Nano WG April 2020

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

NanoFASE

UK Centre for Ecology & Hydrology

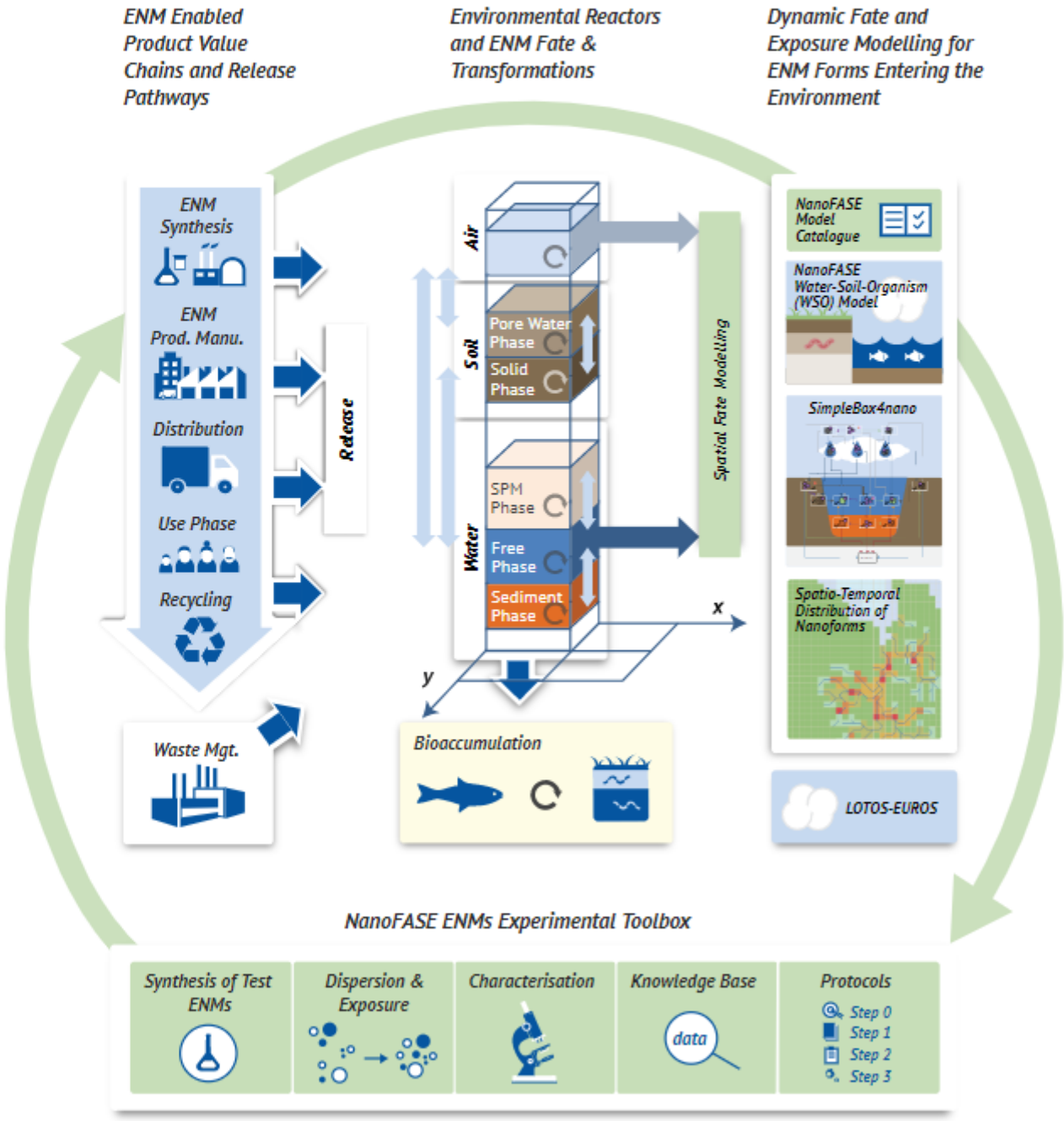
Outline

- 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

Nano WG April 2020

Aims and Objectives

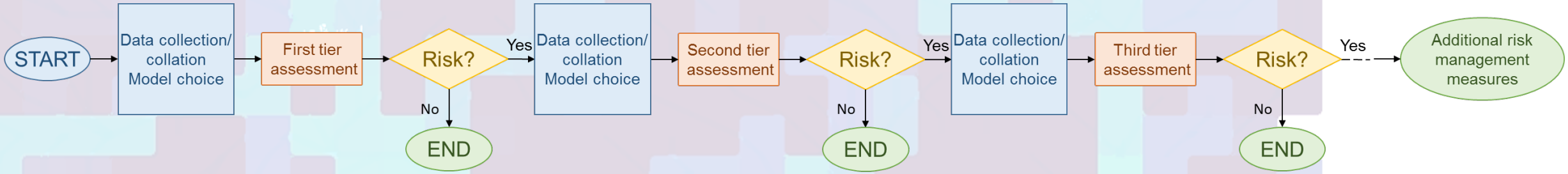
www.nanofase.eu



REGULATORY RELEVANCE

Nano WG April 2020

Tiered exposure assessment



Increasing complexity

Increasing realism

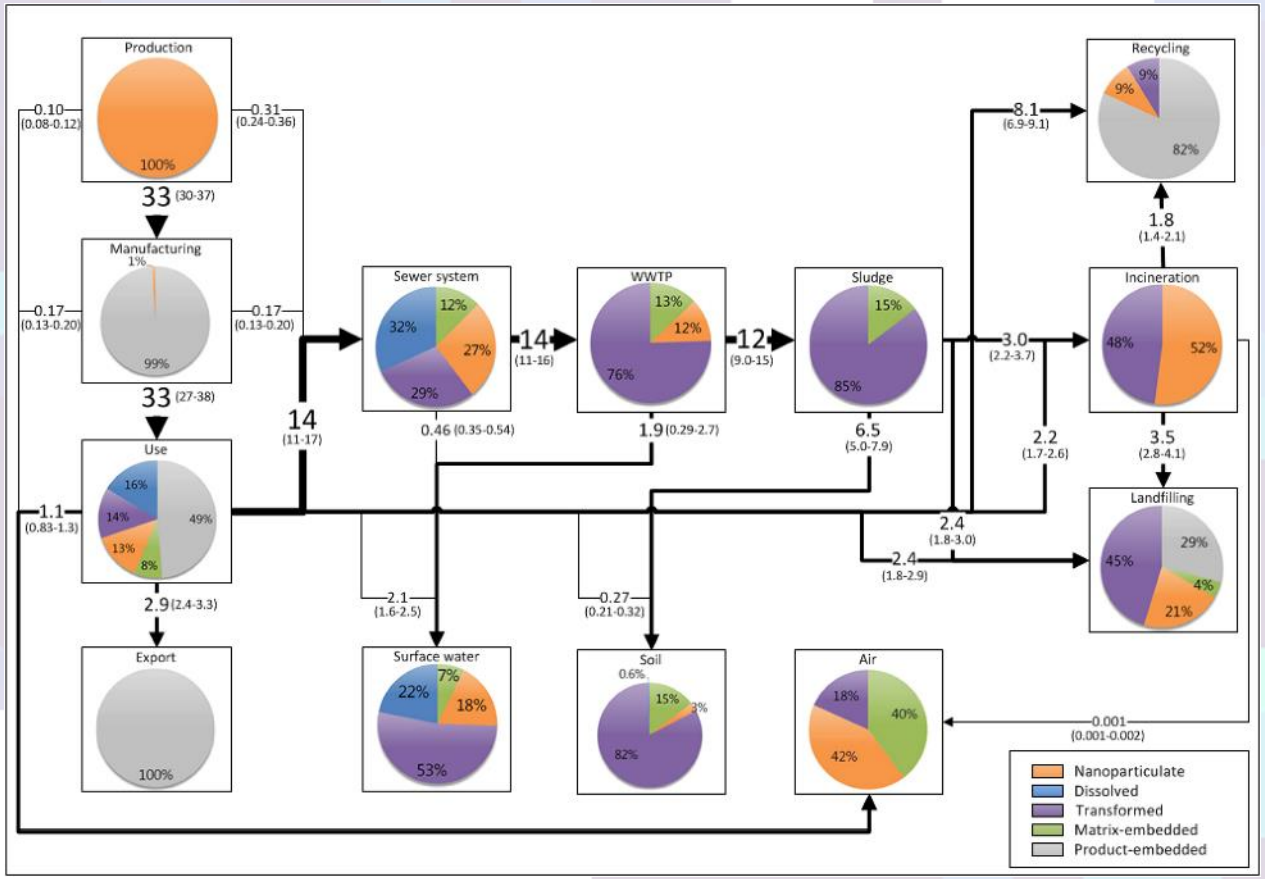
Decreasing conservatism

Increasing data demands and "expertise" required to run

NanoFASE

UK Centre for Ecology & Hydrology

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.

