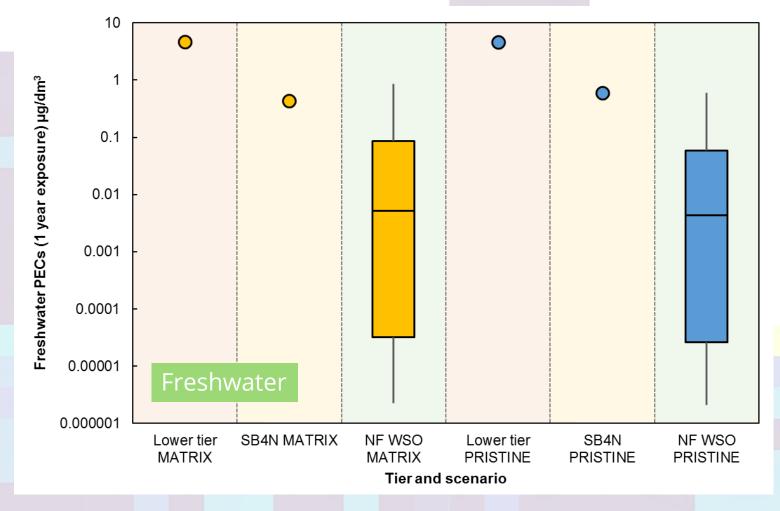
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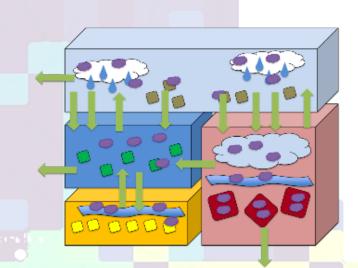


#### DISCUSSION

## Regulatory perspective

- NanoFASE WSO model useful to compare, evaluate and scope changes to screening level tools e.g. SimpleBox4Nano
- Potential occasional use for high level tools in risk assessment where substance fails at lower tiers
- Uptake of tools by regulators...
  - ECHA aware of SimpleBox4Nano
  - Can be a slow process (regulatory conservatism)
  - Industry stakeholder input/pressure important
  - Model parameter needs should be linked to testing requirements if at all possible
  - Linkages to databases…?







### Future

Risk Governance and Safe by Design

Appropriate **model choice** for early
stages of product
development

Utility of model outcomes in the design cycle

### **Usability of models**

- Exposure scenarios
- Parameter selection

Links to data for parameter derivation?





### NanoSolv eIT

#### **Knowledge Base**

Exposure data Hazard data

Structural Specifications Compositional data

## **Fingerprint formulation**

Descriptors

Meta-models for properties (intrinsic and extrinsic)

#### **IATA**

Exposure estimation

Adverse Outcome prediction Human and environmental exposure and risk assessment





Nano WG



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 An overview of the NanoFASE model with some commentary on its reception, lessons learned, value of the NIKC to your modeling, and what would be required to be a priority at the next EUSUS



