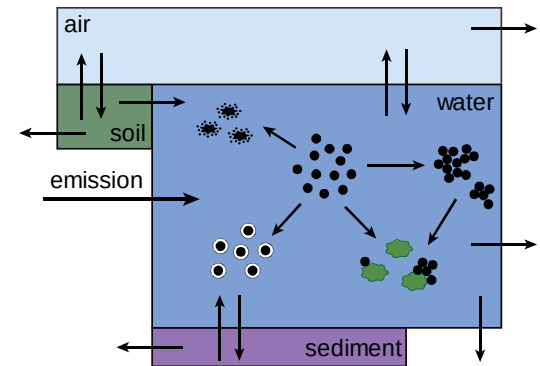


What do we need to create good models for the development of a sustainable nanotechnology?

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Frank von der Kammer, Thilo Hofmann

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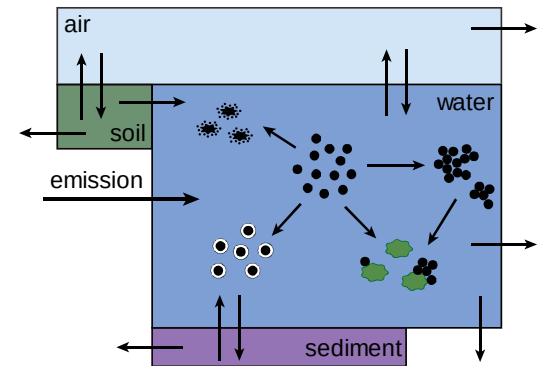
What do we need to create good models for the development of a sustainable nanotechnology?

→ bridging the gap between experiments and models

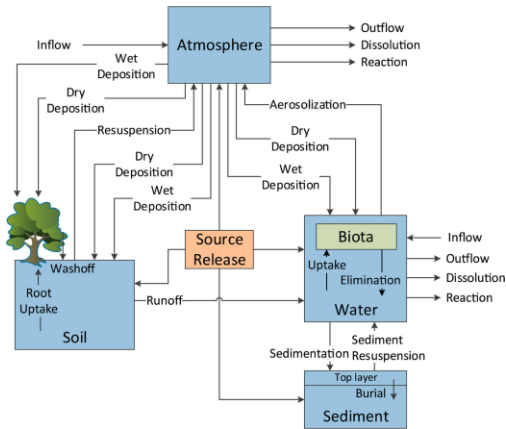
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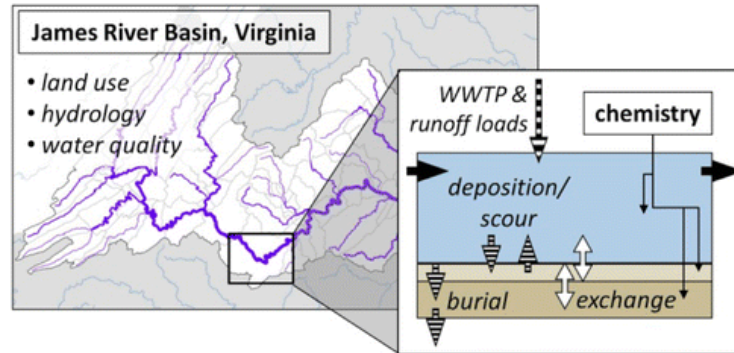
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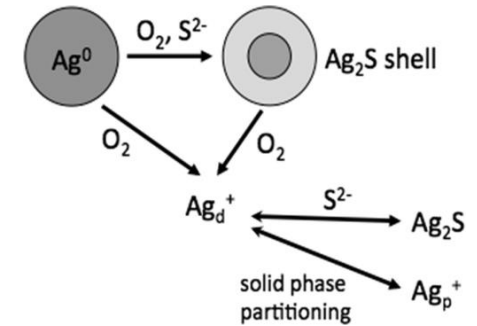
Different models for different purposes and scales



