Modeling Nanomaterial Fate and Exposure

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NanoFASE Meeting September 6, 2019, Vienna

Environmental Fate Modeling

NM Sources/Inputs

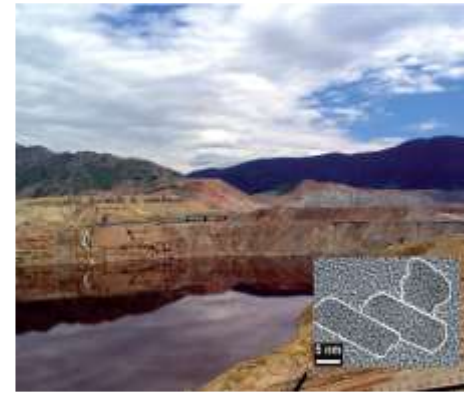
Environmental Processing

Where are the NMs?
What form are the NMs?
What are the NMs doing?

Exposure Route 1

Exposure Route 2

Exposure Route 3



Effects of Interest

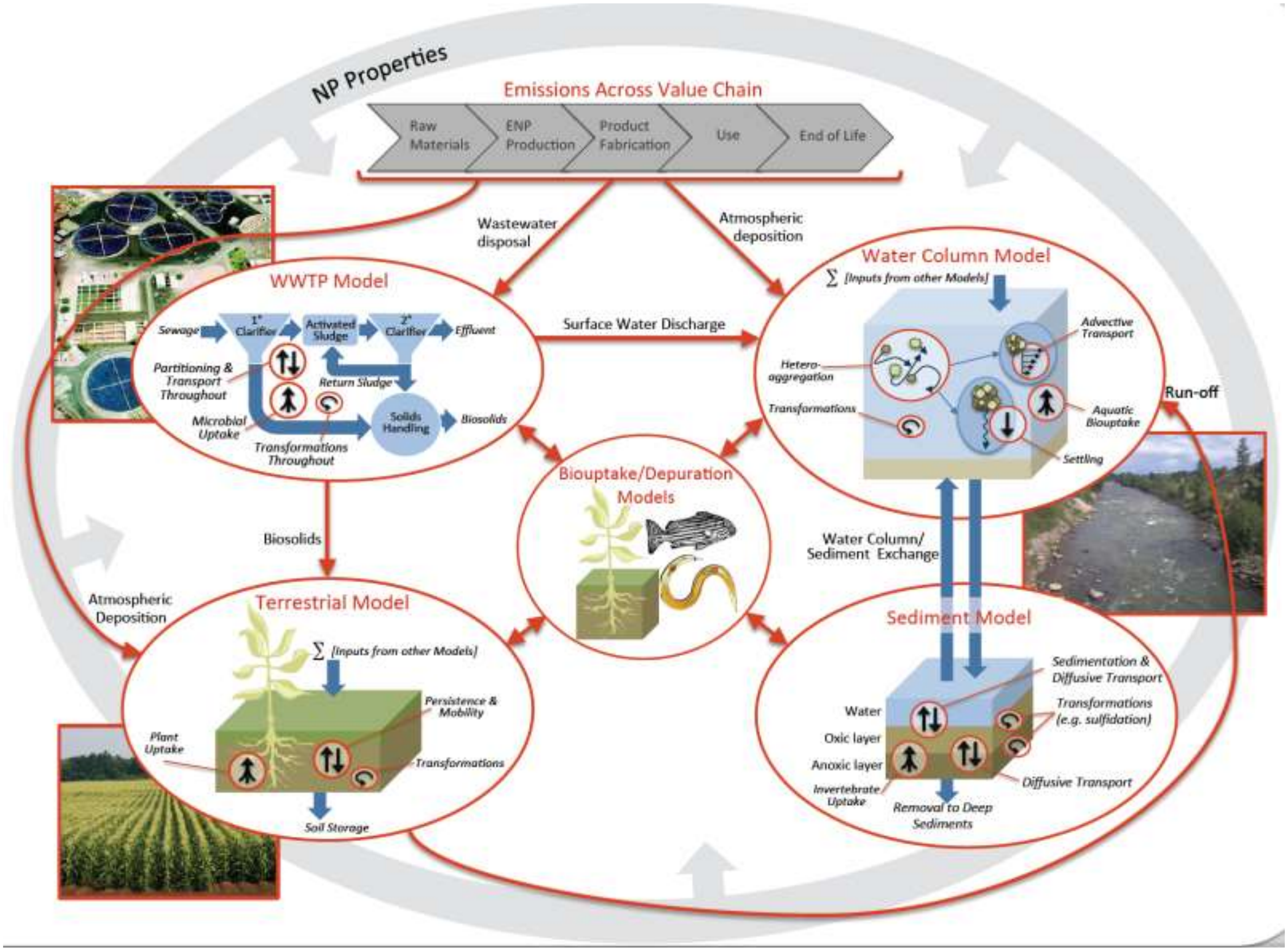
Acute Toxicity

Chronic/Multigenerational Effects

Ecosystem Function/Services

SUN-Nano March 2015?

Some Key Models Required (CEINT 2008)



Engineering models must <u>compromise</u> between *simplicity* and *realism*.

“The best solution emphasizes the former without undue violence to the latter”

Dominic Di Toro, 2001

Key Questions to Address?

- What modeling frameworks make sense?
  - Spatial and temporal resolution
- What processes and parameters are essential?
  - Chemistry, chemistry, chemistry!!
- How do we parameterize models in complex systems?
  - Model sensitivity to each parameter
- How can we validate our models?

How Important is Spatial and Temporal Resolution in models?