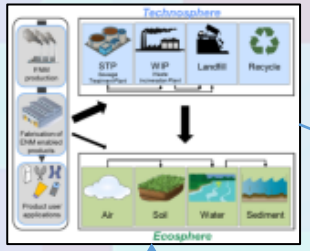
Adams, V et al 2018 Environmental Pollution, 243, pp 17-27

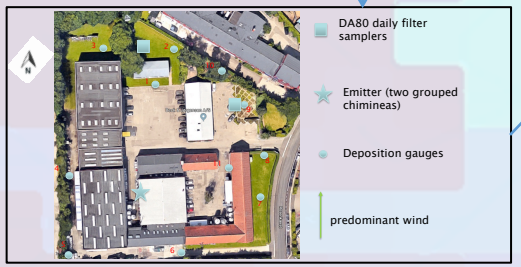
NanoFASE

UK Centre for Ecology & Hydrology

LOTOS-EUROS

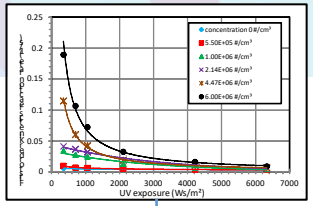
Emission inventory





Measured ENM emissions used as input data

Chemical reactions added to model



LOTOS EUROS

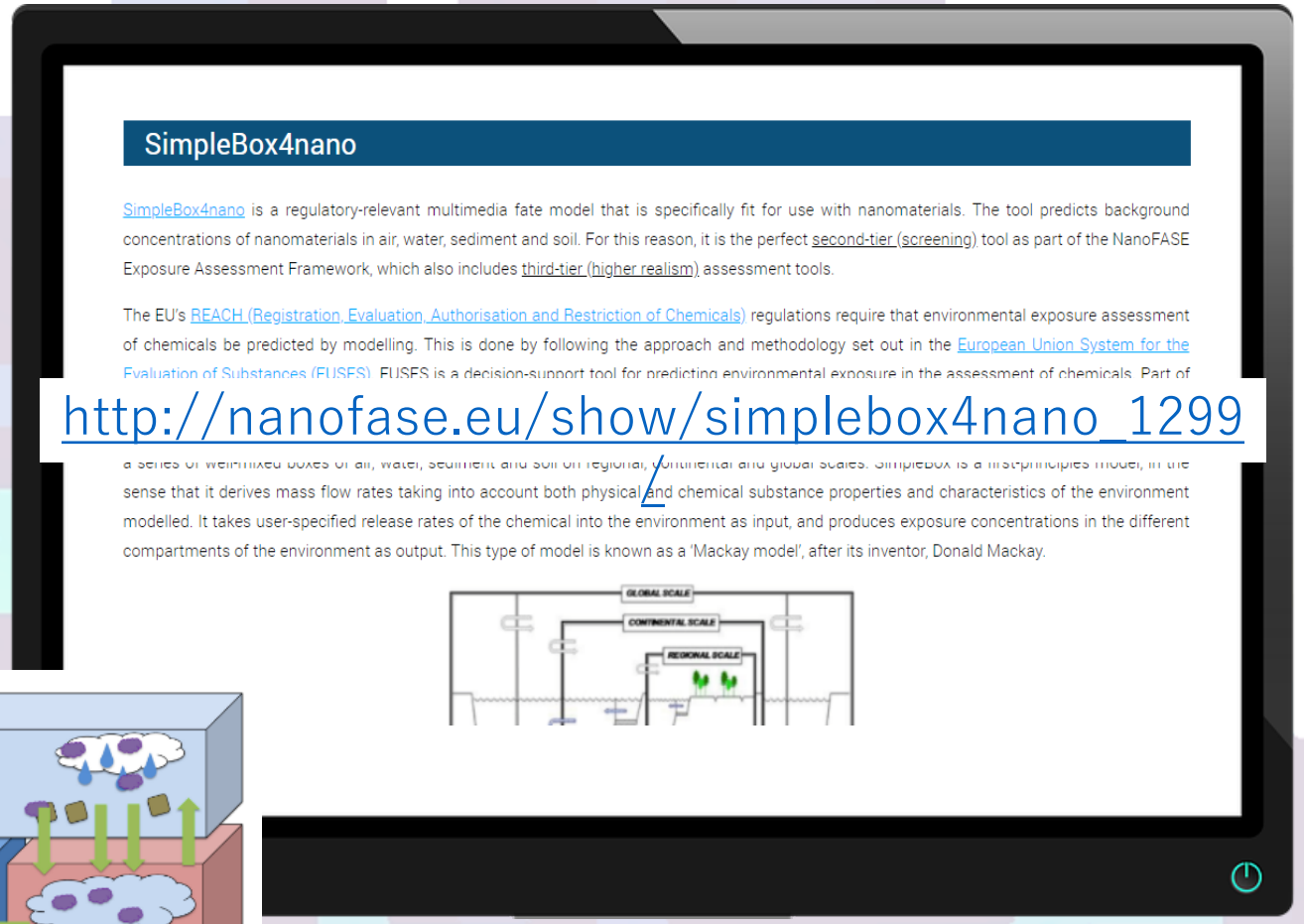
NanoFASE

TNO innovation for life

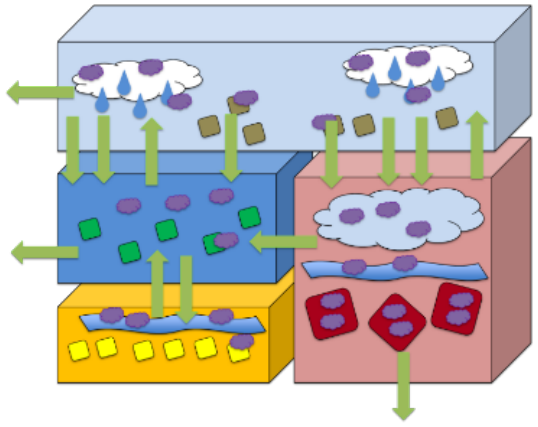
SimpleBox4Nano

Nano WG April 2020

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



http://nanofase.eu/show/simplebox4nano_1299



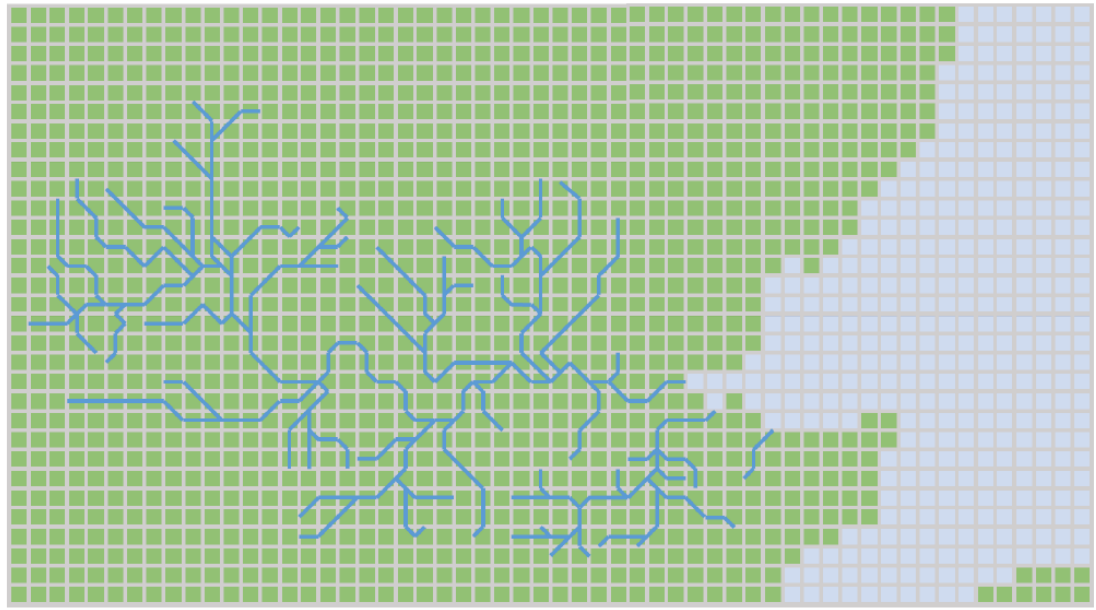
NanoFASE

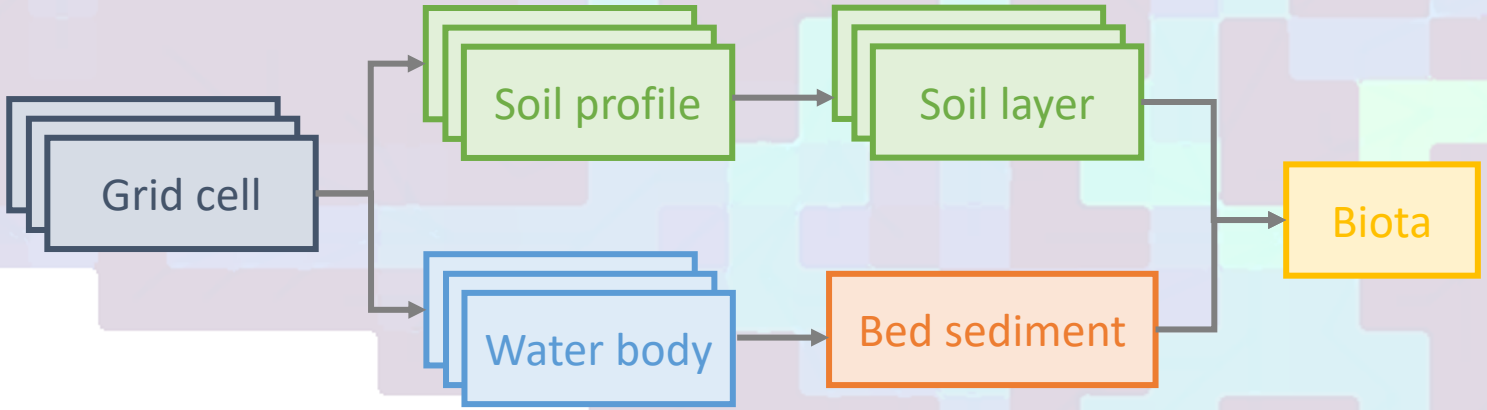
UK Centre for Ecology & Hydrology

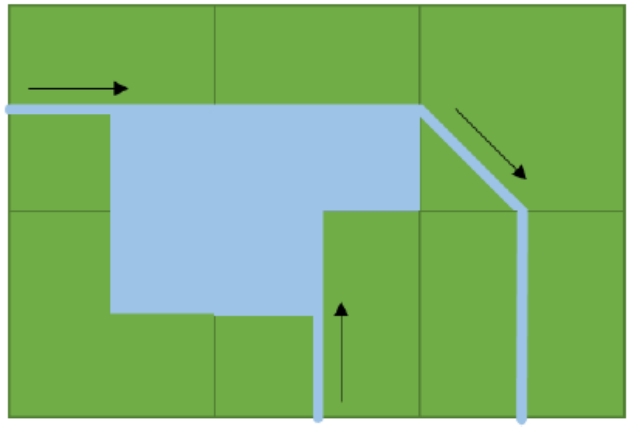
NANOFASE MODEL

The NanoFASE water–soil–organism model

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







NanoFASE

UK Centre for Ecology & Hydrology

NANOFASE MODEL

Soil profile

Transformations: e.g. **attachment** to soil matrix

Bioturbation rate is function of earthworm density:

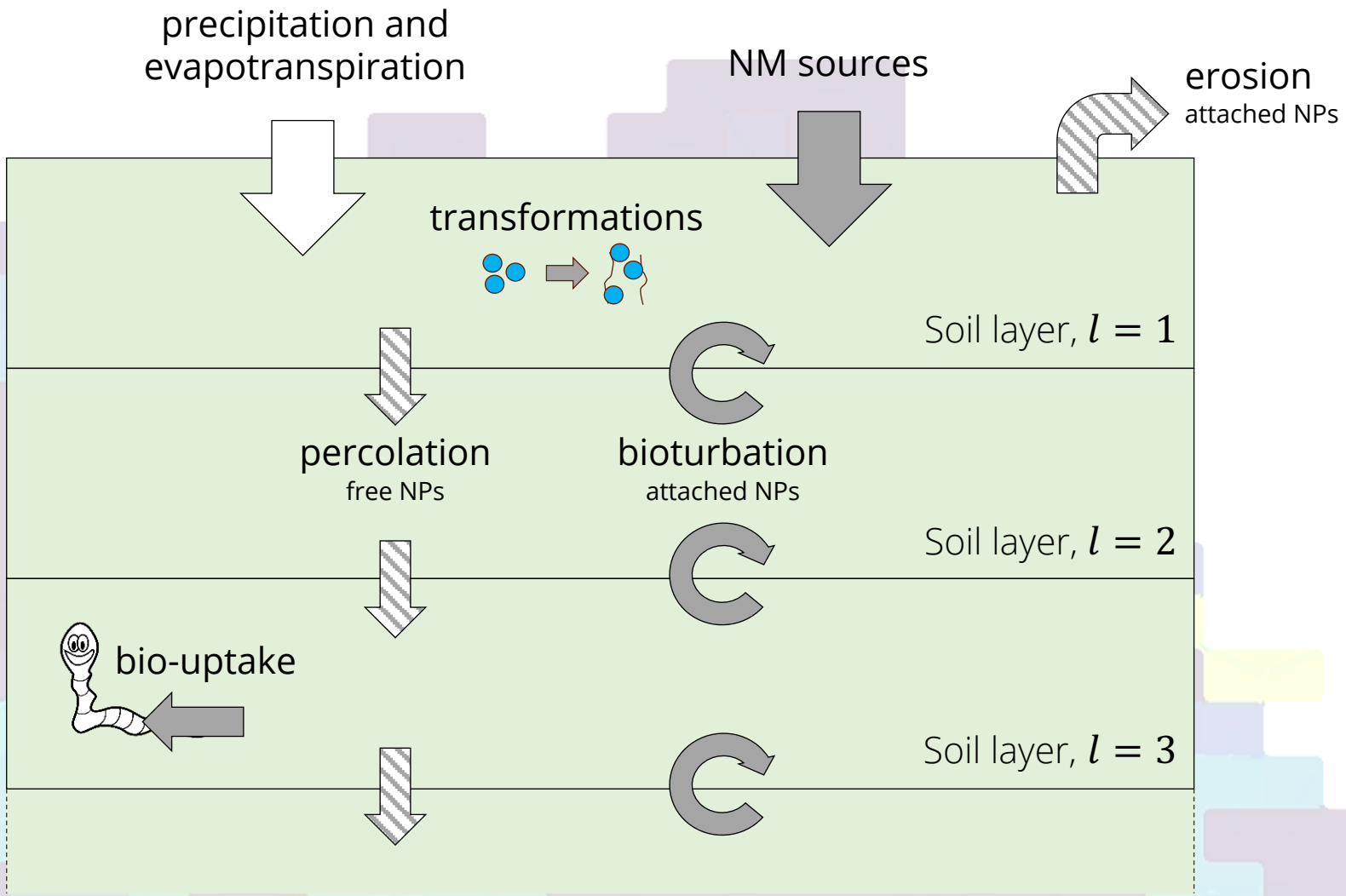
Empirical bioturbation parameter

$$k_{\text{bioturb},l:l+1} = \frac{\beta w_l}{d}$$

Bioturbation rate

Layer depth

Worm density



NanoFASE

UK Centre for Ecology & Hydrology

NANOFASE MODEL

Rivers and estuaries

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

Attachment efficiency

Collision frequency

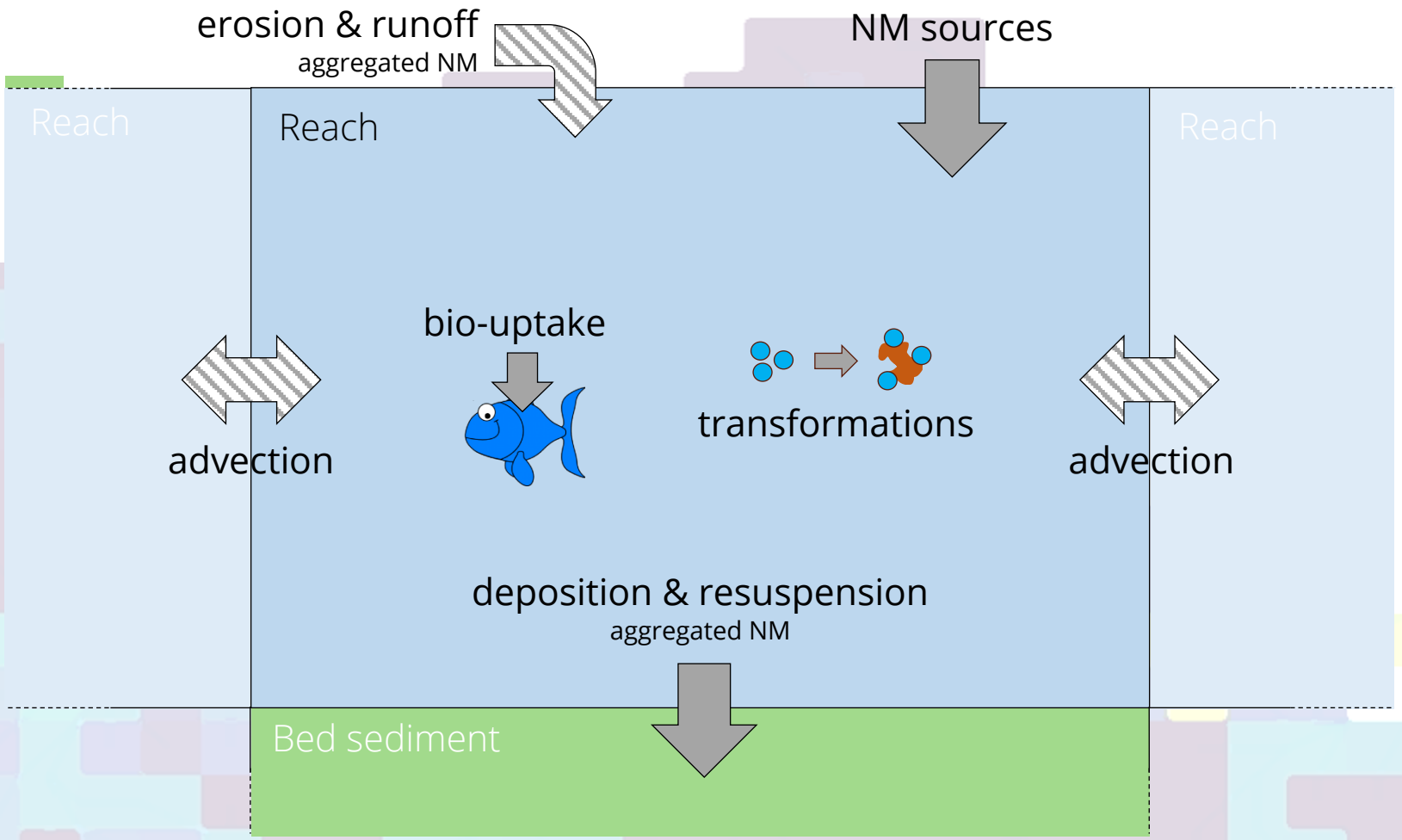
$$k_{\text{hetero}} = \alpha_{\text{hetero}} k_{\text{coll}} C_{\text{spm}}$$

