



Modelling atmospheric fate of TiO₂ and its impact on atmospheric chemistry

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TNO

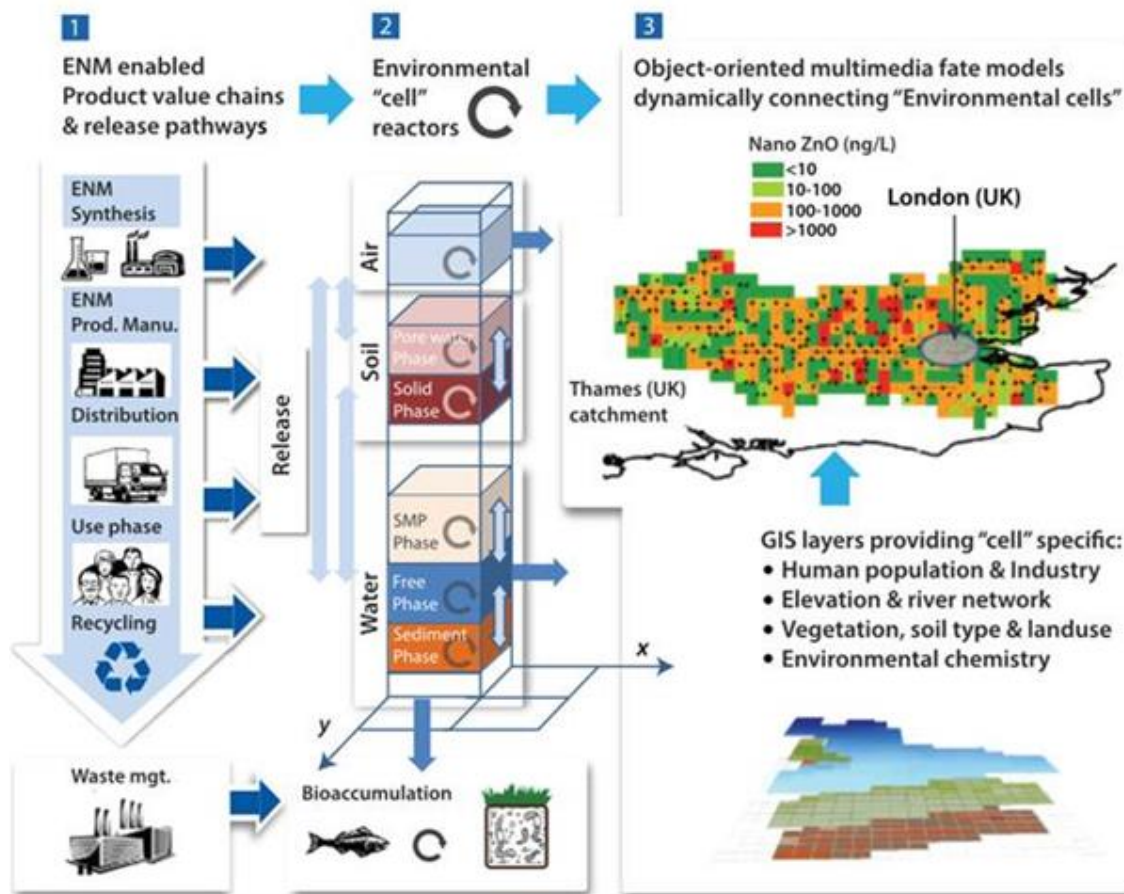
INERIS
controlling risks
for sustainable development



Nanofase project

- Nanomaterial may behave differently from conventional material, environmental risks
- Describe environmental fate of engineered nanomaterial (ENM)
- Concentrations resolved in space and time, for [air](#), water and soil
- Consistency with screening-level model (SB4N)

Nanofase project



- Focus on metal oxides (TiO_2 , CeO_2) for air

Challenges

- Emissions poorly known
- Particle properties of emitted material poorly known
- Potential impact on atmospheric chemistry, what are reaction rates?

