

Environmental hazard and risk of nanomaterials: grouping concepts for aquatic and terrestrial toxicity

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Scientific Workshop - Grouping of Nanomaterials

NanoReg2 and Gracious H2020 projects

12-13 September 2018, OECD, Paris

Contributions

Kerstin Hund-Rinke



Overall coordination

Aquatic tox.: algae

Terr. tox testing

Risk matrix

Monika Herrchen

Exposure: release

Risk matrix

Dana Kühnel



Hazard matrix

Aquatic tox.: daphnia (acute),
ZFE

Carmen Nickel



Fate matrix

PC characterisation

Esther van der Zalm



Aquatic tox.: algae

Daphnia (chronic)

Perspectives of grouping

Hazard

Comparable PC-properties result in groups of ENM with similar hazard

READ-ACROSS -> Detailed

SEG4nano
(sophisticated environmental grouping for nanomaterials)



Risk

Combination of hazard grouping with grouping schemes for exposure (release + fate)

HIGHLY CONDENSED

AEG4nano
(aggregated environmental grouping for nanomaterials)



Publications under preparation

Systematic data set

Aquatic tests

(algae, daphnids acute / chronic, fish embryo: OECD 201, 202, 236)

Terrestrial tests

(microflora, earthworm: ISO 15689, OECD 222)

PC parameters

Intrinsic parameters

- *Size*
- *Crystalline structure*
- *Surface area*

Media dependent parameters

- *Solubility (24 h, 72 h)*
- *Reactivity: CPH, DMPO (+ / - illumination)*
- *Agglomeration / sedimentation*
- *Zeta-potential*

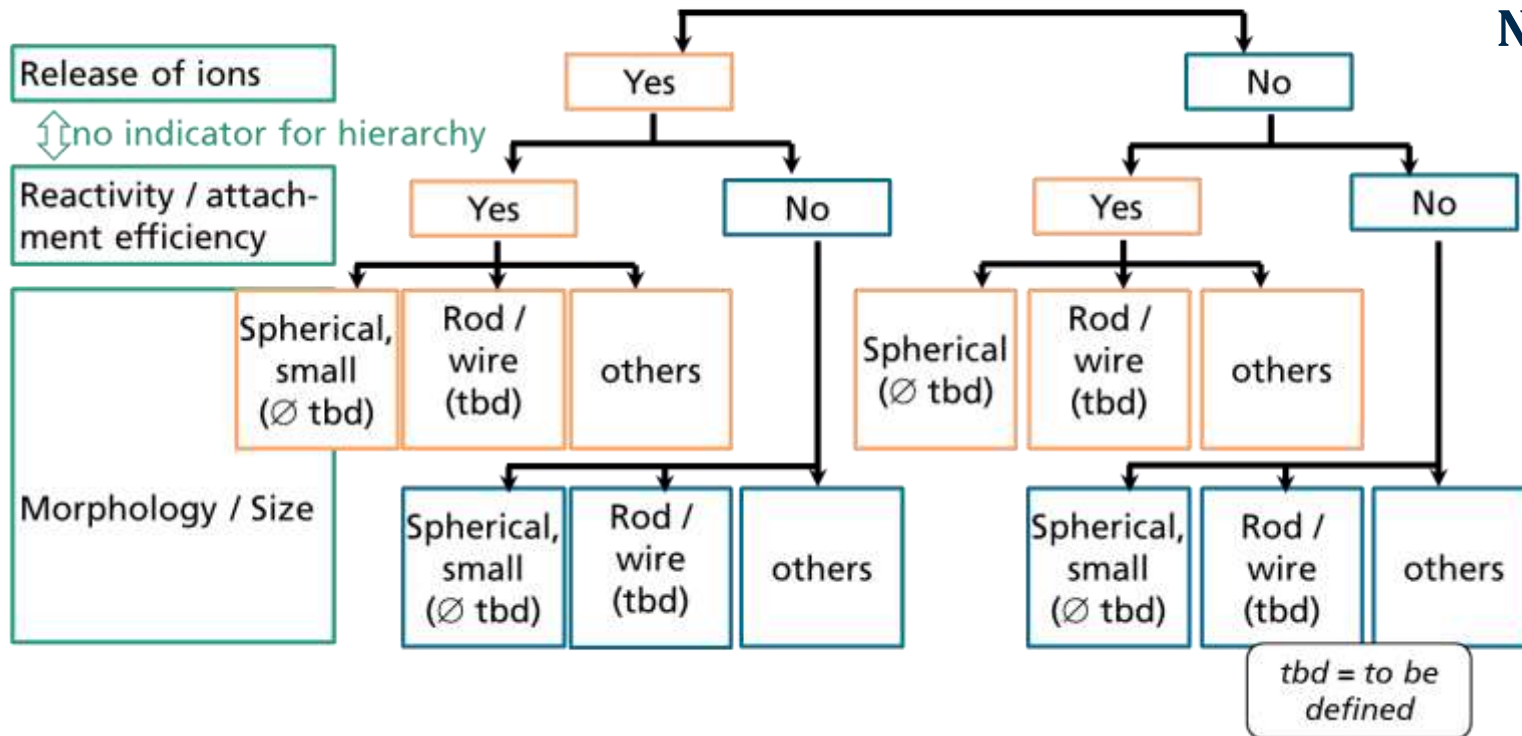
	Variable PC-parameters	Nanomaterial (9 types / 25 sub-types)
Ion-release	Morphology	Ag Batch SRM 110525 Batch 1340, NM-300K
	Size	nCu, CuO
	Hydrophobicity	ZnO NM110; NM111; NM113
Non-ion release	Size, surface modification	CeO ₂ NM-211, NM212; NM213; Eu doped
	Crystalline structure, surface modification	TiO ₂ NM-104; NM-105; Eu doped, Fe doped
	Morphology, size	Fe ₂ O ₃ _nano_A; nano_B, _larger
	Surface modification	SiO ₂ untreated; _amino; _larger
	Surface charge	CuPhthalo_nano; _halogen