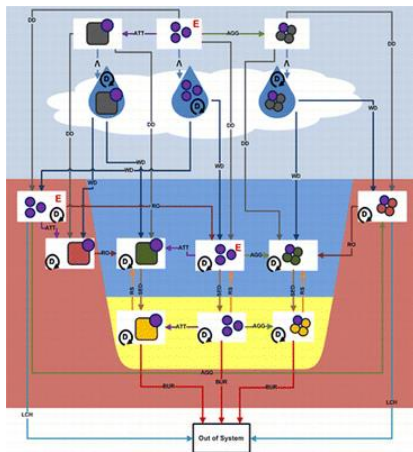
Liu & Cohen, ES&T 2014



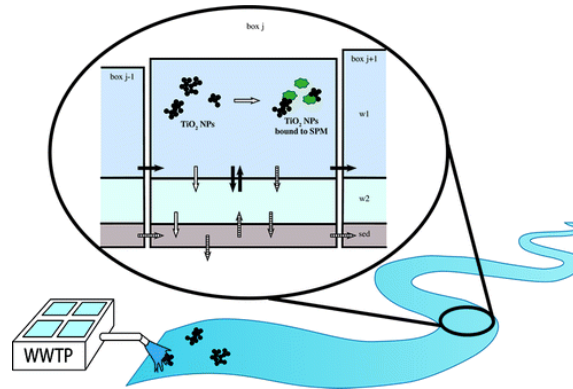
Dale et al., ES&T 2015



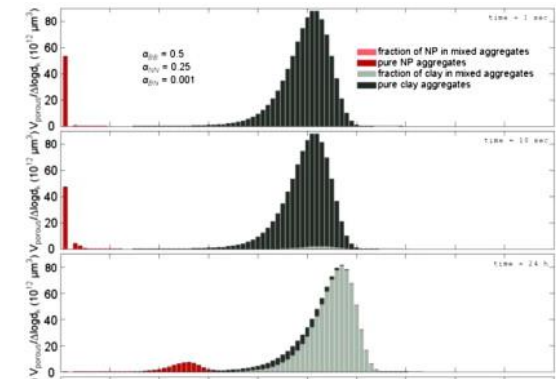
Dale et al., ES&T 2012



Meesters et al., ES&T 2014

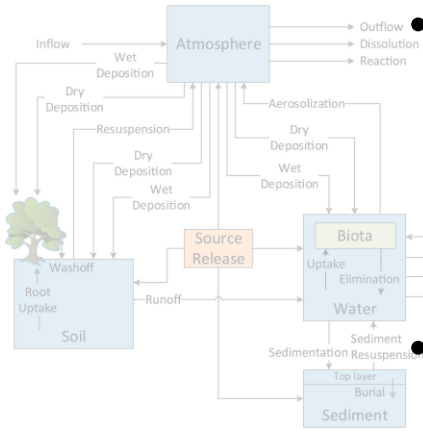


Praetorius et al., ES&T 2012



Therezien et al., ES&T 2014

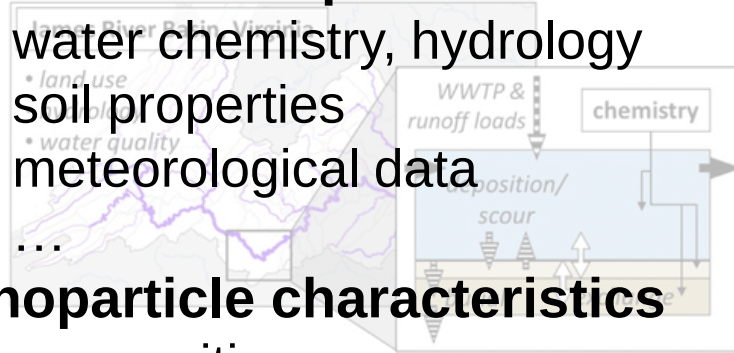
All models need input parameters



Liu & Cohen, ES&T 2014

Environmental parameters

- water chemistry, hydrology
- soil properties
- meteorological data
- ...



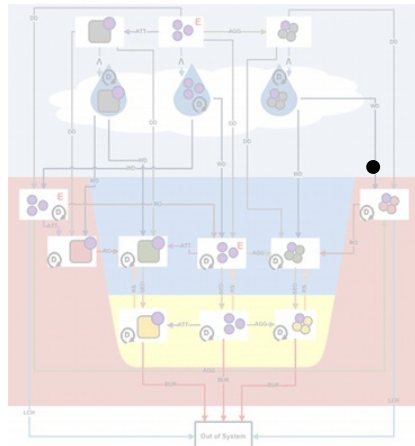
Dale et al., ES&T 2015

Nanoparticle characteristics

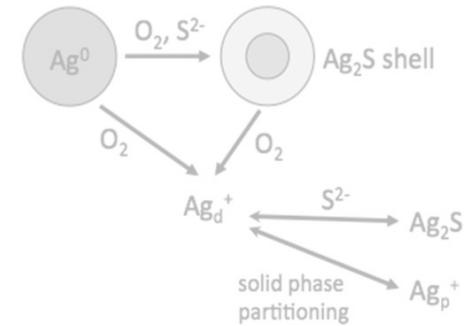
- composition
- size
- shape
- surface properties/coatings
- ...