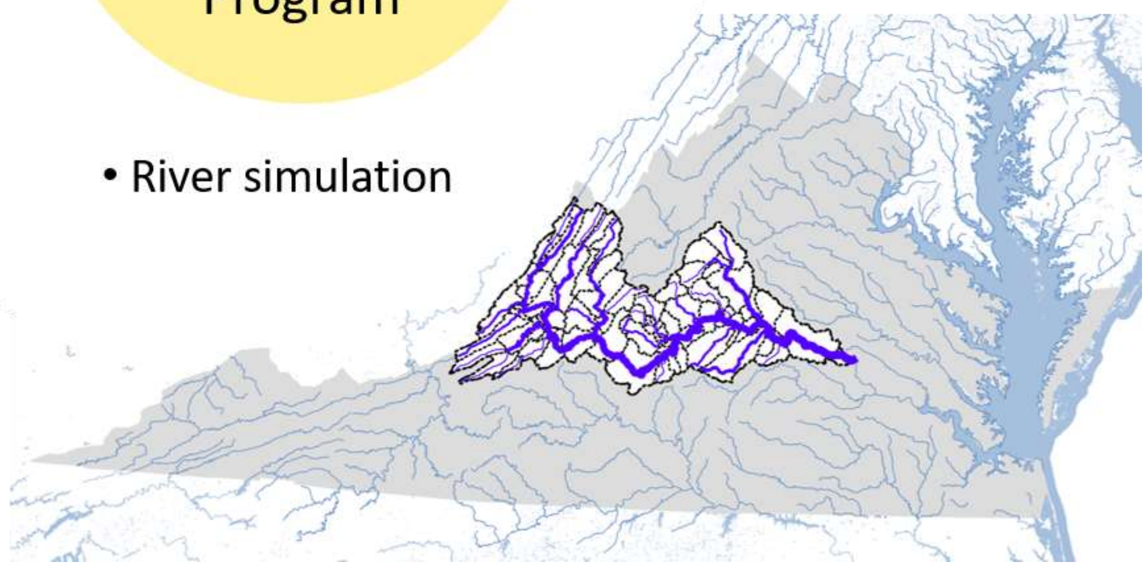
River Model Framework

WSM:
Chesapeake Bay Watershed Model (HSPF)

- Meteorology
- Land simulation (crop runoff)
- Stream hydrology
- Point sources (WWTP effluent)

WASP7:
Water Quality Analysis Simulation Program

- River simulation



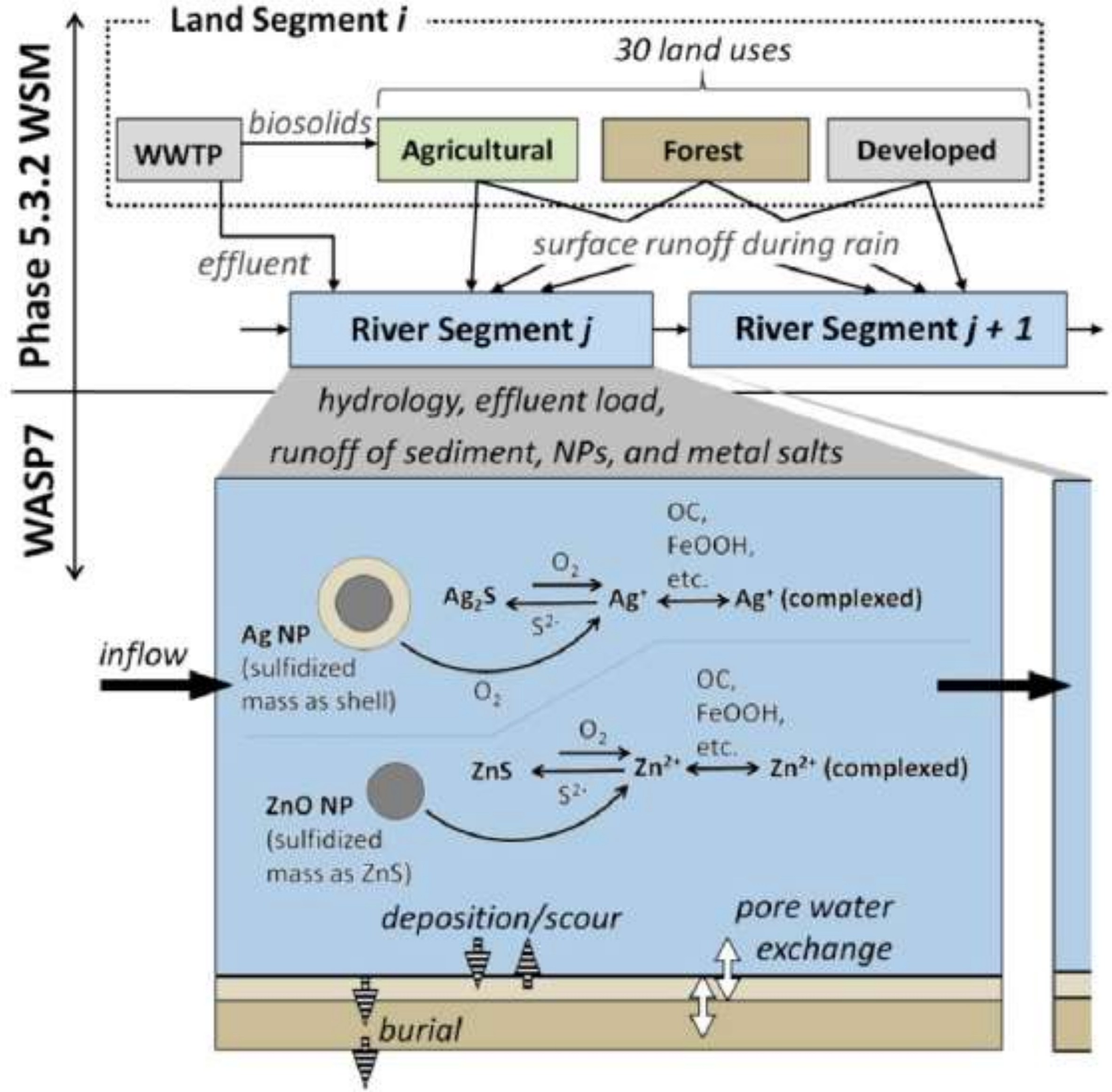
Dale et al., 2015 ES&T 49 (12), pp 7285

Model Framework

What is NP distribution in river?

What controls the distribution?