Approach – SEG4nano

Aim: grouping of ENMs regarding their hazard to the **aquatic** environment

Flow-chart on grouping regarding aquatic ecotoxicity









Sophisticated
Environmental
Grouping for
Nanomaterials



Trigger values to be defined

Approach – SEG4nano

Aim: grouping of ENMs regarding their hazard to the aquatic environment

Group (based on various combinations of properties)	Nanomaterial (type and designation of sub-type)	Ecotox profile (sensitivity of organisms)	Magnitude of ecotoxicity (most sensitive organism) within the group (range of EC50 [mg/L])
Ions, reactive, fibers	Ag : Batch SRM 110525; Batch 1340	daphnids > algae > FE	
Ions, reactive, others	Ag : NM-300K nCu : nCu	algae = daphnids > FE	
Ions, non-reactive, others	ZnO : NM-110; NM-111; NM-113	algae > daphnids > FE	
Non-ions, attachment, others	CeO ₂ : NM-211, NM-212; Eu doped Fe ₂ O ₃ : _nano_A; nano_B	algae > daphnids, FE	
Non-ions, no/low attachment, others	CeO ₂ : NM-213 Fe ₂ O ₃ : _larger SiO ₂ : _untreated; _amino; _phosphonate	algae > daphnids, FE	
Organics	CuPhthalo: _nano; _halogen	none	
Non-ions, attachment, others	TiO ₂ : NM-104; NM-105; Eu doped, Fe doped, undoped	algae > daphnids, FE	
Ions, reactive, others	CuO : CuO	daphnids > algae > FE	

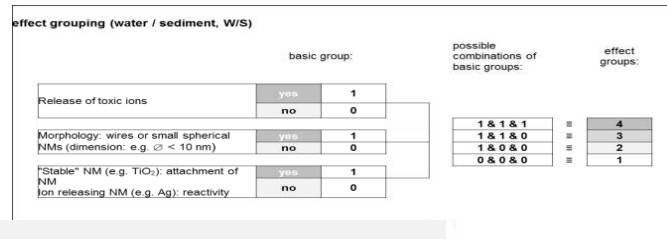
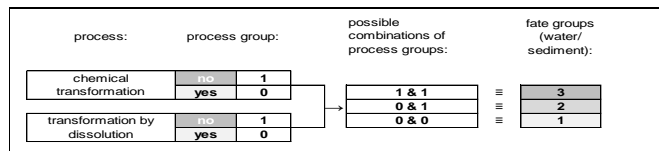
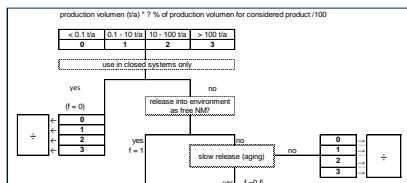
Summary – SEG4nano

Aim: grouping of ENMs regarding their hazard to the **aquatic** environment

- Most ENMs from the test data set group according to their ecotoxicity
- unambiguous, clear indication which parameters are responsible for grouping
- For some ENMs, the selected parameters do not allow a good hazard grouping
- Additional parameters, trigger values
- Restricted to aquatic hazard and metal/metal oxide ENMs

Approach – AEG4nano

Aim: grouping of ENMs regarding their risk to the **aquatic** and **terrestrial** environment

