

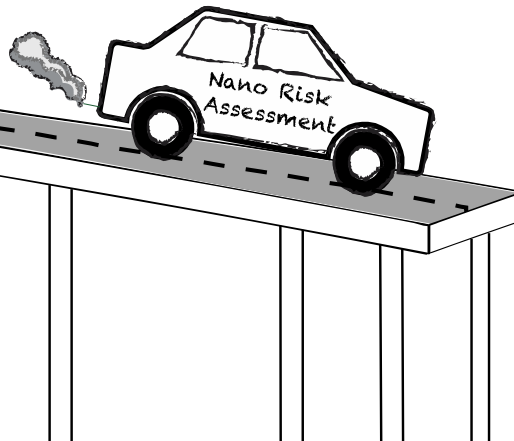


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Implications of using inappropriate fate descriptors for engineered nanoparticles



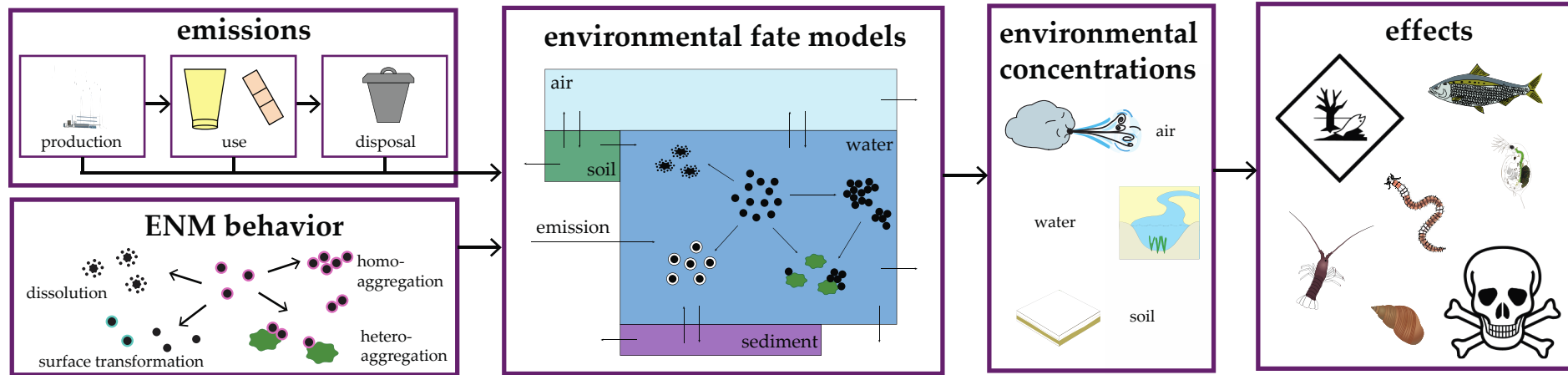
Antonia Praetorius

Frank von der Kammer

Thilo Hofmann

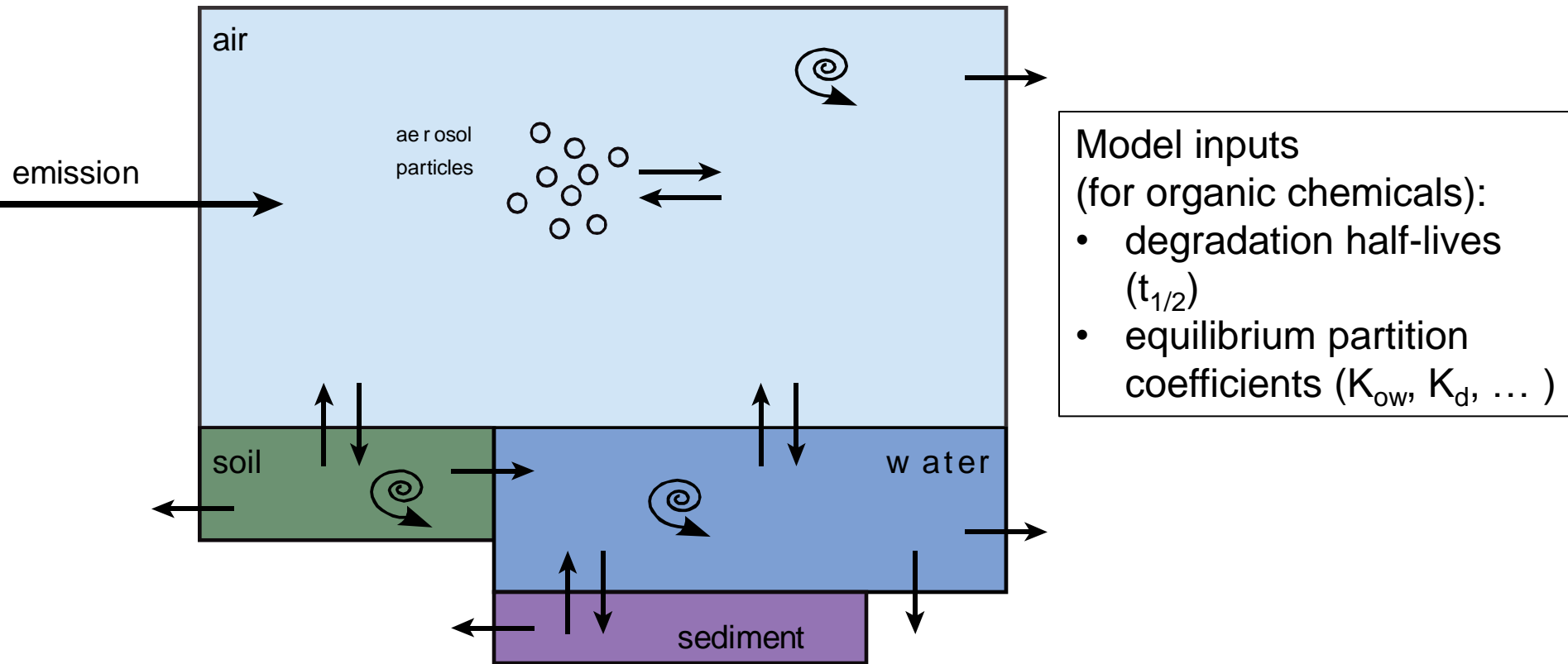
antonia.praetorius@univie.ac.at

Motivation

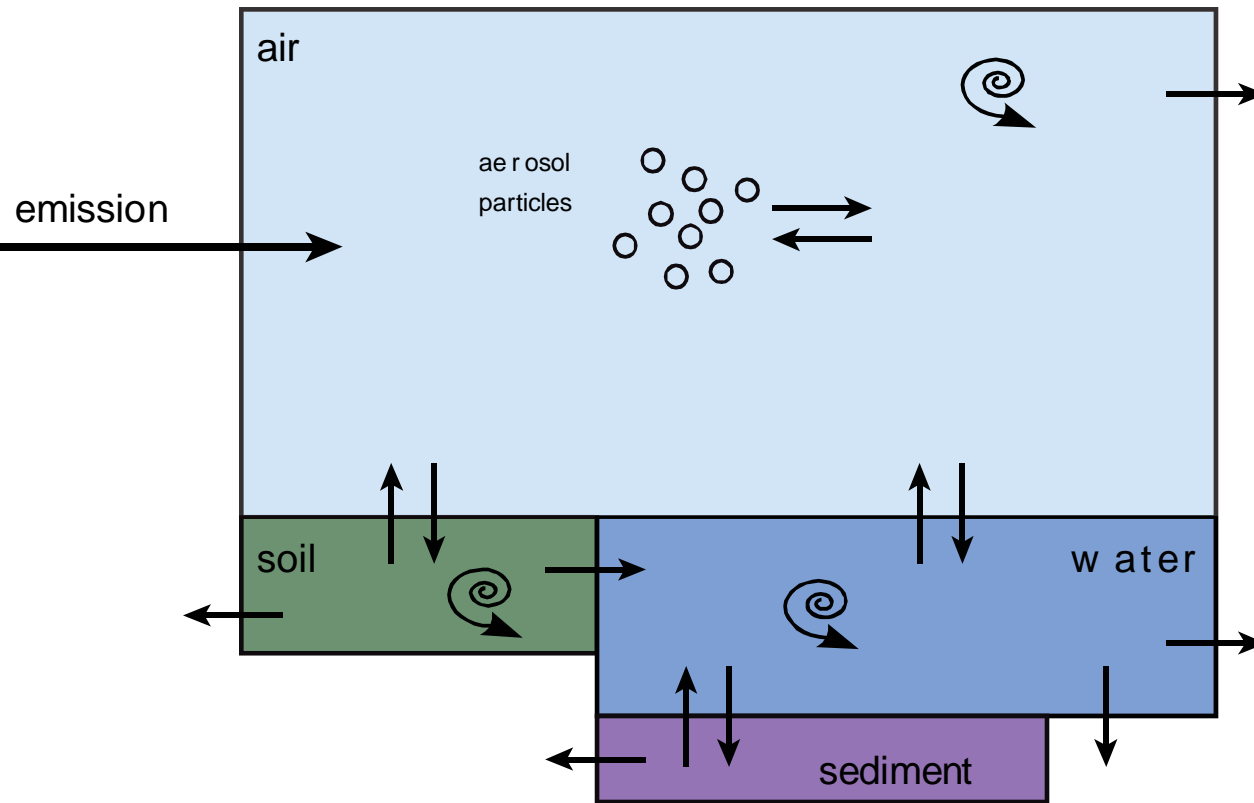


- we need adequate fate predictors for engineered nanoparticles (ENPs) to use as input parameters in models to predict ENP behaviour, transport and fate in different environmental systems (e.g. for risk assessment)
- the selection of adequate fate descriptors requires a careful selection and understanding of the underlying physical chemical properties of ENPs

Fate models & fate descriptors for "conventional" pollutants



Fate models & fate descriptors for "conventional" pollutants

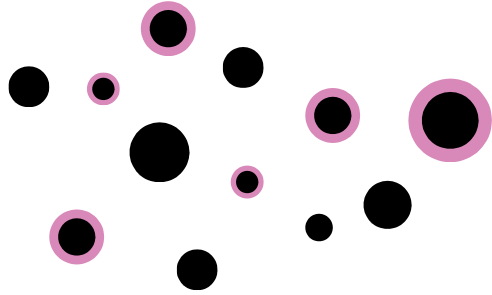


Model inputs

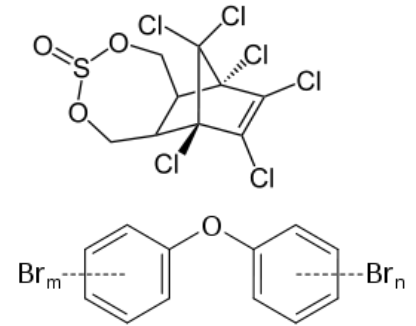
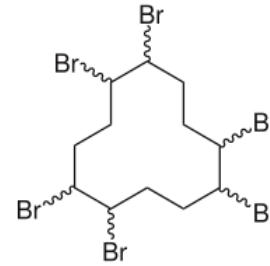