<u>Key assumption</u>: NPs moved with larger particles (α=1)



Dale et al., 2015 ES&T 49 (12), pp 7285

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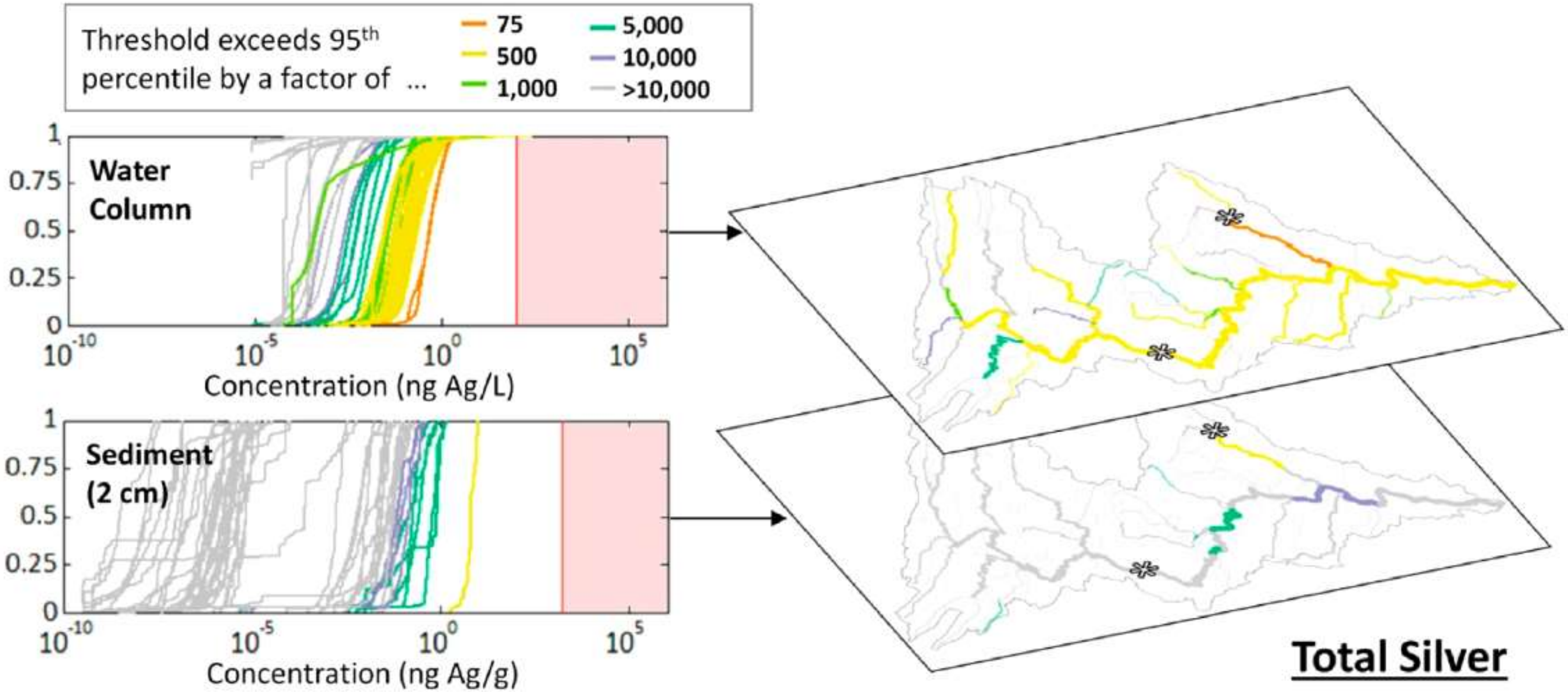
⦿ Spatial variation is very high! (hot spots!)

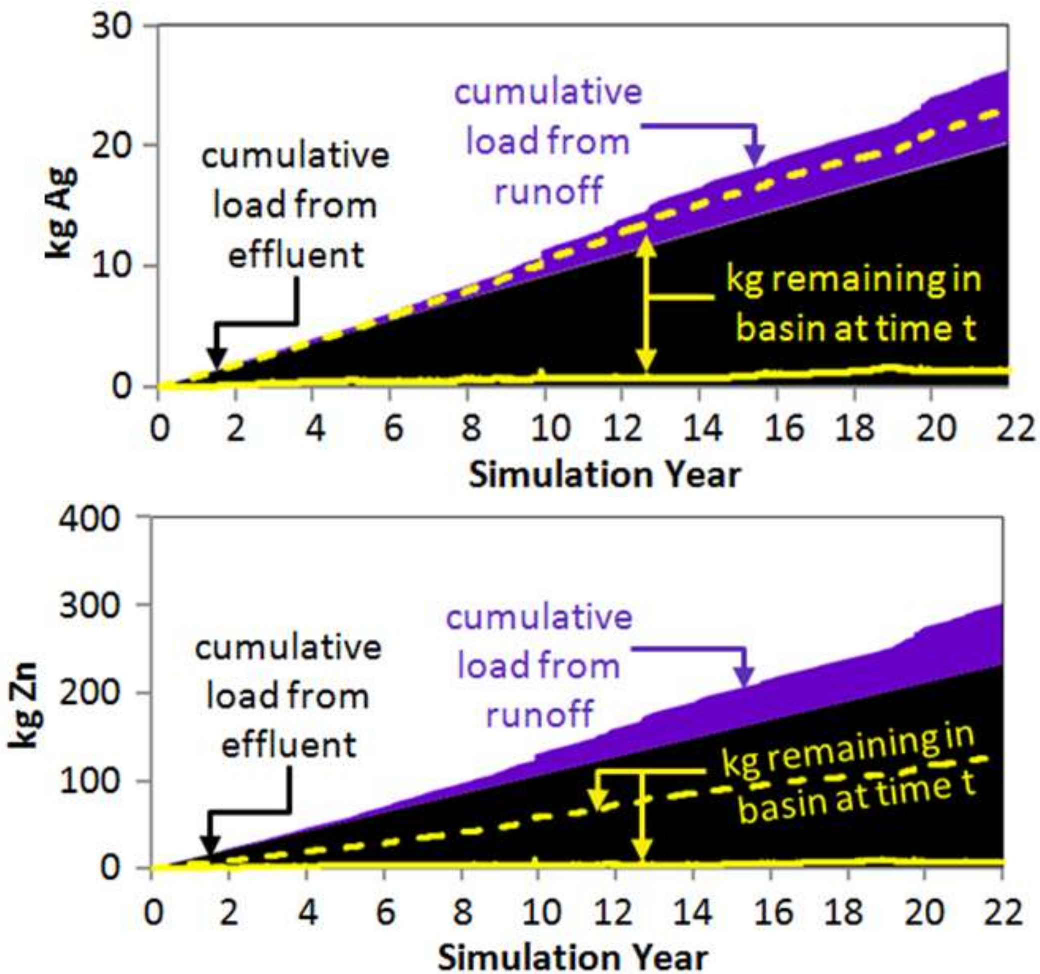
⦿ PECs never exceed EPA regulatory thresholds for total metals



- Hydrology, sediment transport, chemical transformations, and spatial variation in loads strongly impact NP fate.