Solutions

- Emissions poorly known
- First spatially resolved emission inventory
- Particle properties of emitted material poorly known
- Field campaigns+ approximations
- Potential impact on atmospheric chemistry, what are reaction rates?
- Laboratory study

CTM used to assess overall concentrations and deposition

Emissions

Spatially resolved emissions of TiO_2 to air, water determined for 5 classes:

- Pristine
- Transformed
- Matrix-embedded
- Product-embedded
- Dissolved

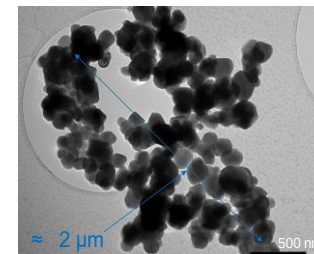
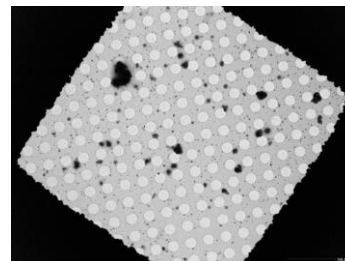
Adam, V., Caballero-Guzman, A., & Nowack, B. (2018). *Environmental pollution*, 243, 17-27.

+ manuscript in preparation on spatial and temporal distribution

Particle Properties

- No free nanoparticles released to air under normal conditions, only at accidental release->near field modelling needed
- Particles can be treated as conventional particles on regional scale
- Density & shape based on field experiments+ other considerations
- TiO₂ can act as a catalyst for NO₂-reactions, but only at very high concentrations effects are found

	LOTOS-EUROS size class (μm)	Density of particles (kg/m ³)
Pristine	0.33	2000
Transformed	0.33	1500
Matrix-embedded	8.0	1800



Modelling

- LOTOS-EUROS model
- $1/2 \times 1/4^\circ$ for European continent
- $1/8 \times 1/16^\circ$ for UK Thames Catchment
- Year 2015
- Emission timing like industrial processes for emissions to air
- Passive tracers, sensitivity studies
- Chemically active tracer, sensitivity study with unrealistically high concentrations

Annual mean concentration and deposition

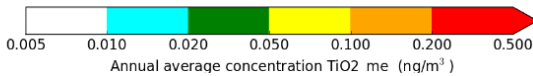
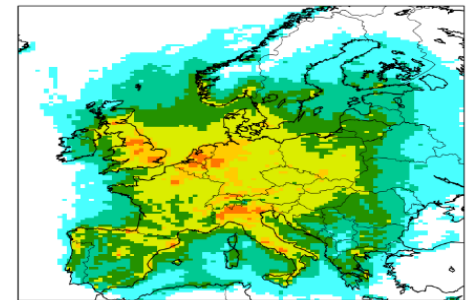
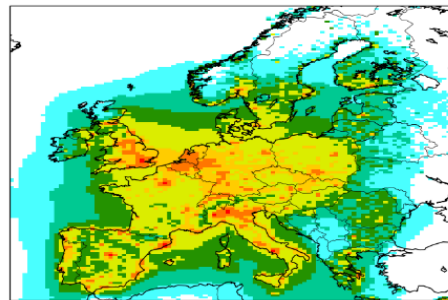
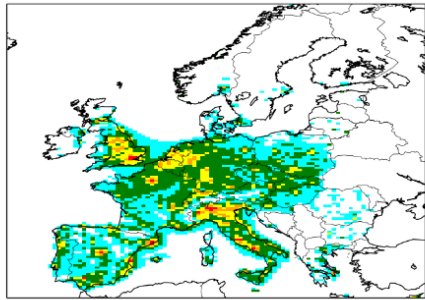
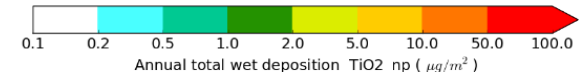
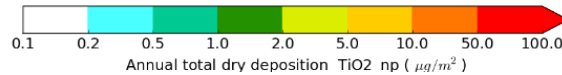
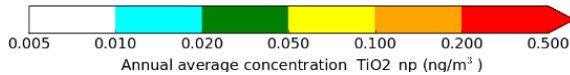
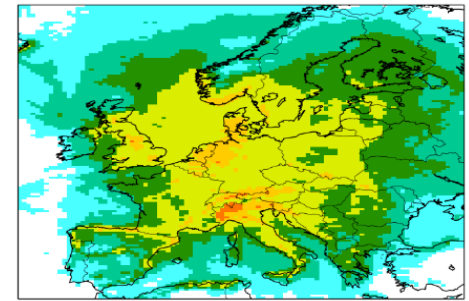
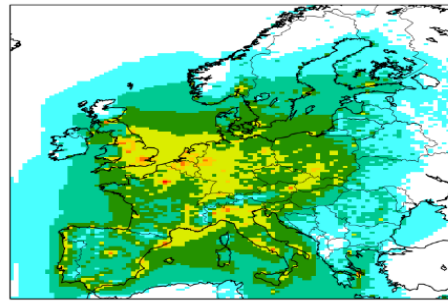
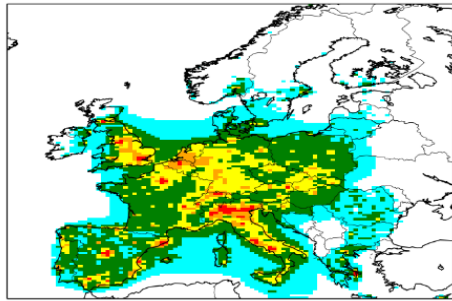
Concentration