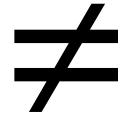
(for organic chemicals):

- degradation half-lives ($t_{1/2}$)
- equilibrium partition coefficients (K_{ow} , K_d , ...)

ENP versus "conventional" organic contaminants

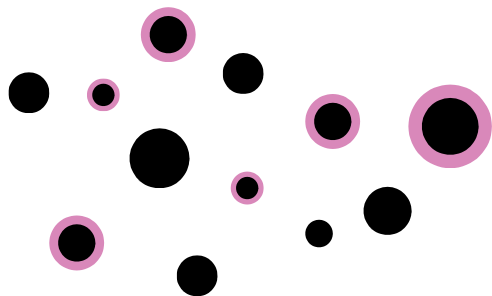


nanoparticles

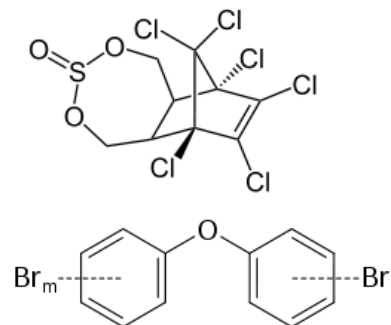
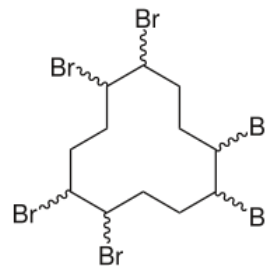


organic chemicals

ENP versus "conventional" organic contaminants



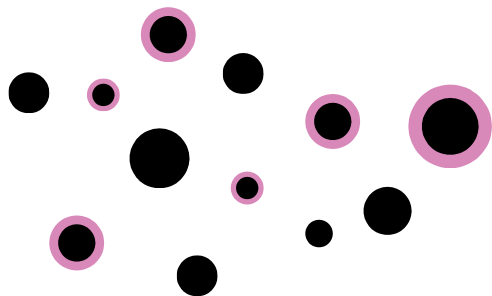
nanoparticles



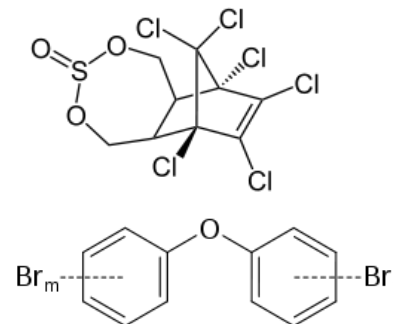
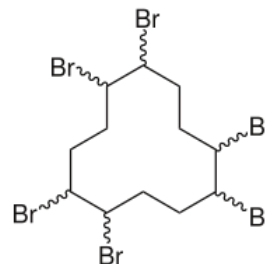
organic chemicals

- NPs do not form solutions but **colloidal dispersions**
→ thermodynamically unstable multiphase systems

ENP versus "conventional" organic contaminants



nanoparticles



organic chemicals

- NPs do not form solutions but **colloidal dispersions**
→ thermodynamically unstable multiphase systems

→ we cannot simply apply existing concept as they are for these new materials

What are appropriate fate descriptors for ENPs?