- Models that exclude these features may be limited in their ability to characterize environmental risks.

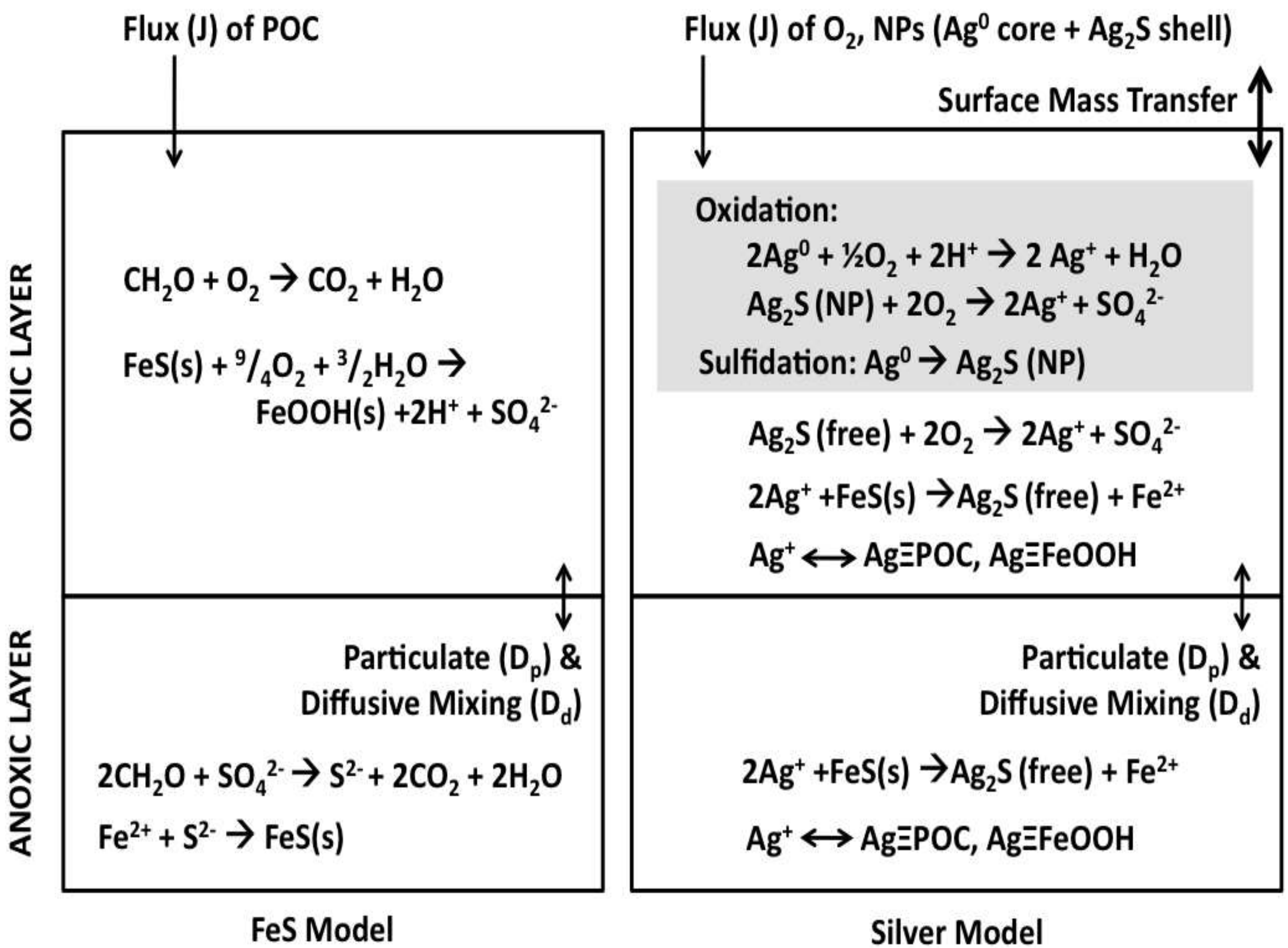
- Runoff is roughly a quarter of total stream loads
- Metal mobility is surprisingly high (<6% accumulation)
  - NP-derived Zn is twice as mobile as Ag



Setting deposition and resuspension rates to commonly used <u>average constant</u> values dramatically overpredicted accumulation

Dale et al., 2015 ES&T 49 (12), pp 7285

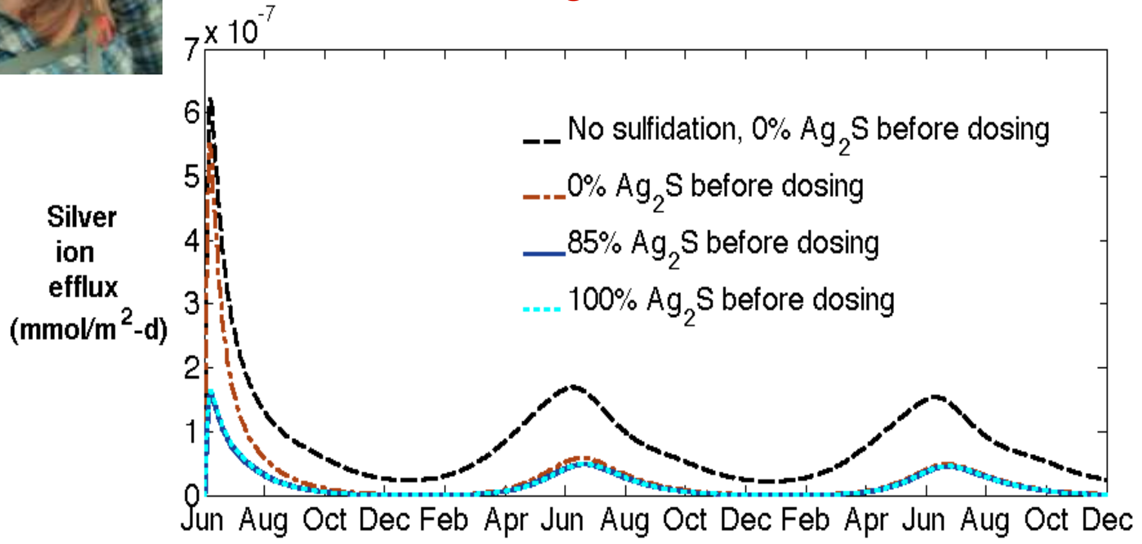
How can we model the effects of Ag NP transformations on metal bioavailability?