Heteroaggregation rate

SPM particle concentration

$\alpha_{\text{hetero}} = 0.01$ freshwater

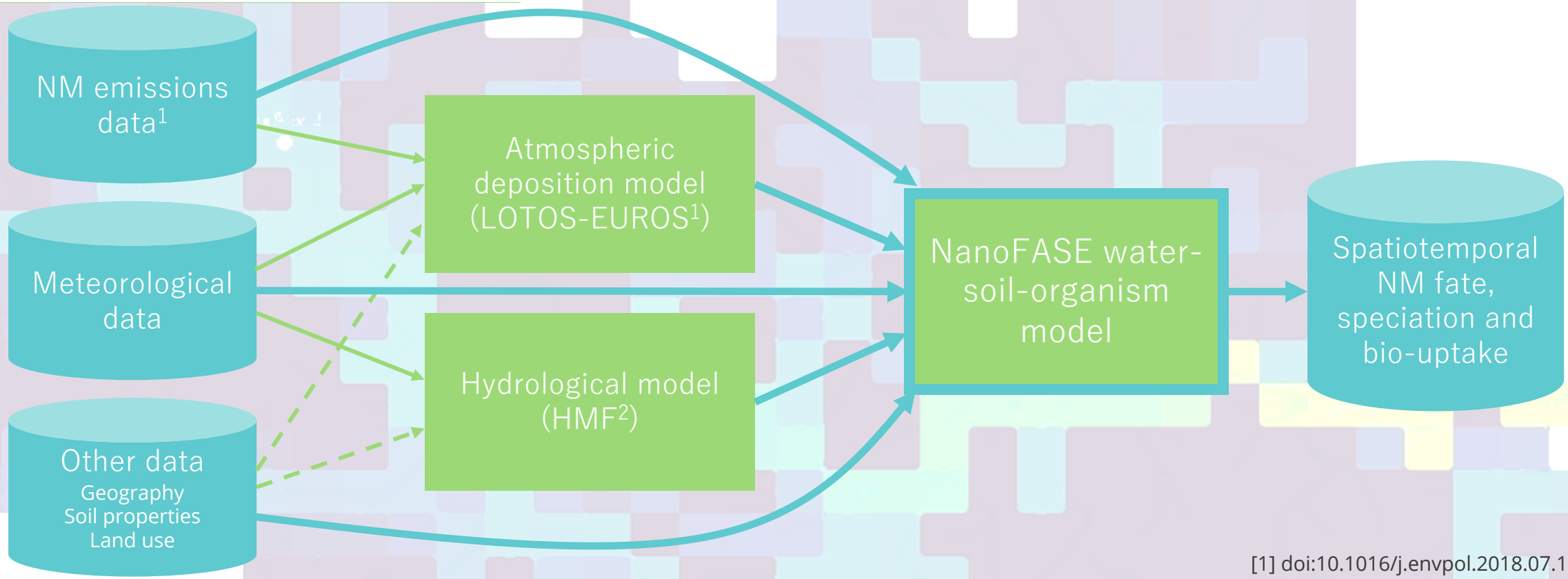
0.1 estuarine



NanoFASE

UK Centre for Ecology & Hydrology

How it all fits together



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

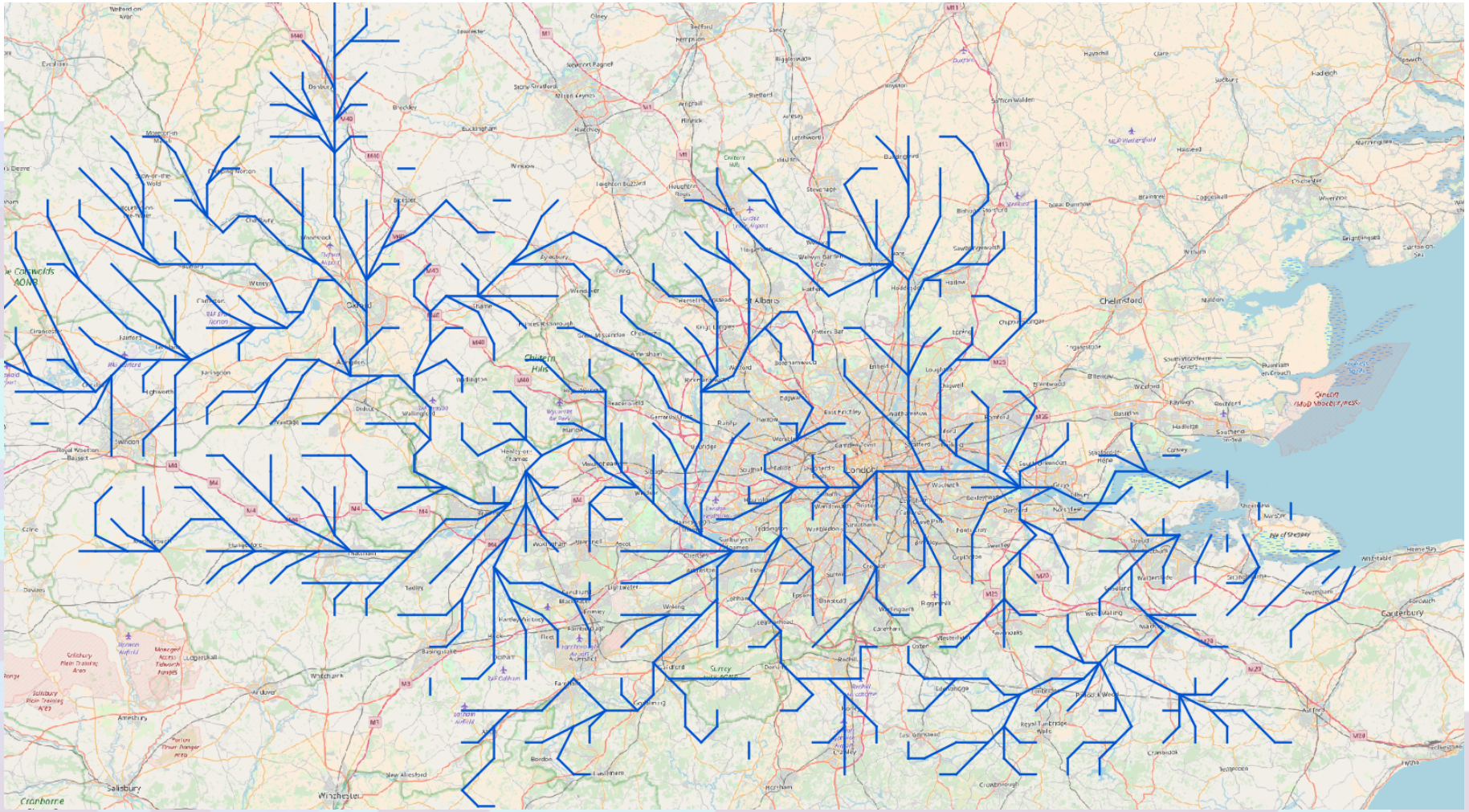
NanoFASE

UK Centre for Ecology & Hydrology

RESULTS

Application to the Thames catchment

- Resolution: 5x5 km
- Years: 2000-2020
- Materials: TiO_2



NanoFASE

UK Centre for Ecology & Hydrology

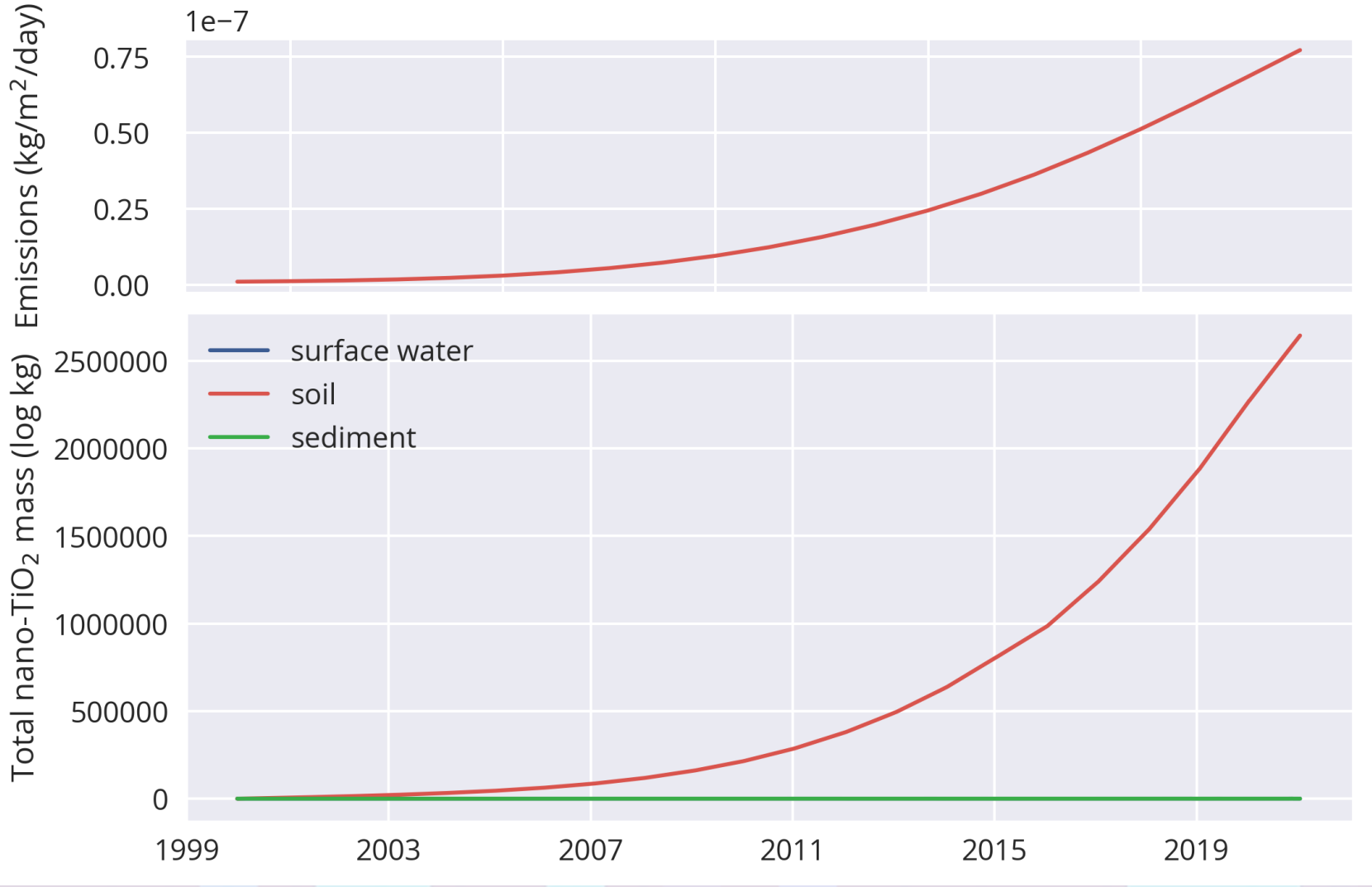
RESULTS

Where do NMs end up?

Total mass of nano-TiO_2 in the entire catchment, split by environmental compartment.