Fate descriptor debate

Environmental
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Nano



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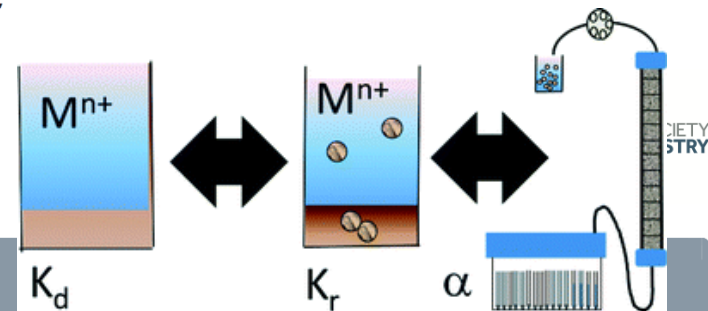
The road to nowhere: equilibrium partition coefficients for nanoparticles

Cite this: *Environ. Sci.: Nano*, 2014, 1, 317

Antonia Praetorius,^{*a} Nathalie Tufenkji,^b Kai-Uwe Goss,^c Martin Scheringer,^a Frank von der Kammer^d and Menachem Elimelech^e

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Cite this: *Environ. Sci.: Nano*, 2015, 2, 19

Fate descriptors for engineered nanoparticles: the good, the bad, and the ugly

Geert Cornelis

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Cite this: *Environ. Sci.: Nano*, 2015, 2, 27

Much ado about α : reframing the debate over appropriate fate descriptors in nanoparticle environmental risk modeling

Amy L. Dale,^{*abc} Gregory V. Lowry^{bc} and Elizabeth A. Casman^{ac}



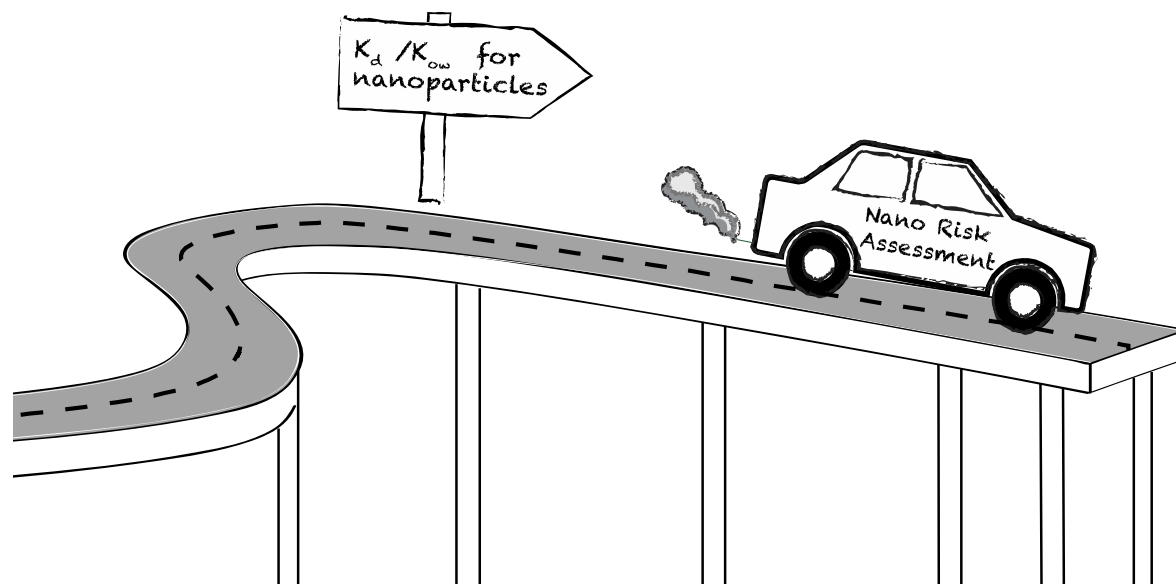
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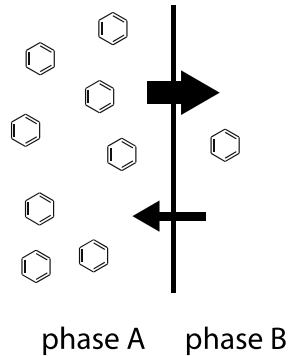
Antonia Praetorius,^{*a} Nathalie Tufenkji,^b Kai-Uwe Goss,^c Martin Scheringer,^a Frank von der Kammer^d and Menachem Elimelech^e



Underlying theoretical concepts

organic chemicals

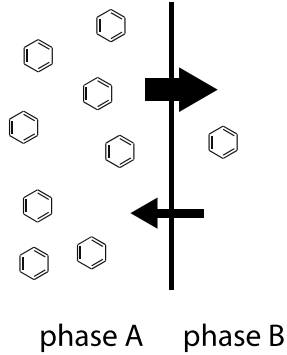
t_0
initial mixing



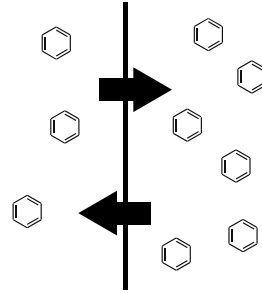
Underlying theoretical concepts

organic chemicals

t_0
initial mixing



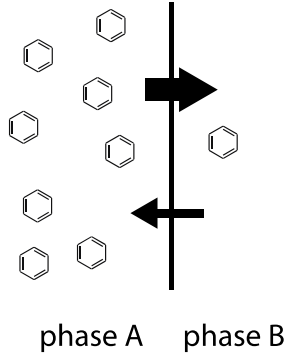
t_1
equilibrium
 $K_{AB} = \frac{3}{6} = 0.5$