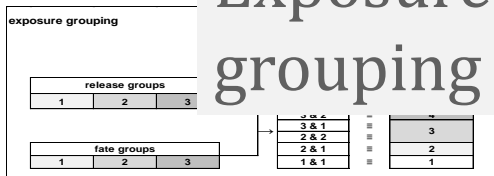


Release grouping

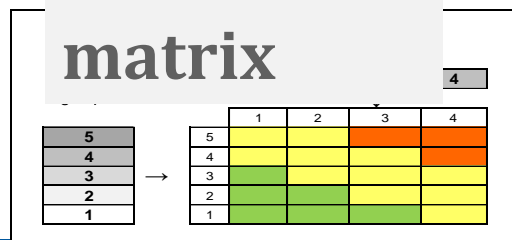
Fate grouping

Exposure grouping

Hazard grouping



Risk matrix



Aggregated Environmental Grouping for Nanomaterials

Approach – AEG4nano

Release grouping

- (estimated) production volumes
- portion relevant for the respective use
- use in closed / open systems
- slow / fast release into the environment

Fate grouping

Surface water / sediment:

- Chemical transformation
- Transformation by dissolution

Soil:

- Chemical transformation
- Transformation by dissolution
- Transport (agglomeration and movement)



Exposure grouping

- Combination of release groups and fate groups 5 exposure groups (1 - low exposure, 5 - high exposure potential)
- Same grouping for water/sediment and soil compartment

ATEG4nano - hazard grouping

Surface water/sediment

basic group:

Release of toxic ions	yes	1
	no	0
Morphology: wires or small spherical NMs (dimension: e.g. $\varnothing < 10$ nm)	yes	1
	no	0
"Stable" NM (e.g. TiO_2): attachment of NM Ion releasing NM (e.g. Ag): reactivity	yes	1
	no	0

possible combinations of basic groups:

1 & 1 & 1	≡	4
1 & 1 & 0	≡	3
1 & 0 & 0	≡	2
0 & 0 & 0	≡	1

effect groups:

Group 1
(low hazard) -
Group 4
(high hazard)

Soil

basic group:

release of toxic ions	yes	1
	no	0

possible combinations of basic groups:

1	≡	2
0	≡	1

effect groups:

2 Groups

ATEG4nano - hazard grouping of 25 test ENMs

Surface water/sediment

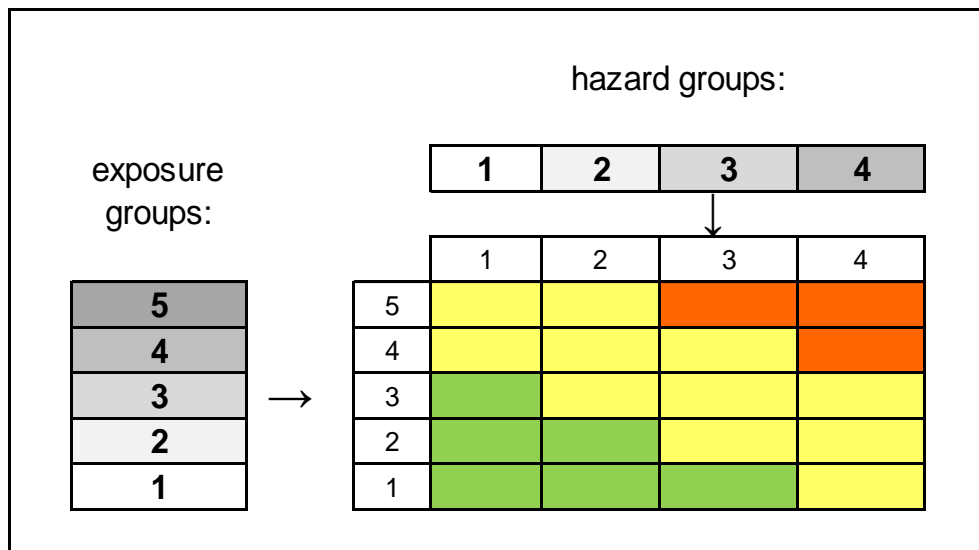
Effect group	Combination of basic groups	Nanomaterial (type / sub-type)	Ecotox profile (sensitivity of organisms)	Magnitude of ecotoxicity (most sensitive organism) within the group (range of EC50 [mg/L])
1	0 & 0 & 0	CuPhthalo_nano; _halogen SiO ₂ untreated; _amino; _larger Fe ₂ O ₃ _larger CeO ₂ NM-213	--- algae > daphnids, FE algae > daphnids, FE algae > daphnids, FE	
2	1 & 0 & 0	ZnO NM-110; NM-111; NM-113 Fe ₂ O ₃ _nano_A; nano_B CeO ₂ NM-211, NM-212; Eu doped TiO ₂ NM-104; NM-105; Eu doped, Fe doped, undoped	algae > daphnids > FE algae > daphnids, FE algae > daphnids, FE algae > daphnids, FE	
3	1 & 1 & 0	Ag Batch SRM 110525, NM-300K nCu CuO	daphnids > algae > FE algae = daphnids > FE algae = daphnids > FE daphnids > algae > FE	
4	1 & 1 & 1	Ag Batch 1340	daphnids > algae > FE	