dry deposition

wet deposition

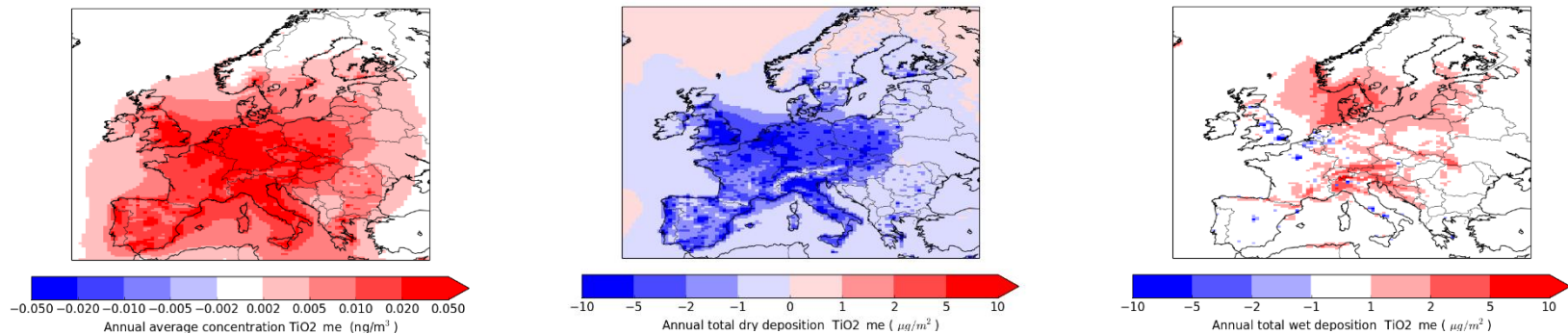
nanoparticulate

matrix-embedded



Annual mean concentration and deposition

- Impact of particle size and density mainly for larger particles, up to factor 2 difference



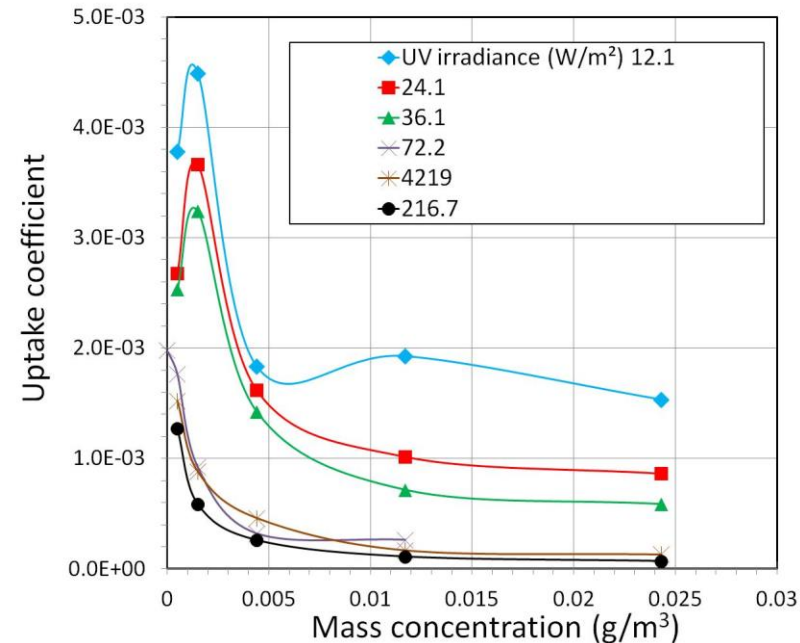
Impact of reducing particle size from 8 to 3 μm , increasing concentrations and transport distance