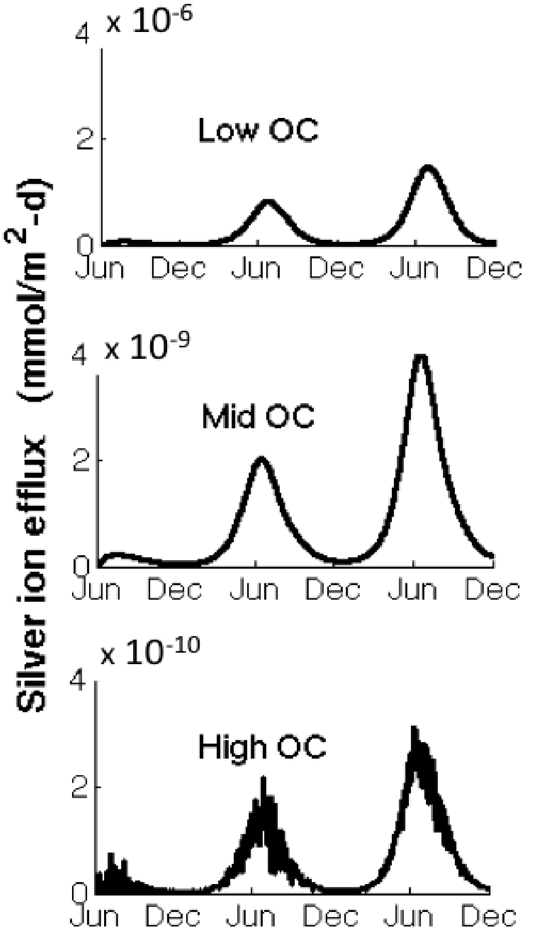
Dale et al., 2013 ES&T 47 (22) 12920

Modeling Ag ion Efflux from Sediment

Effect of Degree of Sulfidation



Effect of Organic Carbon



Dale et al., 2013 ES&T 47 (22) 12920

Transformations of ENMs in soil

Environmental Science & Technology

Article

Cite This: Environ. Sci. Technol. 2019, 53, 4959−4967

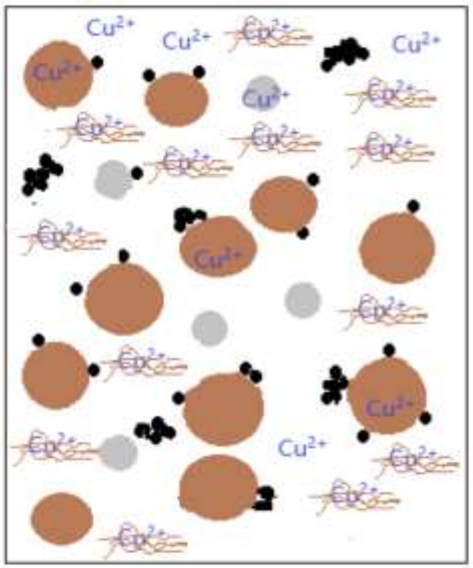
pubs.acs.org/est

Effect of Soil Organic Matter, Soil pH, and Moisture Content on Solubility and Dissolution Rate of CuO NPs in Soil

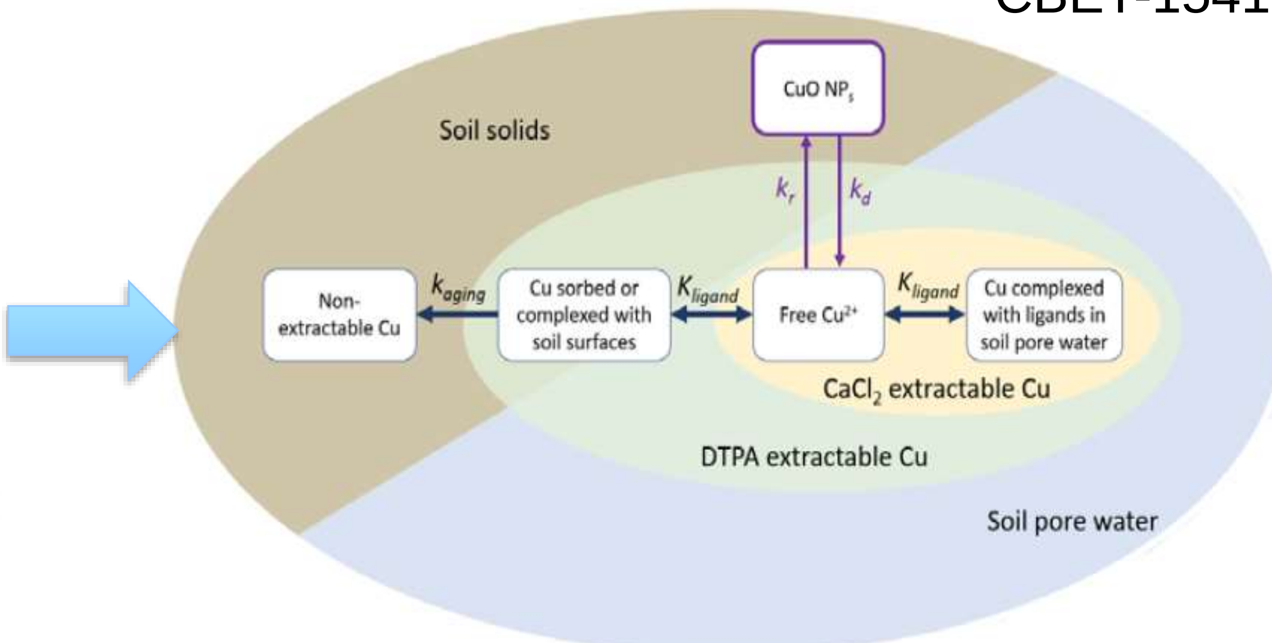
Xiaoyu Gao,[†,§] Sónia M. Rodrigues,[‡] Eleanor Spielman-Sun,[†,§] Sónia Lopes,[‡] Sandra Rodrigues,[‡] Yilin Zhang,[†,§] Astrid Avellan,[†,§] Regina M.B.O. Duarte,[‡] Armando Duarte,[‡] Elizabeth A. Casman,[§,∥] and Gregory V. Lowry*[,†,§]