Process descriptions

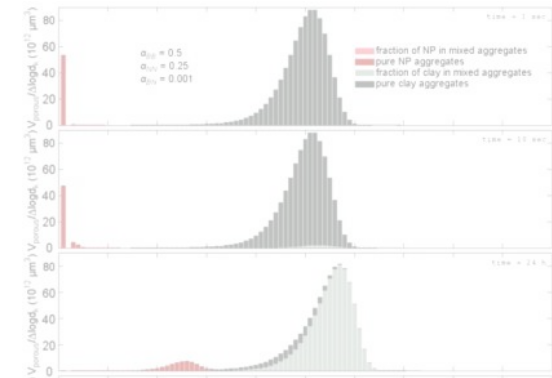
- aggregation rate constants
- attachment efficiencies
- dissolution rate constants
- surface transformation rate constants
- ...



Meesters et al., ES&T 2014



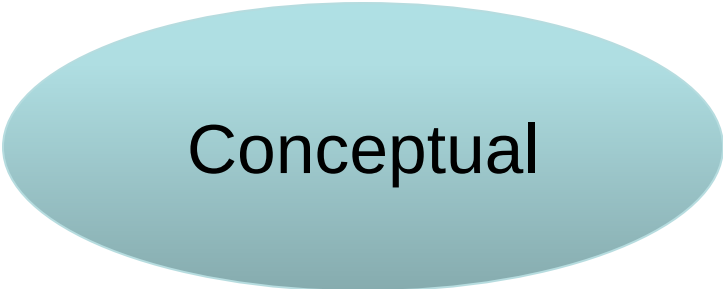
Dale et al., ES&T 2012



Thomazien et al., ES&T 2014

Purpose of models & experiments

Models can be:



Conceptual



Quantitative

Purpose of models & experiments

Models can be:

Conceptual

Quantitative

Experiments can:

Qualitatively
inform models

Provide
quantitative input
parameters



Modelers: “there is not enough data”

Modelers: “there is not enough data”

→ *Is that really true after 10 years of
Nano EHS research?*

We have generated a lot of data in 10 years of Nano EHS research (and already before that)

→ *But a lot of this data cannot be used for modeling*

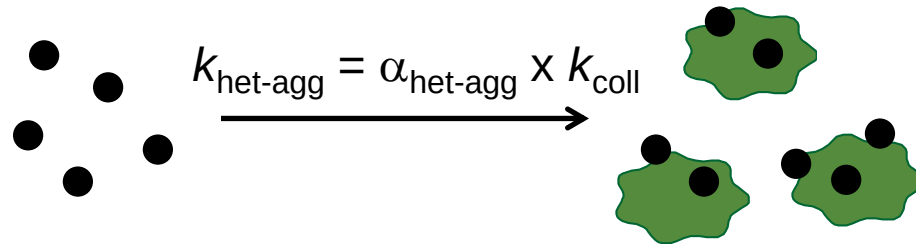
Issues/challenges

experiments

models

1. Data needs for models and experimental outputs do not always align

Example:
heteroaggregation



- aggregation rate constants ($k_{\text{het-agg}}$)
- attachment efficiencies ($\alpha_{\text{het-agg}}$)

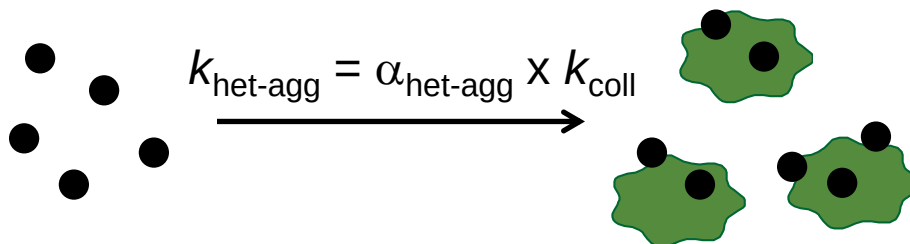
Issues/challenges

experiments

models

1. Data needs for models and experimental outputs do not always align

Example:
heteroaggregation



Experiment outputs

- % removal
- sedimentation rates
- aggregation curves
- distribution coefficients (K_d)*