Chemical reactions

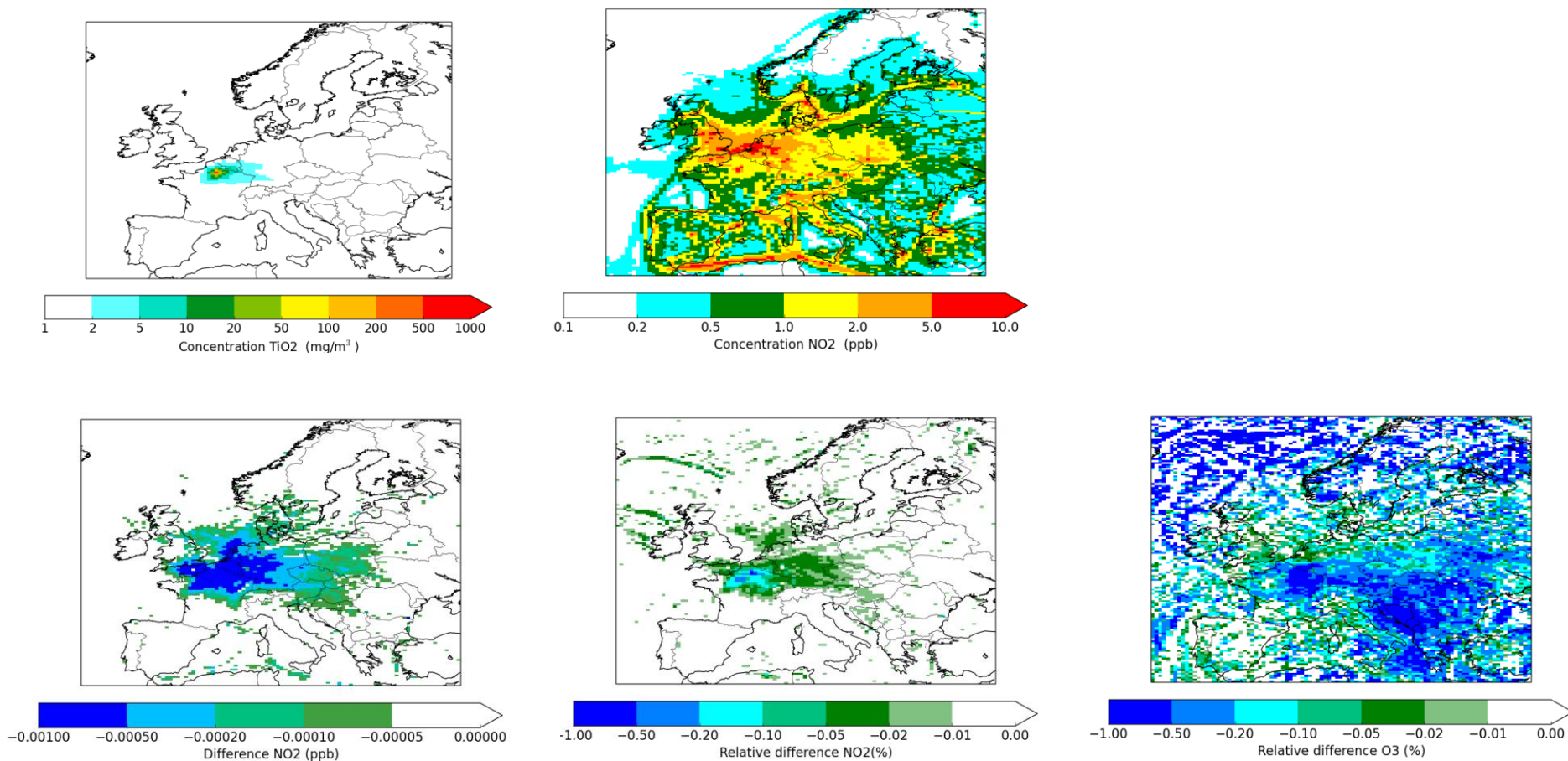
- $\text{NO}_2 \rightarrow \text{NO} + \text{O}$, TiO_2 acts as catalyst
- Experiments in flow chamber with P25
- Effects only at very large concentrations

Modelling experiment

- Emission experiment July 2015
- Fictitious emissions 10^8 (!) kg/hour $\text{TiO}_2\text{_{np}}$ at INERIS location
- $\text{NO}_2 \rightarrow \text{NO} + \text{O}$ and complete removal of NO_2 tested