nano FARM

CBET-1541807

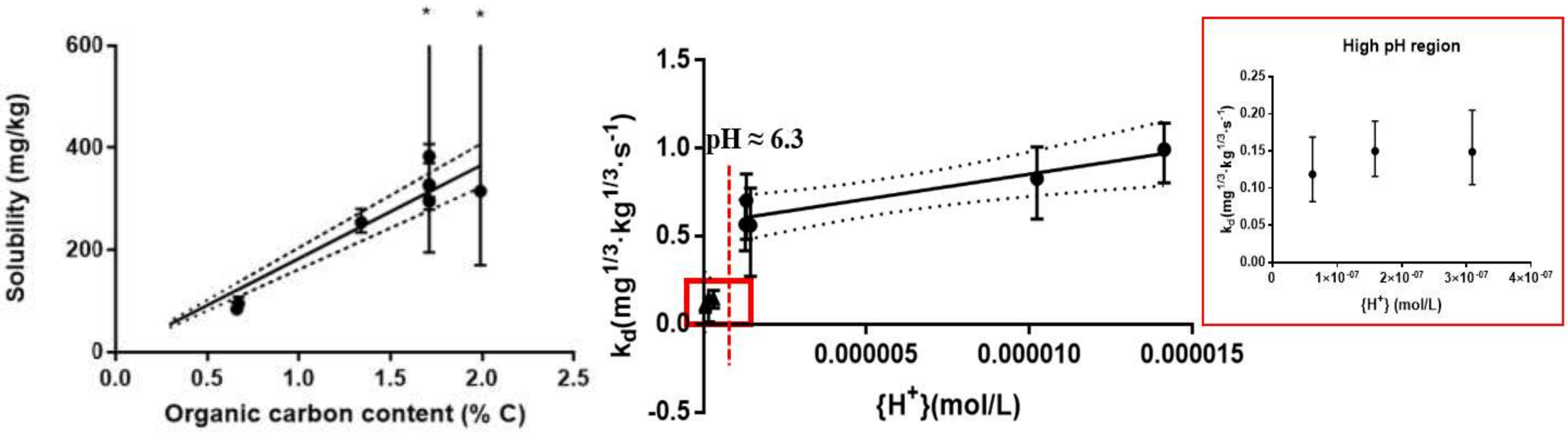


- CuO NPs
- Soil Organic matter
- Clay



Kinetics of dissolution is needed to model NP fate

Relationships between soil properties and dissolution parameters



- Organic carbon correlated with solubility of the CuO NPs
- Soil pH correlated with dissolution rate constant when at pH <6.3

Gao et al., 2019

Most Important Questions to Consider

Environmental Science & Technology

Feature

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Modeling Nanomaterial Environmental Fate in Aquatic Systems

Amy L. Dale,[†,‡,§] Elizabeth A. Casman,[‡,§] Gregory V. Lowry,[†,§] Jamie R. Lead,[‖] Enrica Viparelli,[⊥] and Mohammed Baalousha*[‖,⊥]

Table 1. Proposed Next-Generation Enhancements of Nanoparticle F&T Models Possible through Collaboration of Modelers and Experimentalists

improvements to...	examples
descriptions of NM heteroaggregation and transport	1. Apply kinetic descriptors of heteroaggregation rather than equilibrium descriptors 2. Model heteroaggregate breakup/disaggregation 3. Express heteroaggregation as a function of environmental drivers (e.g., natural organic matter, pH, ionic strength) and NM properties (e.g., particle size, engineered coating, pH_{PZC}) 4. Include bedload shift and other relevant sediment transport processes in stream models
descriptions of reactive NM chemistry	5. Express reaction rates as a function of environmental drivers (e.g., oxygen, temperature, pH) and particle properties (e.g., surface area, size) 6. Express rates as a function of particle transformations (e.g., NM dissolution rate as a function of NM sulfidation) 7. Determine rates for both heteroaggregated and unaggregated nanoparticles 8. Determine rates in complex environmental media (e.g., microbially mediated oxidation rates) 9. Track formation and speciation of reaction byproducts (e.g., metal ions) in models

Key Knowledge Gaps

- Spatially-resolved source characterization
  - MFA models
- Identify and capture all KEY PROCESSES affecting ENM behaviors
  - Heteroaggregation, disaggregation, resuspension, etc.
- Comparison of model frameworks
  - Steady-state vs. spatially-temporally resolved models
- Linking experimental work to modeling needs (parameterization)
- Linking models to bioaccumulation and toxicity
- Model validation

Contents lists available at ScienceDirect

Science of the Total Environment

journal homepage: www.elsevier.com/locate/scitotenv

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Determination of nanoparticle heteroaggregation attachment efficiencies and rates in presence of natural organic matter monomers. Monte Carlo modelling

Arnaud Clavier [a,*], Antonia Praetorius [b], Serge Stoll [a,*]