Soil acts as a sink

Main driver to long-term dynamics ? exponentially increasing emissions



NanoFASE

UK Centre for Ecology & Hydrology

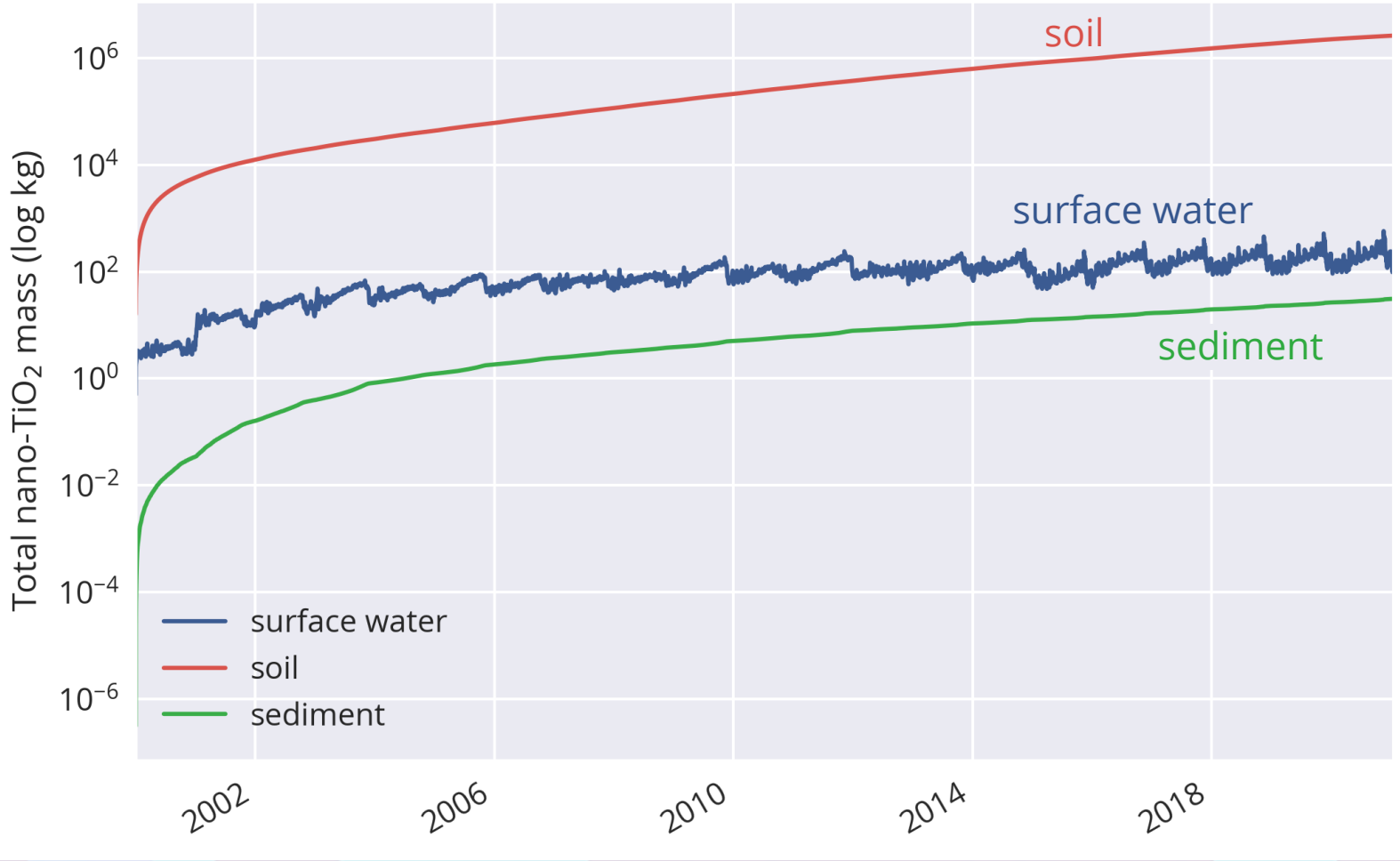
RESULTS

Where do NMs end up?

Total mass of nano-TiO_2 in the entire catchment, split by environmental compartment.

Soil acts as a sink

Main driver to long-term dynamics ? exponentially increasing emissions

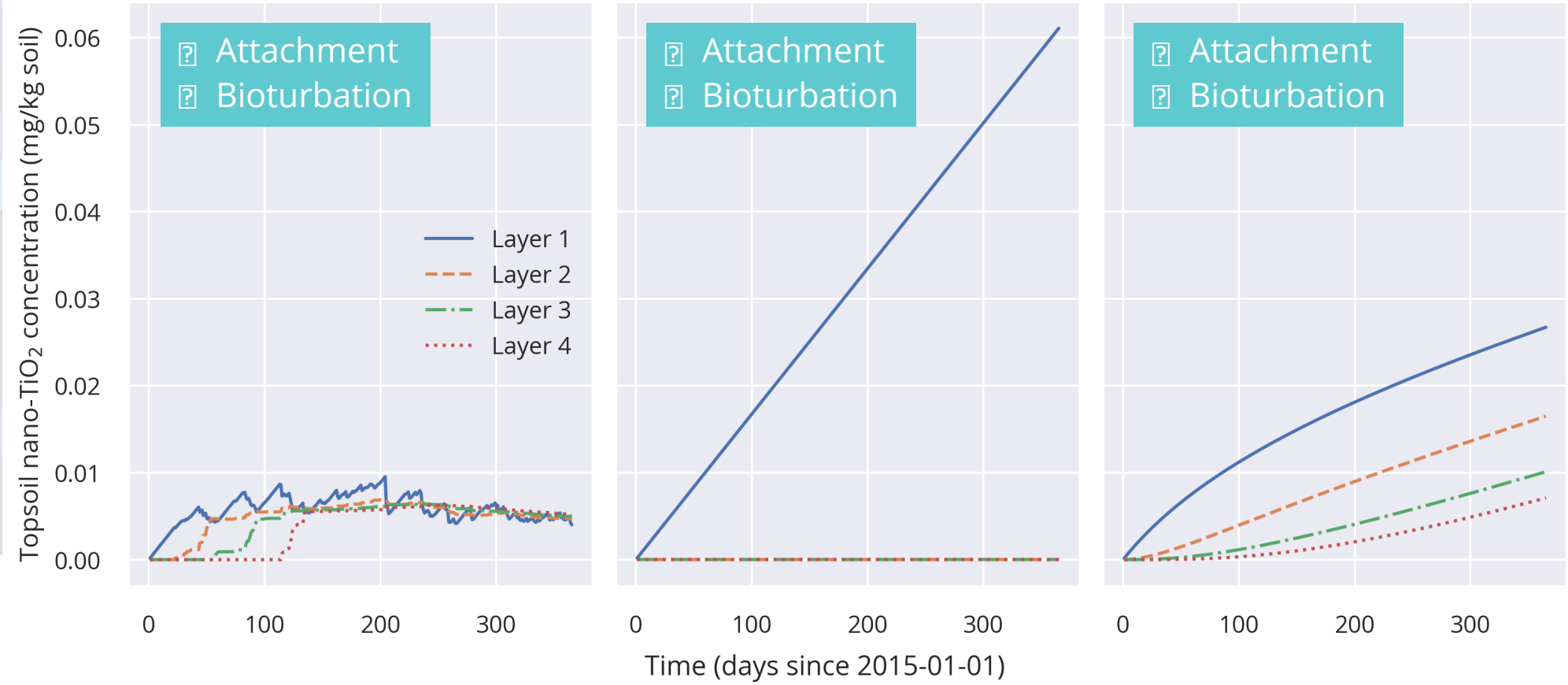


NanoFASE

UK Centre for Ecology & Hydrology

RESULTS

Attachment and bioturbation in soils



NanoFASE

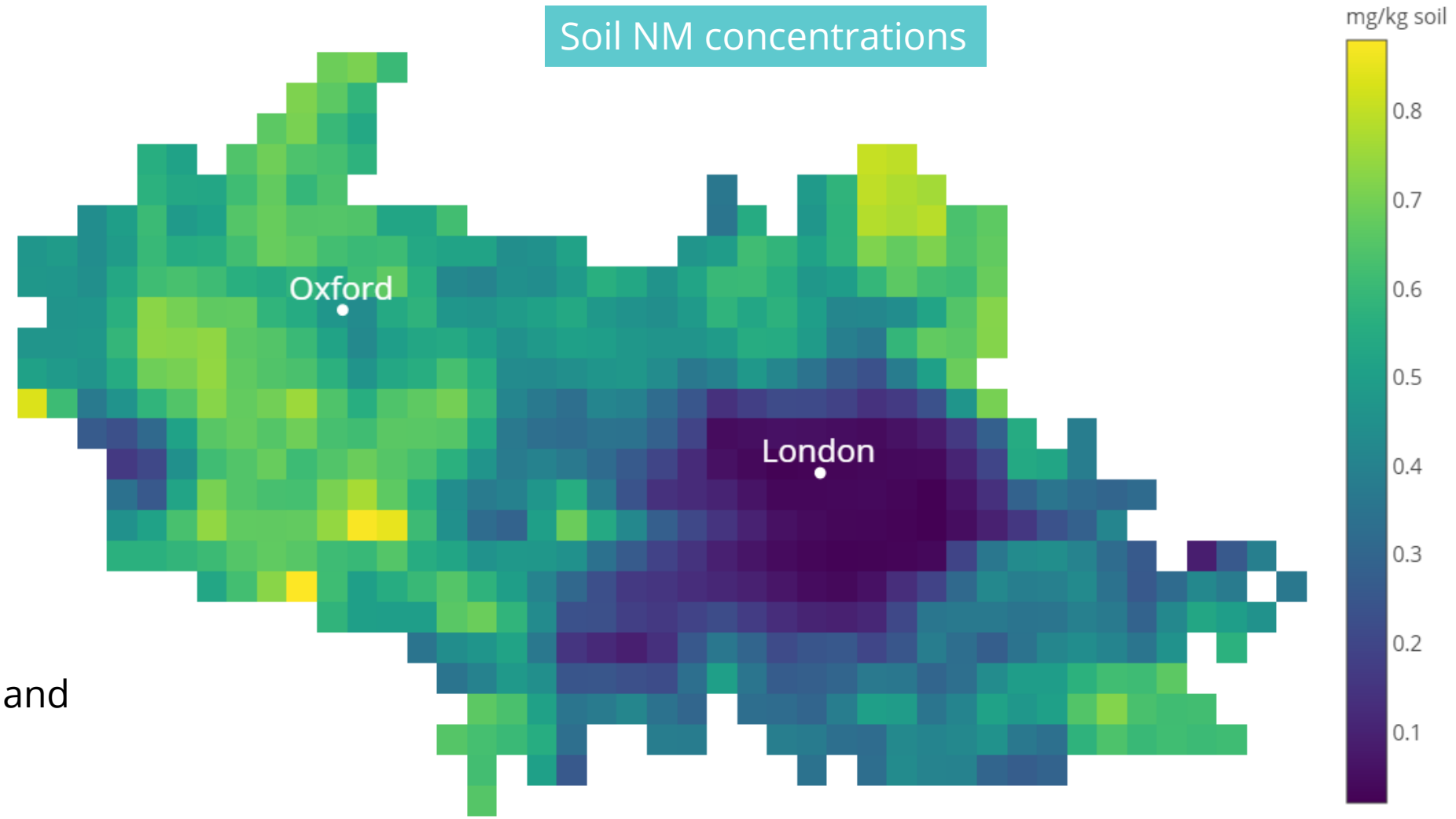
UK Centre for Ecology & Hydrology

RESULTS

Where are the hotspots?