- **aggregation rate constants ($k_{\text{het-agg}}$)**
- **attachment efficiencies ($\alpha_{\text{het-agg}}$)**

**for further information on why K_d is not valid for nanoparticles see:
Praetorius et al. ES Nano 2014*

Issues/challenges

experiments



models

2. Limited application range of experimental method in terms of:

- a) environmental properties (e.g. method does not work at high IS, only without NOM)
- a) nanoparticles types (e.g. method only work for magnetic NPs)
- a) Measured parameter (e.g. many heteroaggregation experiments can resolve a values between 0.01 and 1, but might to assess values of 10^{-7})

Issues/challenges

experiments



models

3. Mismatched levels of accuracy

- a) Large scale models (e.g. regional/global fate & transport models)
 - favor wide range of parameter measurements over high accuracy



3. Mismatched levels of accuracy

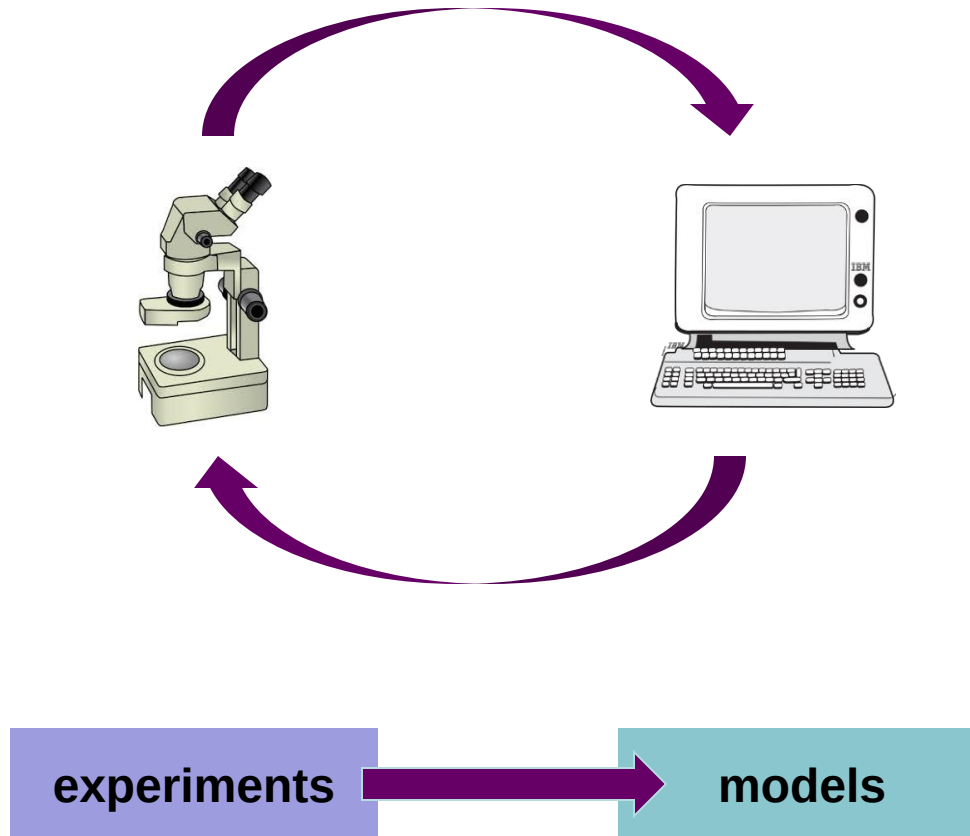
- a) Large scale models (e.g. regional/global fate & transport models)
→ favor wide range of parameter measurements over high accuracy
- b) Small scale models (e.g. detailed aggregation model)
→ need for highly resolved measurements (e.g. property x for several NP sizes)