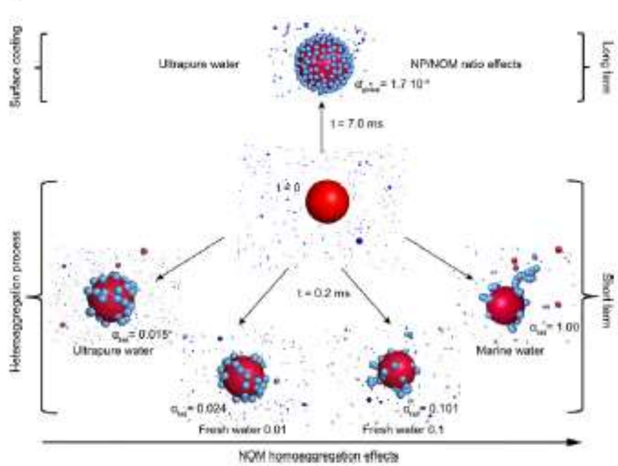
[a] University of Geneva, Institute of Environmental Science, Department F.-A. Forel for Environmental and Aquatic Sciences, Group of Environmental Physical Chemistry, Uni Carl Vogt, 66, boulevard Carl-Vogt, CH-1211 Geneva 4, Switzerland

[b] University of Vienna, Department of Environmental Geosciences and Environmental Science Research Network, Althanstr. 14 UZA2, 1090 Vienna, Austria

HIGHLIGHTS

- A novel and original approach is developed to study heteroaggregation between NPs and NOM molecules.
- Heteroaggregation rates and attachment efficiencies are calculated in contrasting conditions.
- NPs and NOM interactions are playing key roles in controlling the balance between homo and heteroaggregation.
- A clear distinction should be made between individual, primary and global heteroaggregation rates.

GRAPHICAL ABSTRACT



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Considering the forms of released engineered nanomaterials in probabilistic material flow analysis☆

Véronique Adam, Alejandro Caballero-Guzman, Bernd Nowack*

EMPA, Swiss Federal Laboratories for Materials Science and Technology, Technology and Society Laboratory, Lerchenfeldstrasse 5, CH-9014, St. Gallen, Switzerland

NATURE NANOTECHNOLOGY | VOL 13 | NOVEMBER 2018 | 979–985 | www.nature.com/naturenanotechnology

ENGINEERED NANOMATERIALS

Inching closer to realistic exposure models

Engineered nanomaterials are often highly reactive and readily transform to new species. New modelling capabilities incorporate these transformations into estimates of environmental exposure concentrations and associated risks more accurately.

Gregory V. Lowry

Environmental Science Nano

PAPER

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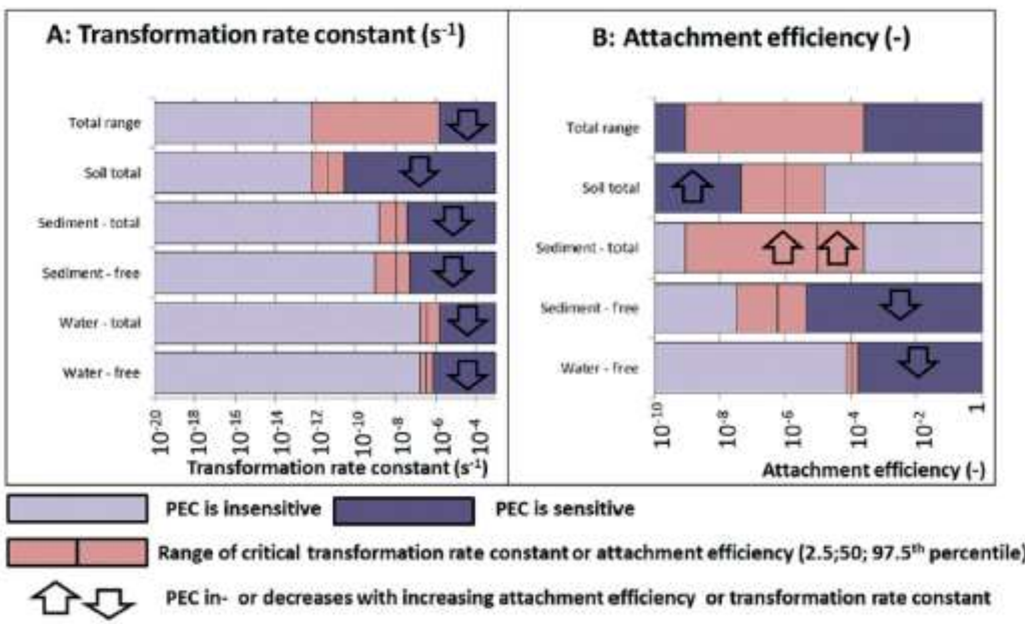
Cite this: *Environ. Sci.: Nano*, 2019, 6, 2049

A model sensitivity analysis to determine the most important physicochemical properties driving environmental fate and exposure of engineered nanoparticles†