Nano-TiO_2 predicted environmental concentrations (PEC) in soil at the end of 2020.

Main determinant of spatial distribution ? land use



NanoFASE

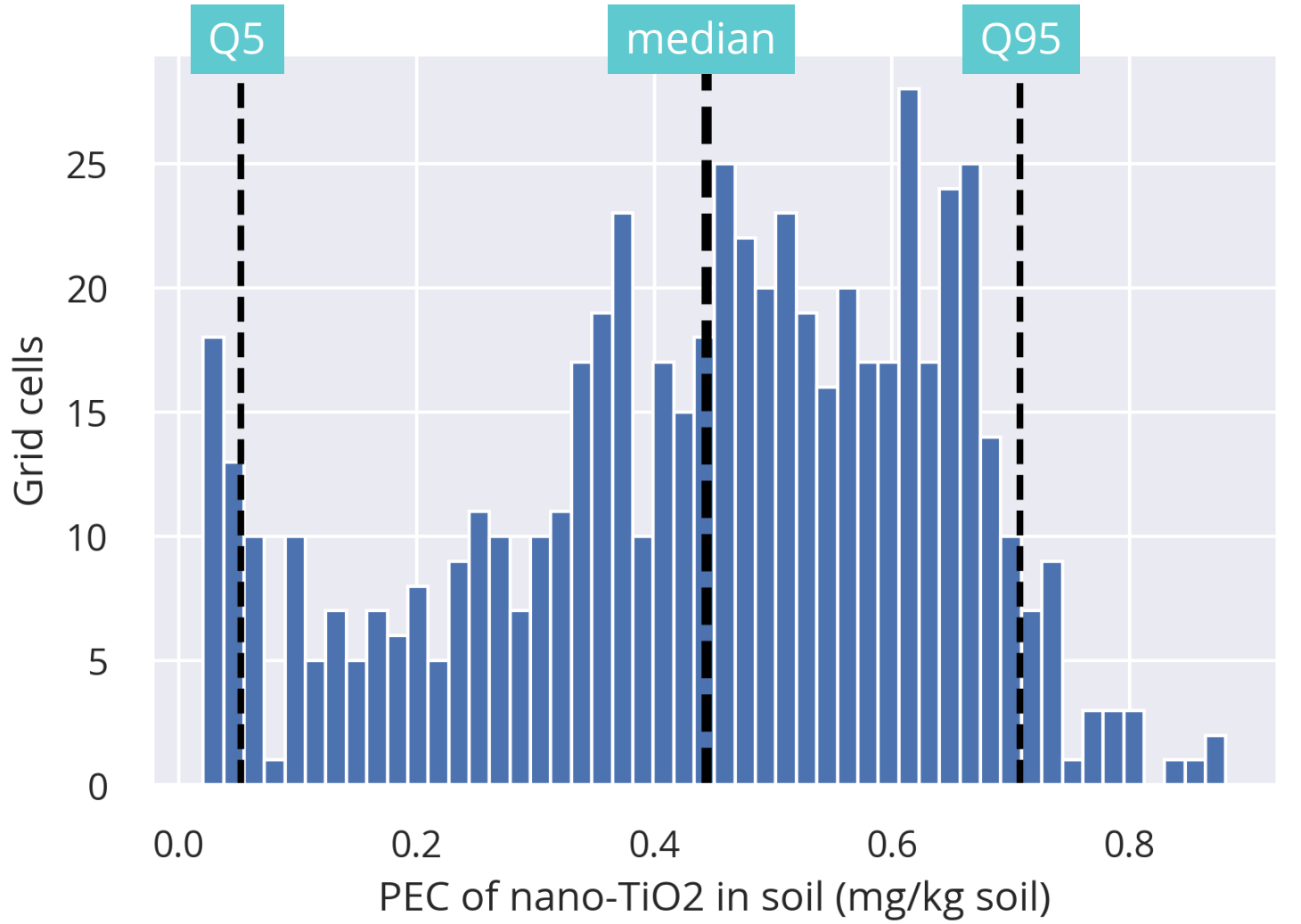
UK Centre for Ecology & Hydrology

RESULTS

What is the spatial distribution?

Nano-TiO_2 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



NanoFASE

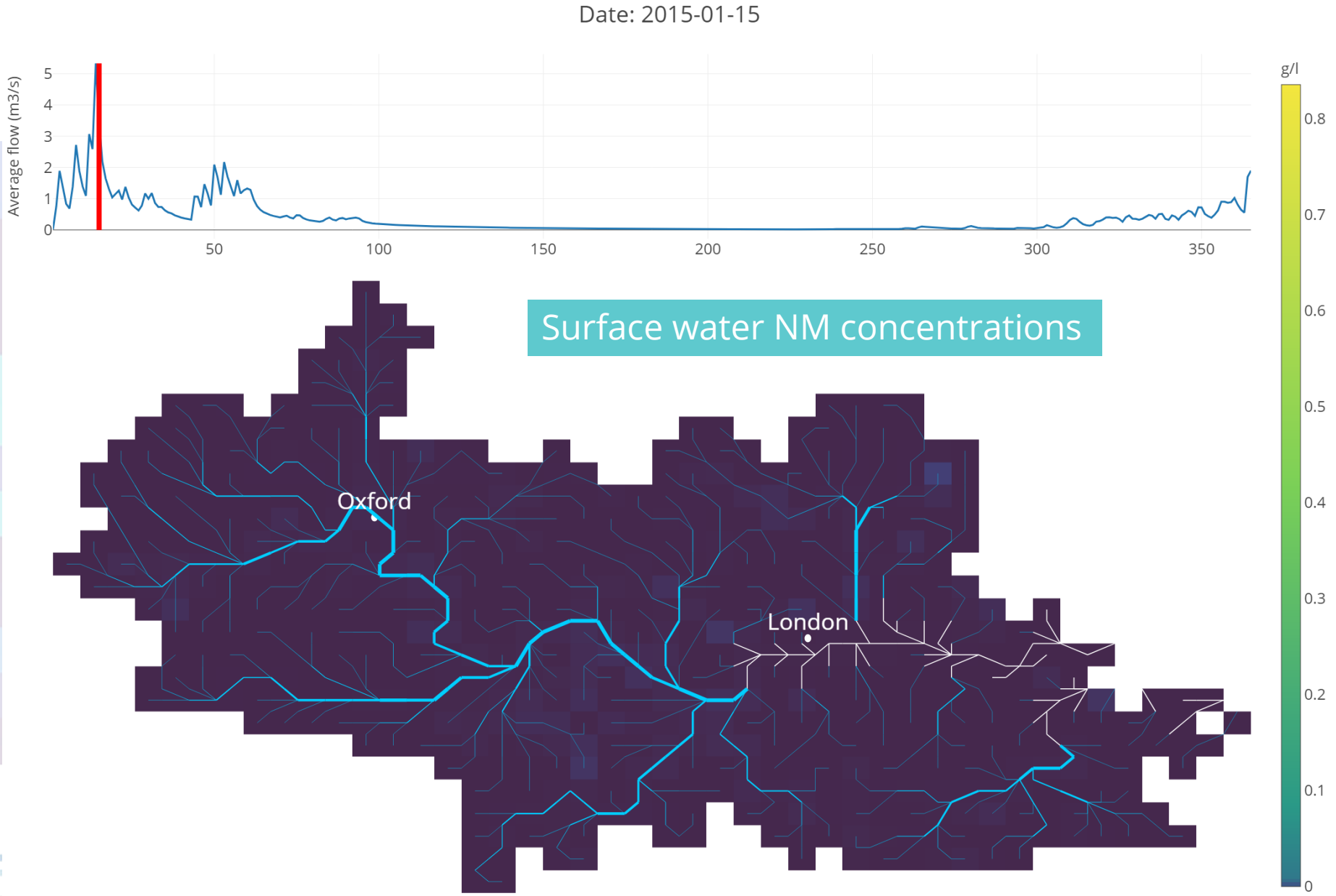
UK Centre for Ecology & Hydrology

RESULTS

What are the dynamics?