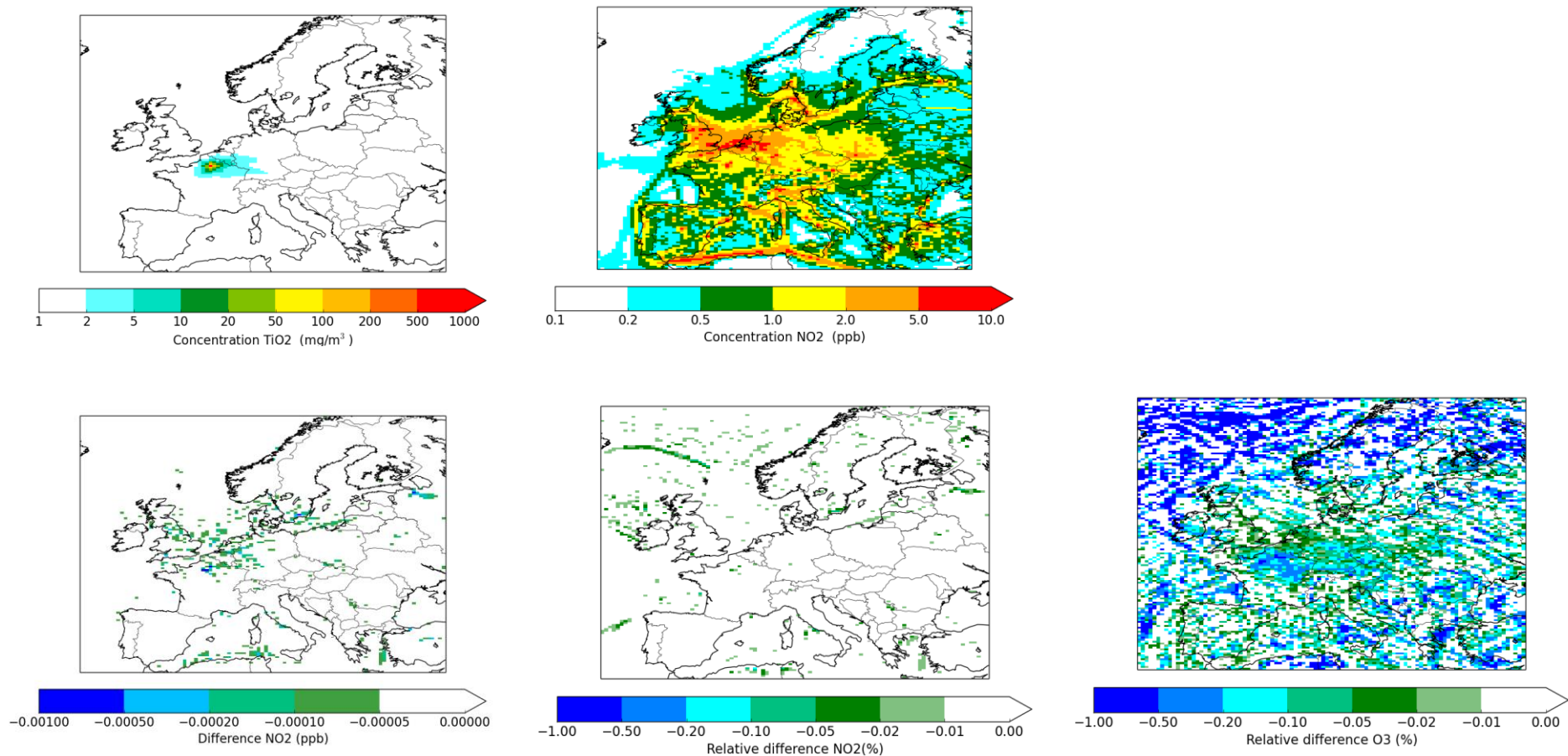


Impact of chemistry



Monthly mean concentration and concentration difference, complete removal case

Impact of chemistry



Monthly mean concentration and concentration difference, $\text{NO}_2 \rightarrow \text{NO} + \text{O}$

Conclusions and outlook

- First estimation of ambient concentrations and deposition of TiO_2
- Under ambient conditions, they occur as larger aggregates or embedded in matrix
- Concentrations are low, cf. EU limit values for BaP, heavy metals 1-5 ng/m³
- Natural contribution TiO_2 in crustal material 10-20 ng/m³
- Impact on atmospheric chemistry can be neglected at current concentration values
- Results will be used by soil/water model and SB4Nano

- Thank you for your attention
- Thank all the NanoFASE people, in particular
 - Jean-Marc Lacomme
 - Christof Asbach, Ali Mohamadi Nasrabadi
 - Jeroen Kuenen
- Time for questions?
- www.nanofase.eu