J. A. J. Meesters, *[ab] W. J. G. M. Peijnenburg, [bc] A. J. Hendriks,[a] D. Van de Meent[a] and J. T. K. Quik [b]



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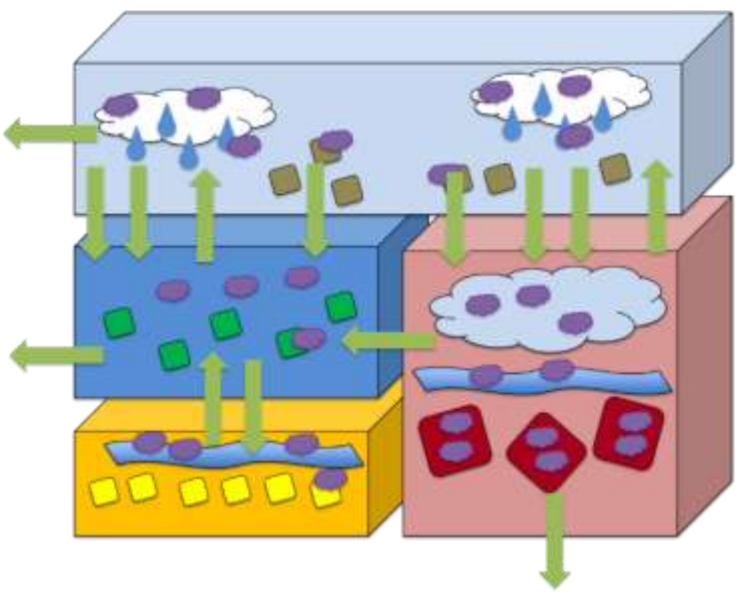
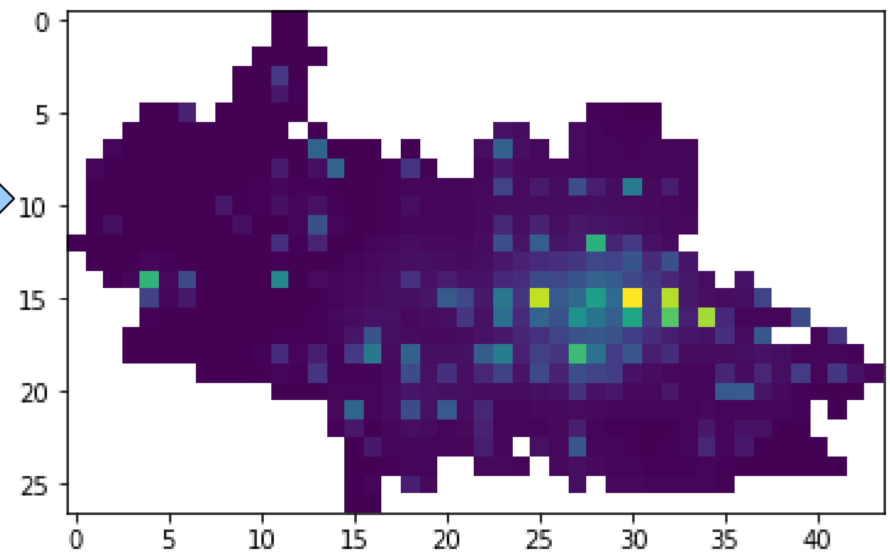
Comparing predicted environmental concentrations from SimpleBox4nano and NanoFASE-WSO

Decision making??





Model consistency is not validation!

5 x 5 km grids?

ACS APPLIED MATERIALS & INTERFACES

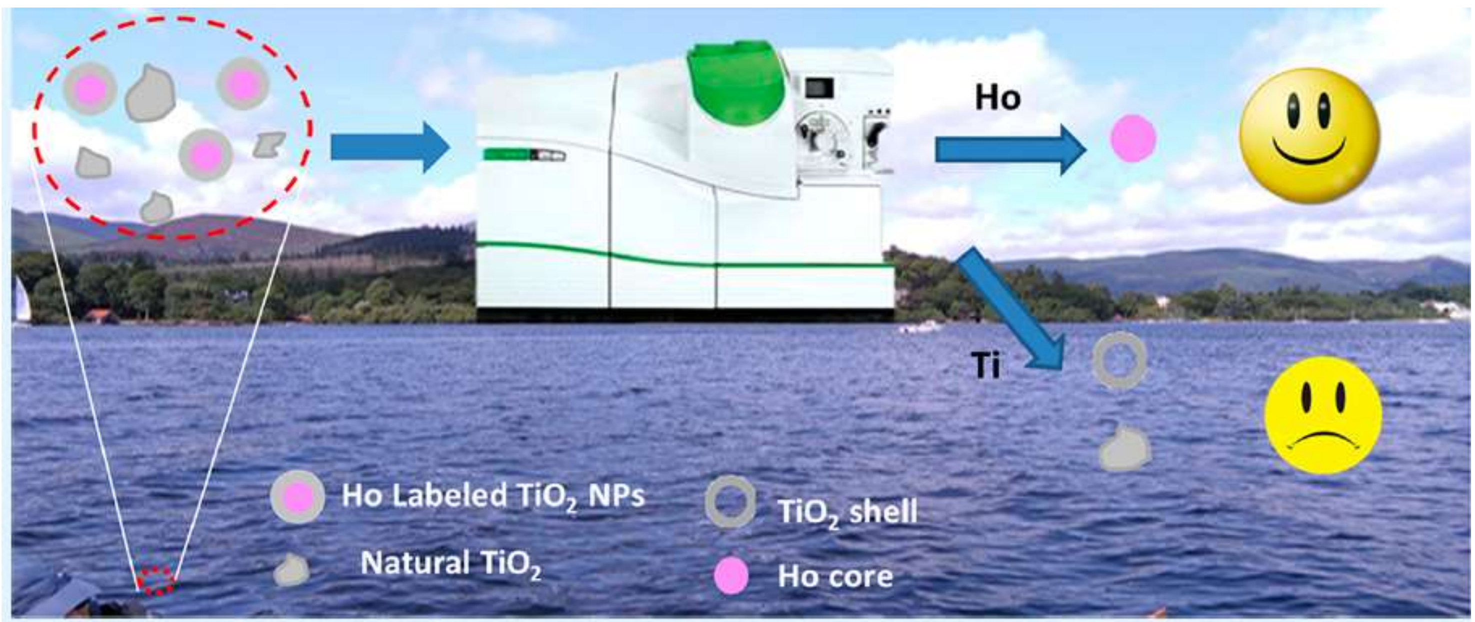
Research Article

Cite This: ACS Appl. Mater. Interfaces 2019, 11, 19452−19461

www.acsami.org

Core–Shell $NaHoF_4$@TiO_2 NPs: A Labeling Method to Trace Engineered Nanomaterials of Ubiquitous Elements in the Environment

Xianjin Cui,[*,†] Benjamin Fryer,[†] Diwei Zhou,[§] Rhys W. Lodge,[‡] Andrei N. Khlobystov,[‡] Eugenia Valsami-Jones,[†] and Iseult Lynch[†]



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Current Opinion in Environmental Sustainability

Models for assessing engineered nanomaterial fate and behaviour in the aquatic environment☆

Richard J Williams[1], Samuel Harrison[2], Virginie Keller[1], Jeroen Kuenen[3], Stephen Lofts[2], Antonia Praetorius[4,5], Claus Svendsen[1], Lucie C Vermeulen[6,7] and Jikke van Wijnen[8]

"ENM-specific processes represented in models are mainly limited to aggregation and, in some instances, dissolution. Transformation processes (e.g. sulphidation), the role of the manufactured coatings, particle size distribution and particle form and state are still usually excluded. "

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Acknowledgements

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Turning bright ideas into brilliant outcomes

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