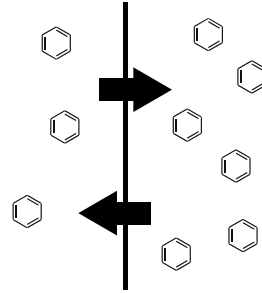
Underlying theoretical concepts

organic chemicals

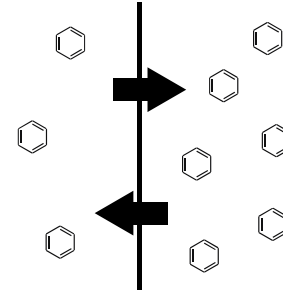
t_0
initial mixing



t_1
equilibrium
 $K_{AB} = \frac{3}{6} = 0.5$



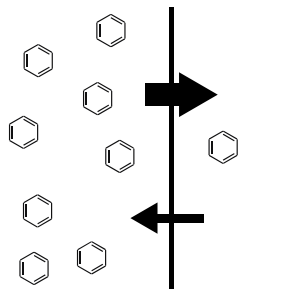
t_2
still equilibrium
 $K_{AB} = \frac{3}{6} = 0.5$



Underlying theoretical concepts

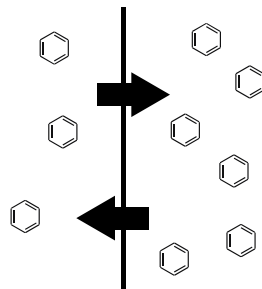
organic chemicals

t_0
initial mixing

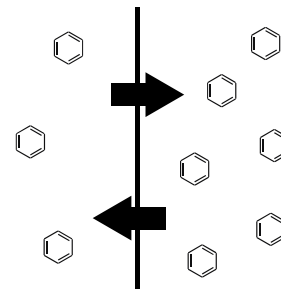


phase A phase B

t_1
equilibrium
 $K_{AB} = \frac{3}{6} = 0.5$

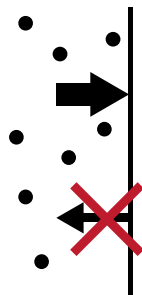


t_2
still equilibrium
 $K_{AB} = \frac{3}{6} = 0.5$



nanoparticles

t_0
initial mixing

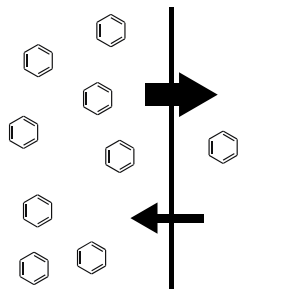


phase A phase B

Underlying theoretical concepts

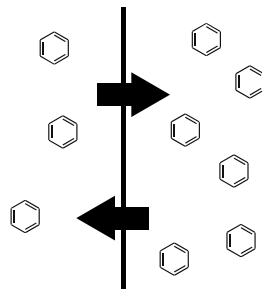
organic chemicals

t_0
initial mixing

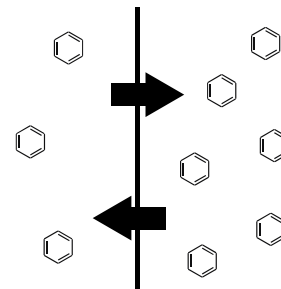


phase A phase B

t_1
equilibrium
 $K_{AB} = \frac{3}{6} = 0.5$

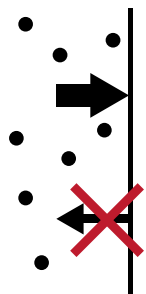


t_2
still equilibrium
 $K_{AB} = \frac{3}{6} = 0.5$



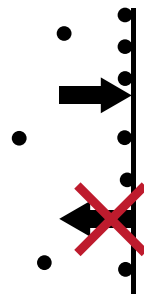
nanoparticles

t_0
initial mixing



phase A phase B

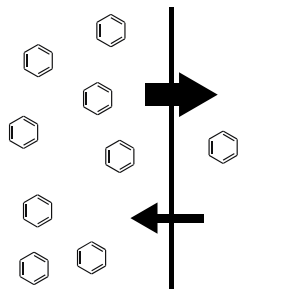
t_1
non-equilibrium
"K_{AB}" = $\frac{3}{6} = 0.5$



Underlying theoretical concepts

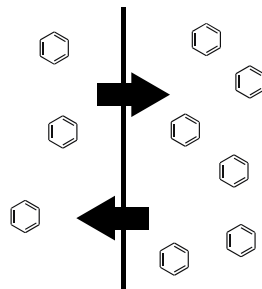
organic chemicals

t_0
initial mixing

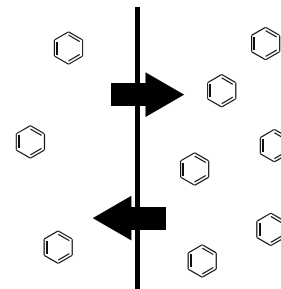


phase A phase B

t_1
equilibrium
 $K_{AB} = \frac{3}{6} = 0.5$

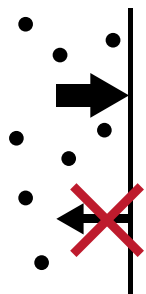


t_2
still equilibrium
 $K_{AB} = \frac{3}{6} = 0.5$



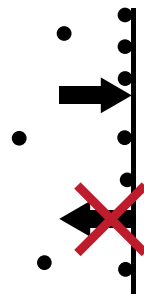
nanoparticles

t_0
initial mixing

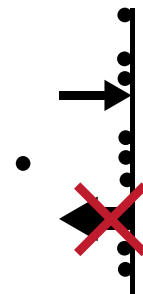


phase A phase B

t_1
non-equilibrium
" K_{AB} " = $\frac{3}{6} = 0.5$

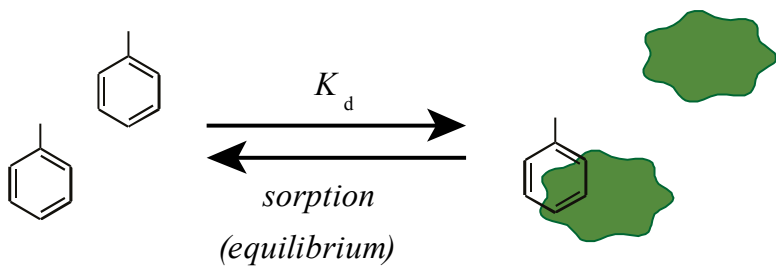


t_2
non-equilibrium
" K_{AB} " = $\frac{1}{8} = 0.125$



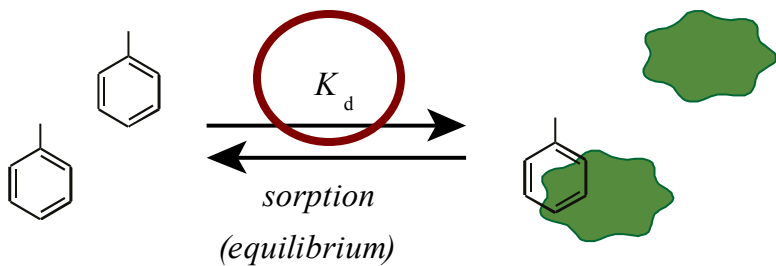
How to describe the interaction of ENPs with surfaces?