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

- Low flows → high concentrations
- Estuary is big → low concentration

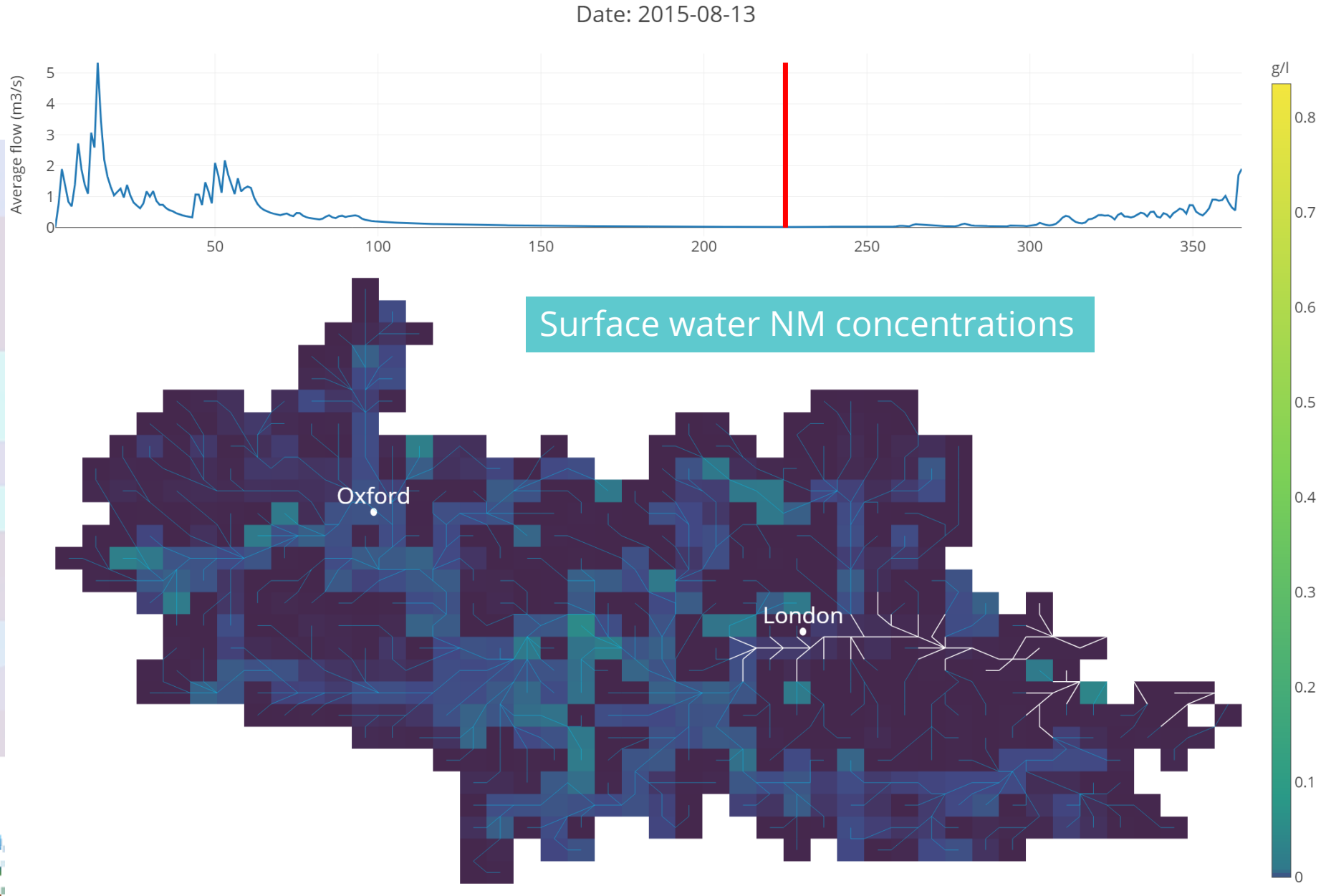


RESULTS

What are the dynamics?

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

- Low flows → high concentrations
- Estuary is big → low concentration

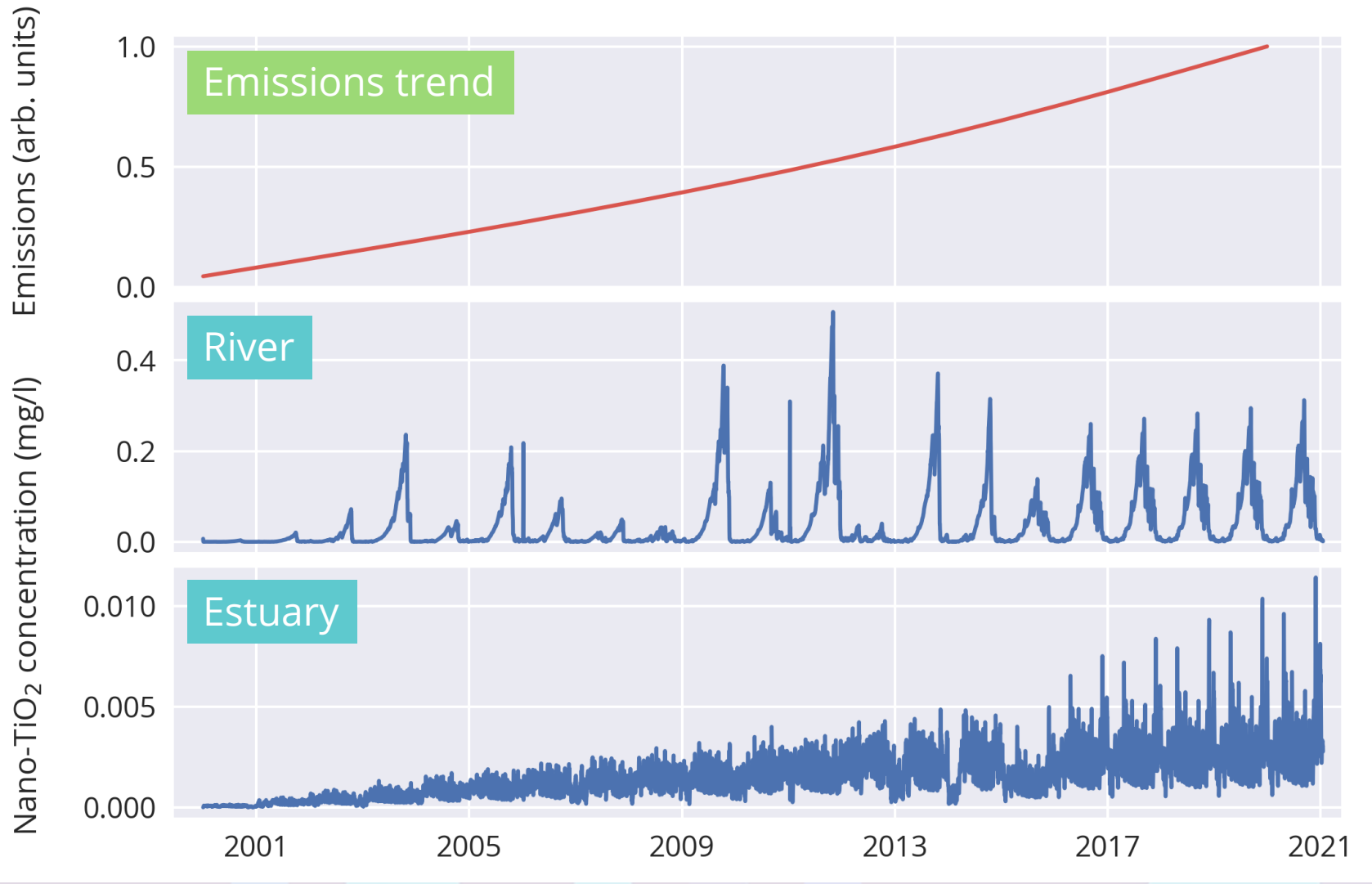


RESULTS

What are the dynamics?