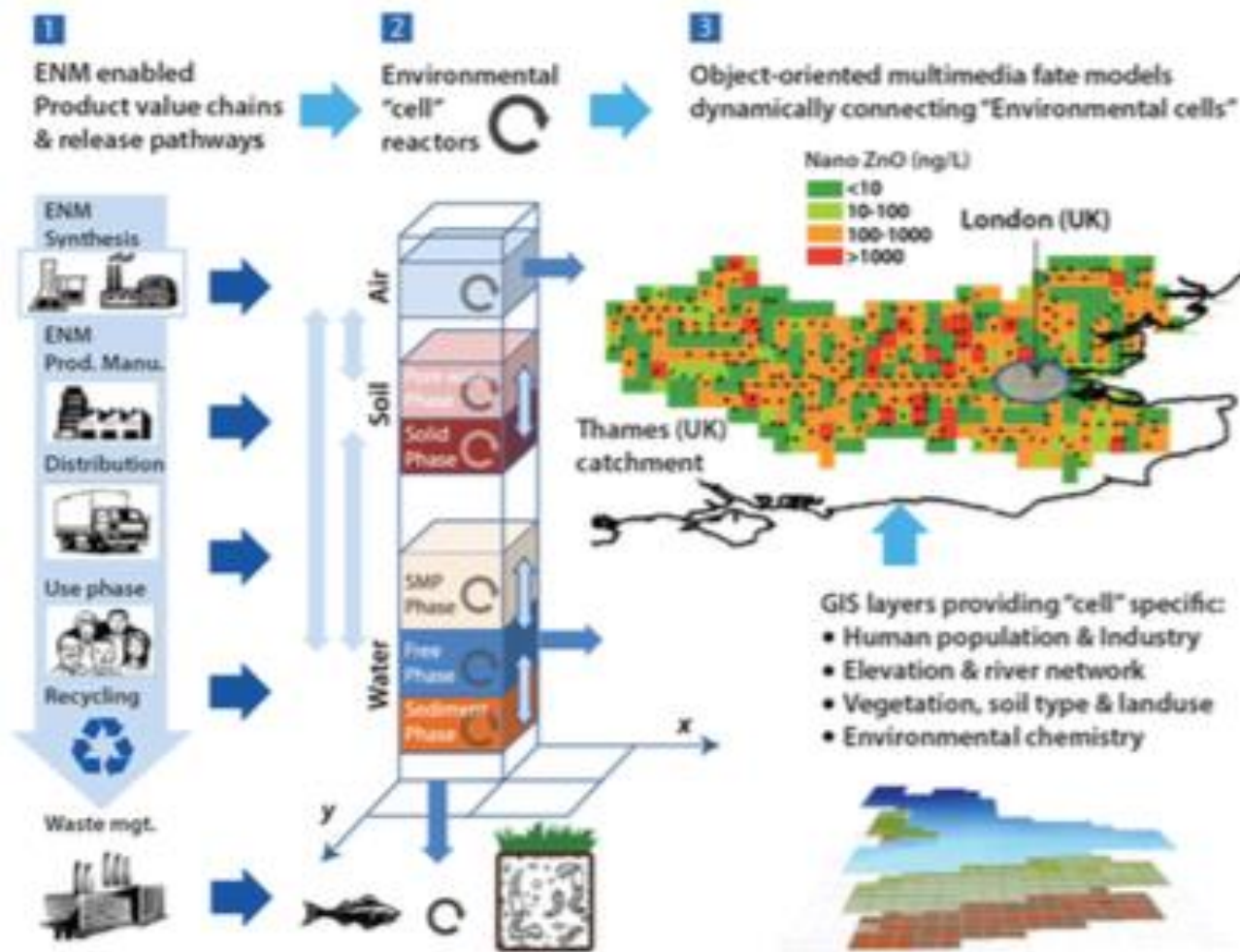
4. Insufficient understanding of measured data

- a) How time consuming/costly is a measurement?
- a) How reliable is the method?
- a) What are common error sources?
- a) Can we quantify the uncertainty?
- b) What are the limits of the method?

→ We need to improve communication and direct collaboration between modelers and laboratory scientists!



NanoFASE project



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

Conclusions

experiments



models

1. We need to align experiment output with data needs of models
2. Choice of experimental method according to required application range and needs for accuracy
3. Need to increase communication between modelers and researchers in the lab
4. Make use of existing knowledge and qualitative results for first estimates before designing new methods

Acknowledgements



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Nano-Norms-Nature Research platform



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