organic chemicals



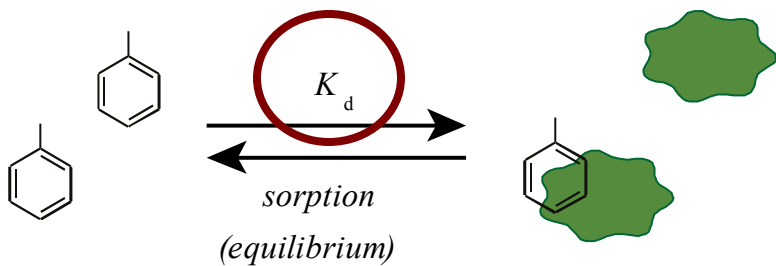
How to describe the interaction of ENPs with surfaces?

organic chemicals

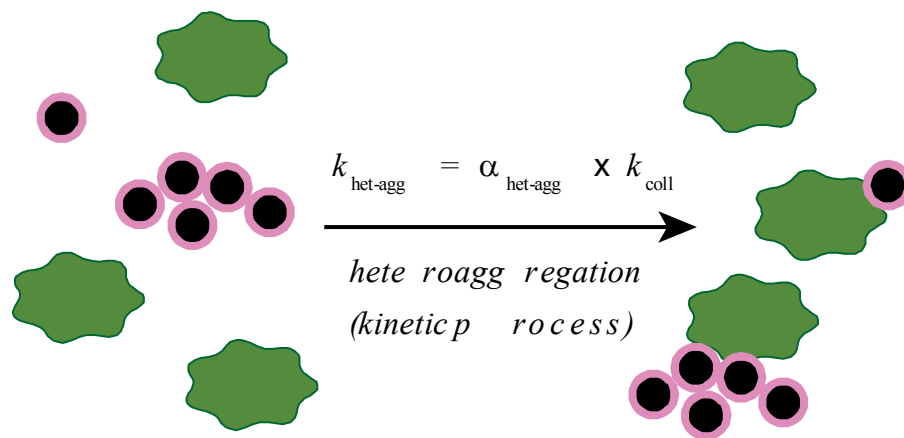


How to describe the interaction of ENPs with surfaces?

organic chemicals

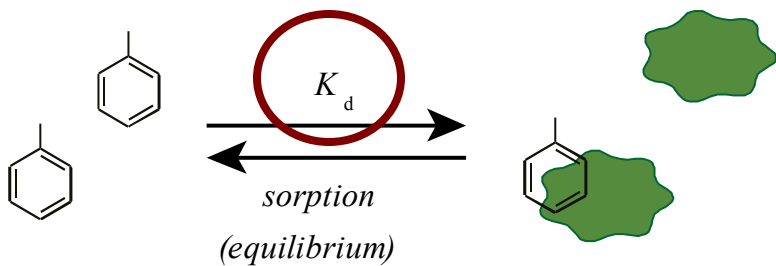


nanoparticles

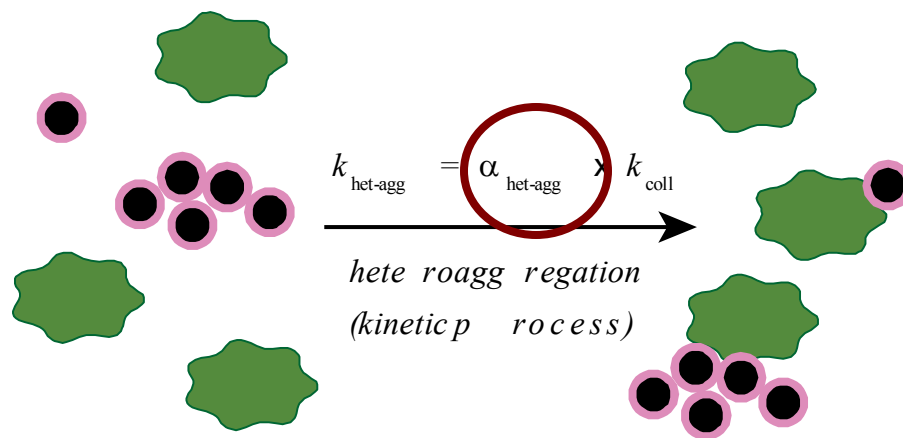


How to describe the interaction of ENPs with surfaces?

organic chemicals

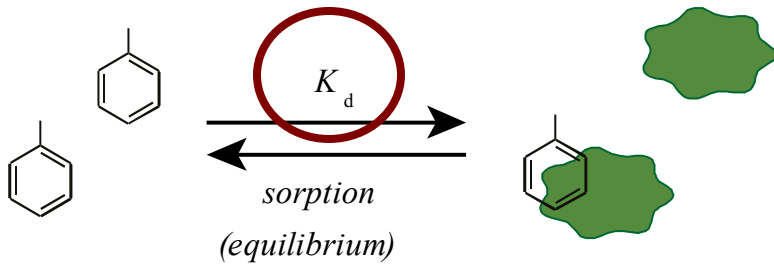


nanoparticles

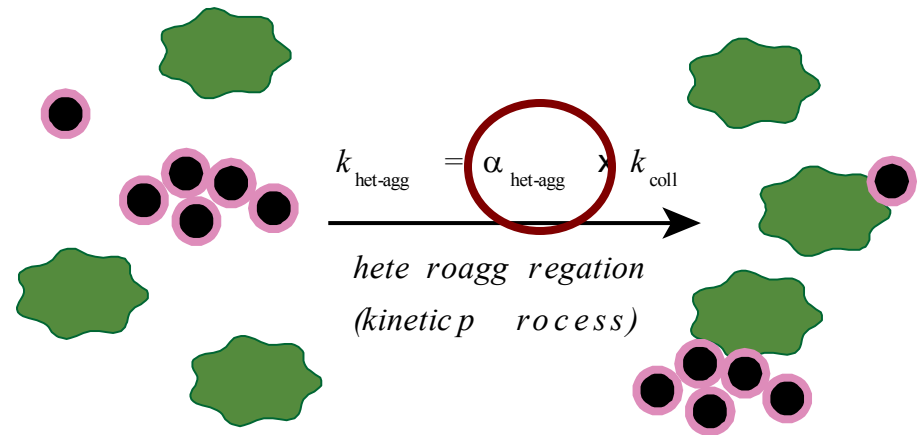


How to describe the interaction of ENPs with surfaces?