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

Riverine temporal trend strongly influenced by hydrology

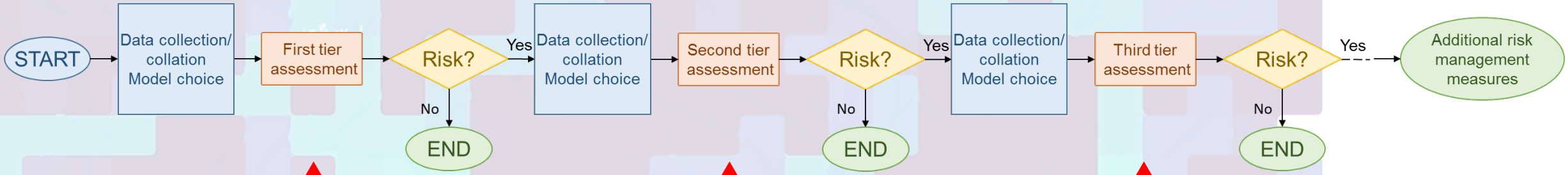


NanoFASE

UK Centre for Ecology & Hydrology

REGULATORY RELEVANCE

Tiered exposure assessment



Simple calculation

SimpleBox4nano

NanoFASE WSO model

NanoFASE

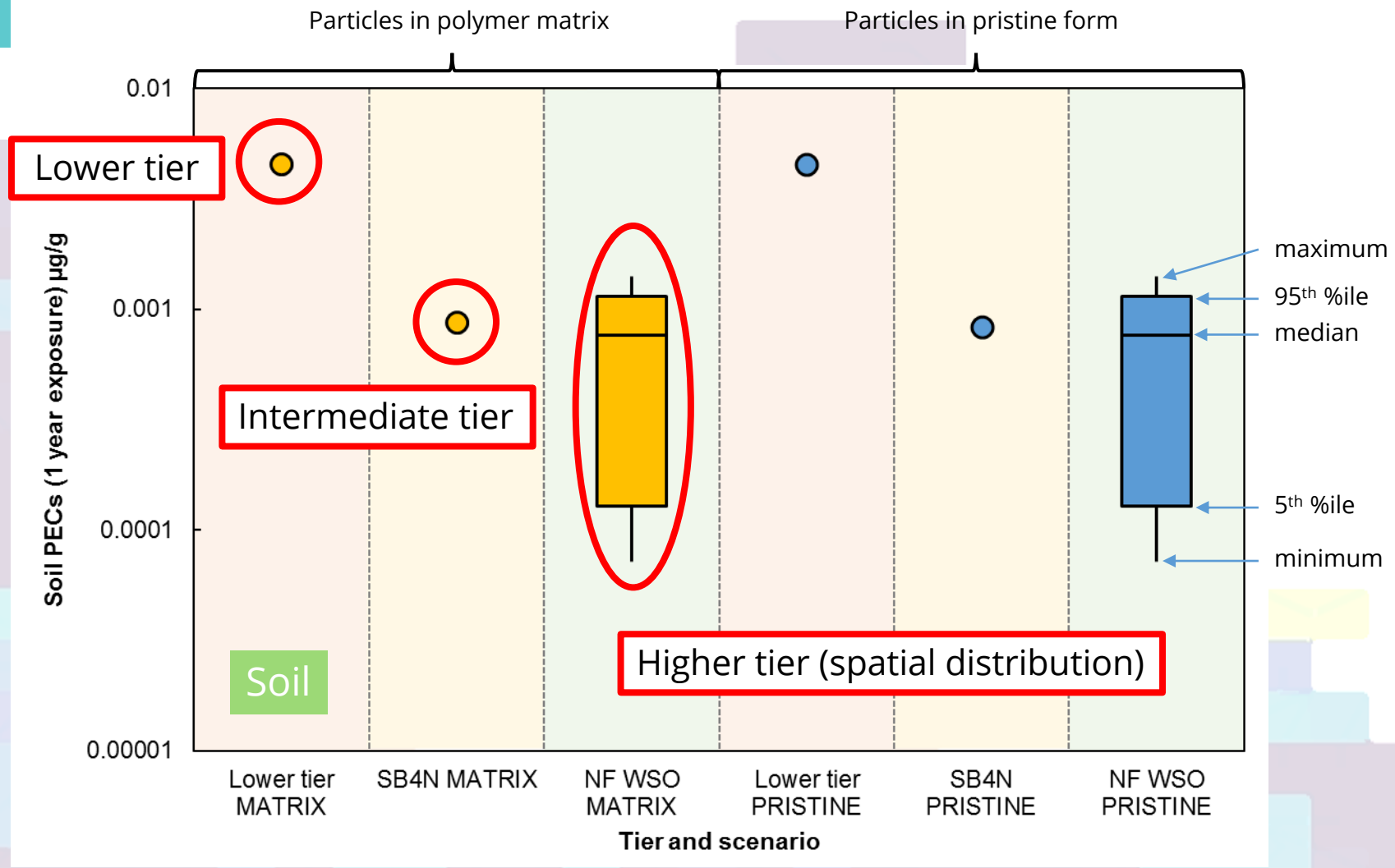
UK Centre for Ecology & Hydrology

Tiered exposure assessment

Case study: TiO_2 applied as road coating in Thames catchment

High tiers = lower PEC

nanofase.eu/exposure_assessment_framework



NanoFASE

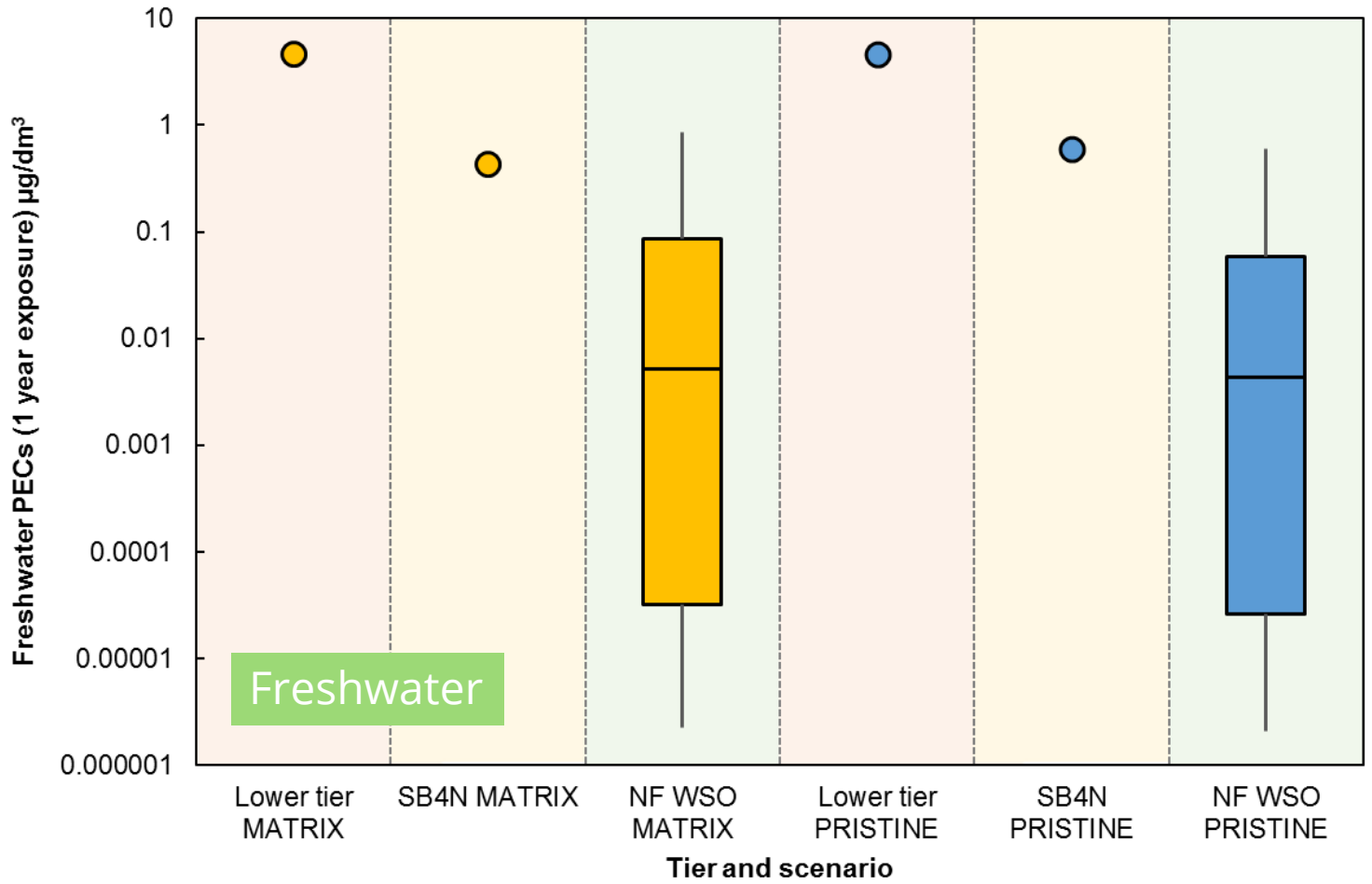
UK Centre for Ecology & Hydrology

Tiered exposure assessment

Case study: TiO_2 applied as road coating in Thames catchment

High tiers ? lower PEC

nanofase.eu/exposure_assessment_framework



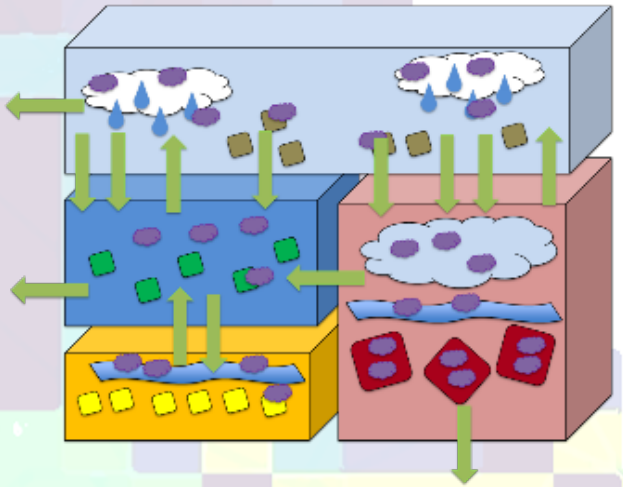
NanoFASE

UK Centre for Ecology & Hydrology

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…?*



NanoFASE

UK Centre for Ecology & Hydrology

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

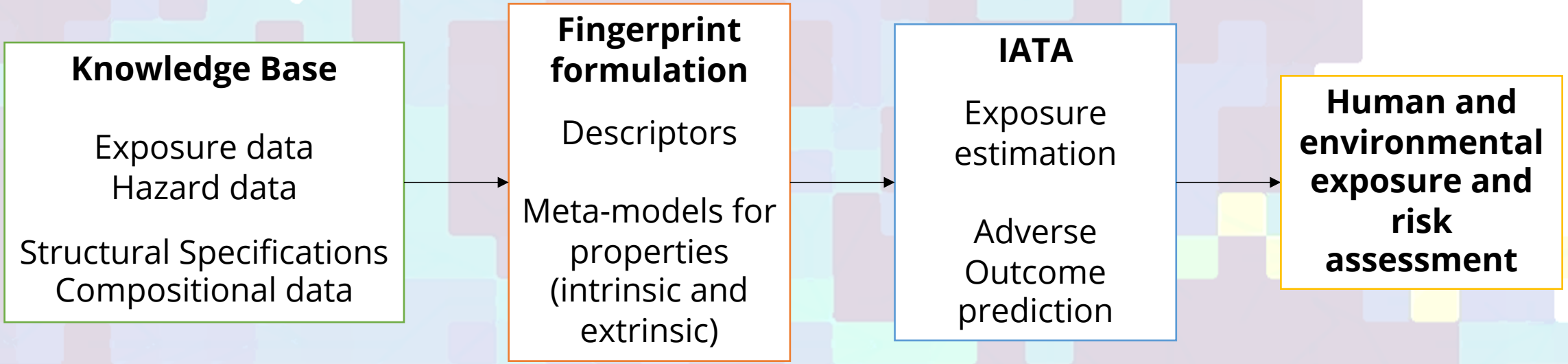
Links to data for parameter derivation?

NanoFASE

UK Centre for Ecology & Hydrology

Nano WG April 2020

NanoSolv eIT



NanoSolveIT

UK Centre for Ecology & Hydrology

Nano WG

This project receives funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 646002.

NanoFASE

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

UK Centre for Ecology & Hydrology

- 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

NanoFASE

UK Centre for Ecology & Hydrology