organic chemicals



nanoparticles



- Challenges:**
- determination of $\alpha_{\text{het-agg}}$ experimentally difficult
 - heteroaggregation process more complex to model than simple equilibrium distribution

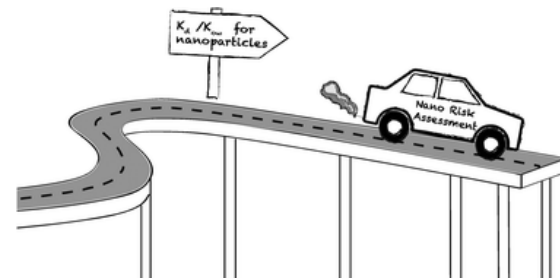
Fate descriptor debate

Environmental
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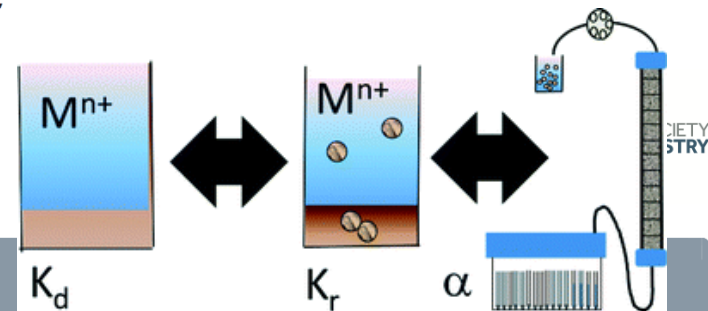
The road to nowhere: equilibrium partition coefficients for nanoparticles

Cite this: *Environ. Sci.: Nano*, 2014, 1, 317

Antonia Praetorius,^{*a} Nathalie Tufenkji,^b Kai-Uwe Goss,^c Martin Scheringer,^a Frank von der Kammer^d and Menachem Elimelech^e

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Fate descriptors for engineered nanoparticles: the good, the bad, and the ugly

Geert Cornelis

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Much ado about α : reframing the debate over appropriate fate descriptors in nanoparticle environmental risk modeling

Amy L. Dale,^{*abc} Gregory V. Lowry^{bc} and Elizabeth A. Casman^{ac}



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scientific principles

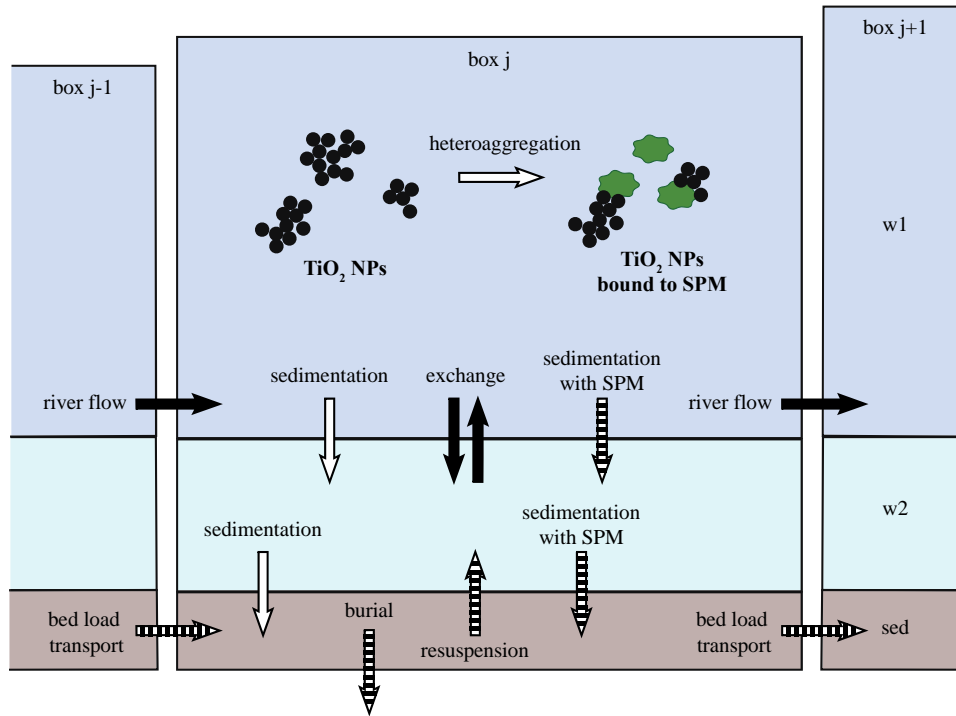
scientific correctness vs practicability

engineering vs scientific models

*appropriate/inappropriate simplifications
in fate modeling*

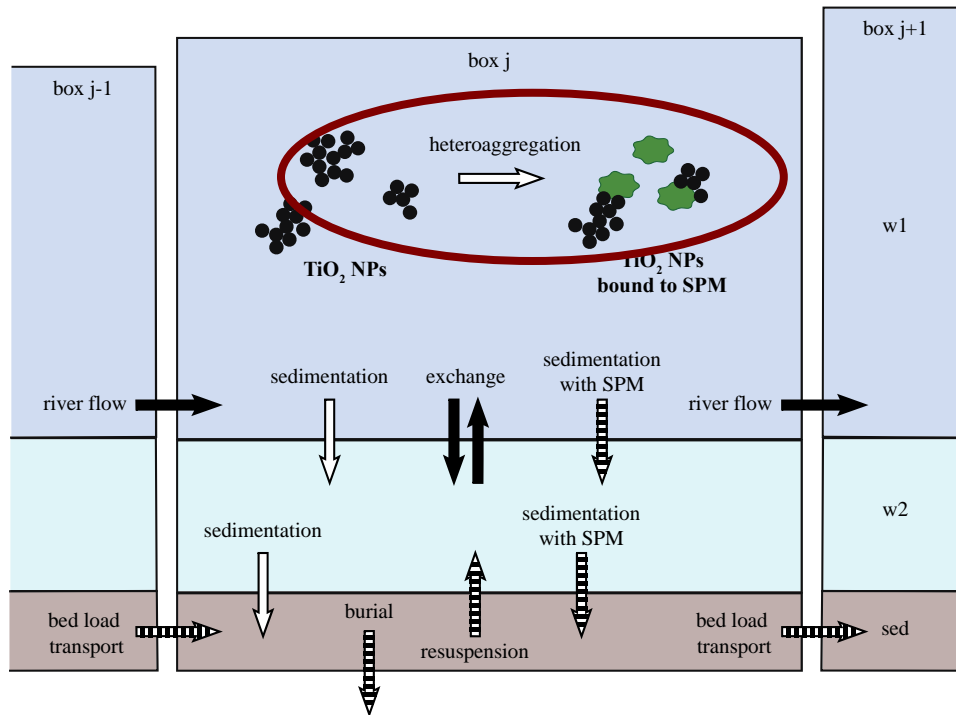
Consequences of using wrong fate descriptors

by replacing a dynamic process with a fixed distribution...



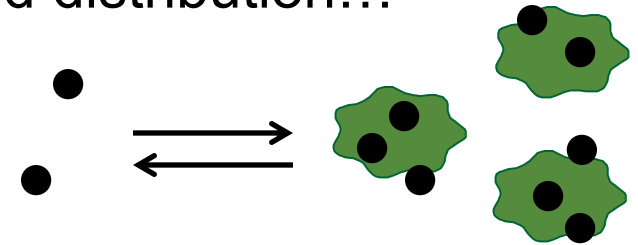
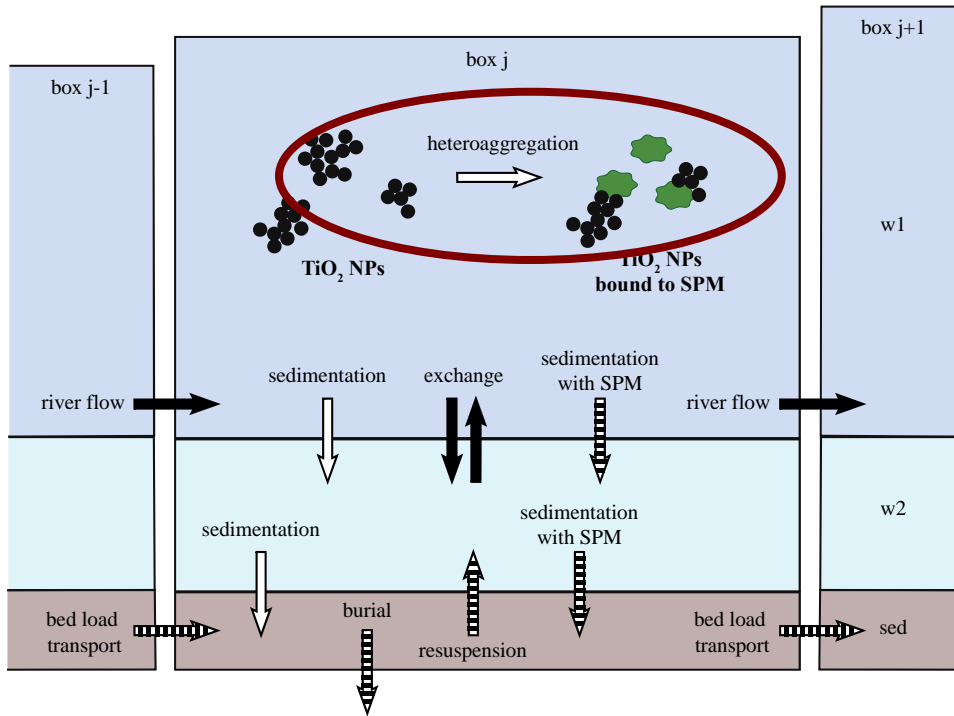
Consequences of using wrong fate descriptors

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Consequences of using wrong fate descriptors

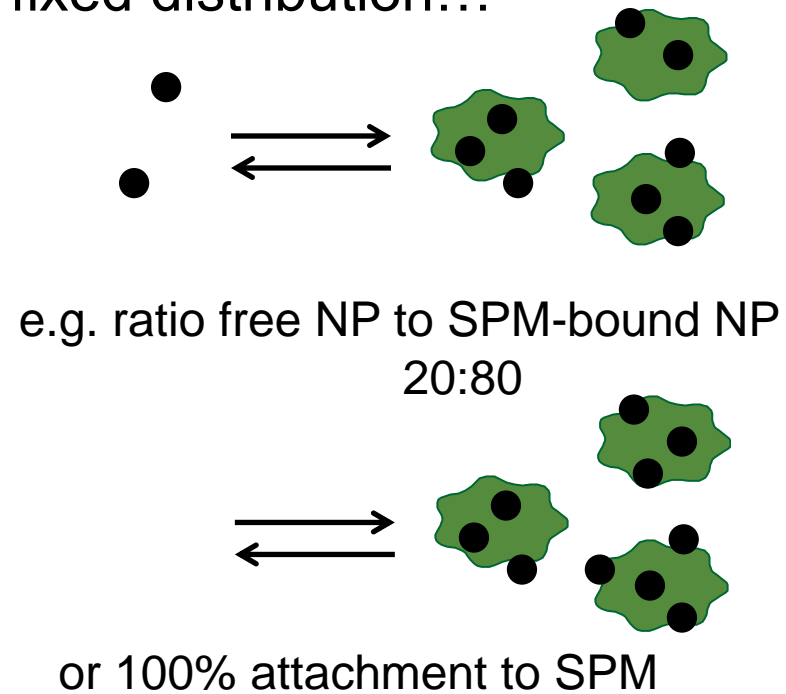
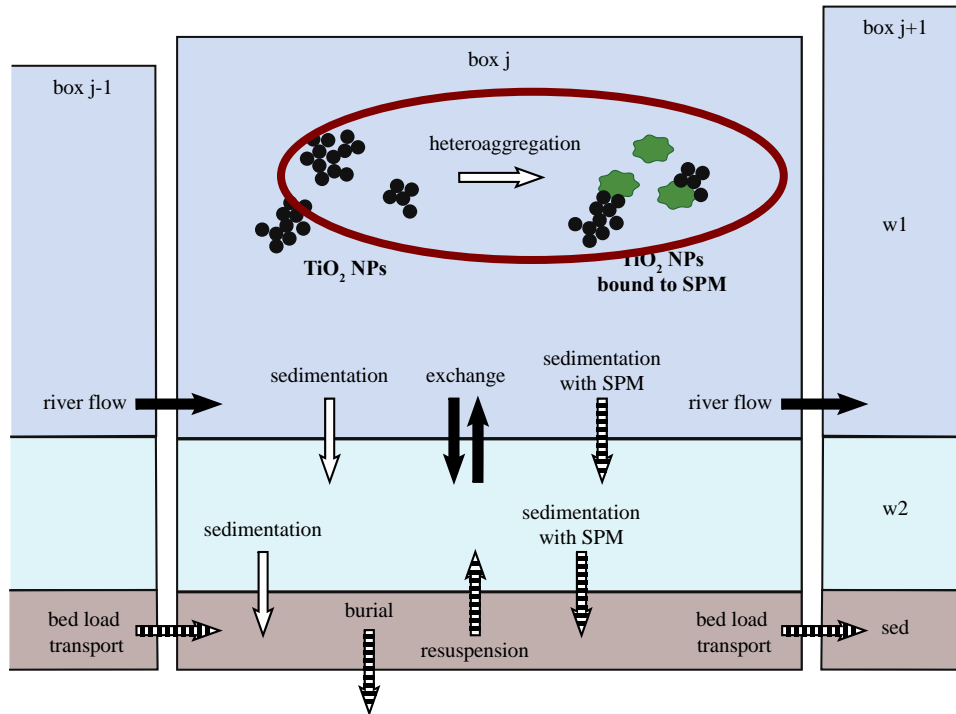
by replacing a dynamic process with a fixed distribution...



e.g. ratio free NP to SPM-bound NP
20:80

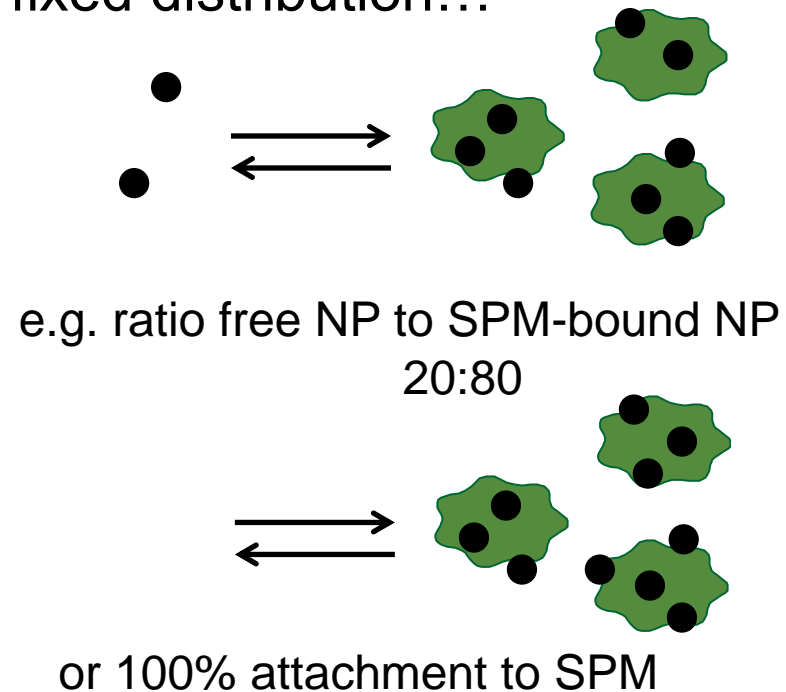
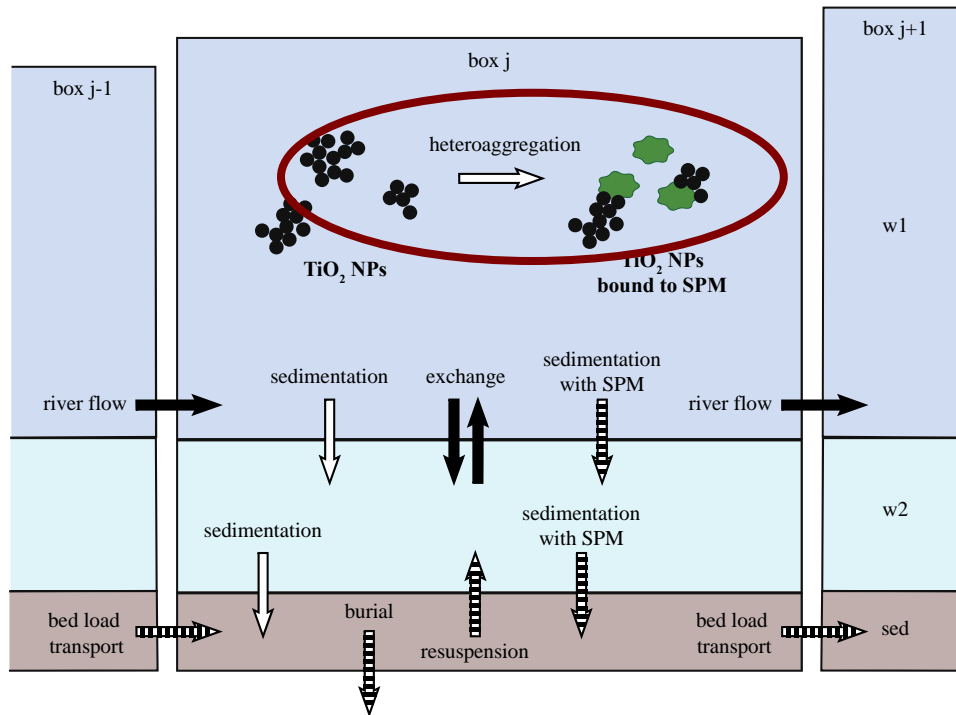
Consequences of using wrong fate descriptors

by replacing a dynamic process with a fixed distribution...



Consequences of using wrong fate descriptors

by replacing a dynamic process with a fixed distribution...

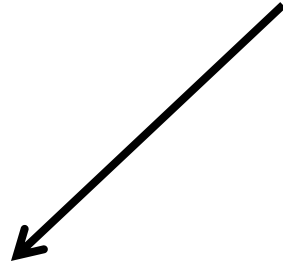


... we risk:

- misrepresentation of fate processes & misinterpretation of transport profiles/trends
- underestimation of free NP concentration close to emission source

ENP fate descriptors?

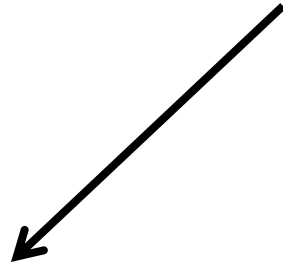
ENP fate descriptors?



distribution coefficients

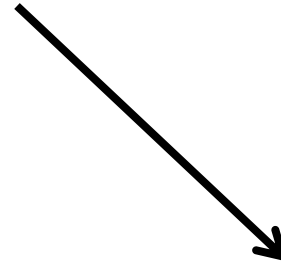
- simple determination and use
- no scientific meaning for ENPs
- risk a meaningless predictions

ENP fate descriptors?



distribution coefficients

- simple determination and use
- no scientific meaning for ENPs
- risk a meaningless predictions



particle-specific fate descriptors (attachment efficiencies or other)

- challenging determination
- more research efforts needed to identify most adequate approach
- more adequate representation of reality (still a model, not actual reality)
- more meaningful prediction, with the possibility of improvement with improved insights

Thank you!

Acknowledgements

- Martin Scheringer
- Nathalie Tufenkji
- Kai-Uwe Goss
- Menachem Elimelech