Soil

Group	Release of toxic ions	Nanomaterial (type / sub-type)	
1	YES	Ag Batch SRM 110525, Batch 1340, NM-300K nCu ZnO NM110, NM111, NM113 CuO	
2	NO	CeO ₂ NM-211, NM212, NM213, Eu doped Fe ₂ O ₃ _nano_A, nano_B, _larger SiO ₂ untreated, _amino, _phosphonate CuPhthalo_nano; _halogen TiO ₂ NM-104, NM-105, Eu doped, Fe doped, undoped	

AEG4nano - risk matrix

Surface water/sediment



Green: low risk -> no further action

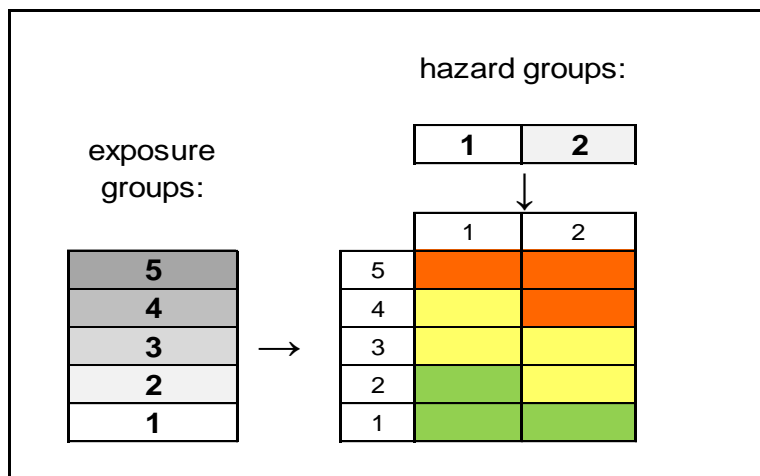
Yellow: plausibility check of grouping (exposure or hazard)

if grouping plausible: effects or exposure refinement, e.g. by higher tier testing

re-grouping

Red: high priority for risk assessment

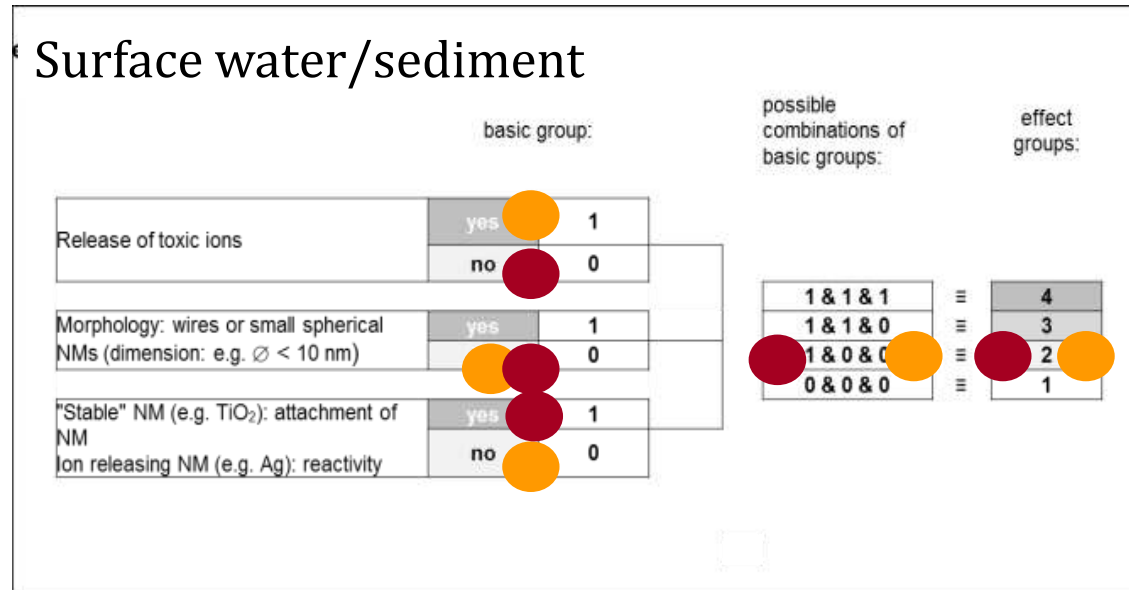
Soil



higher tier testing / sophisticated tests

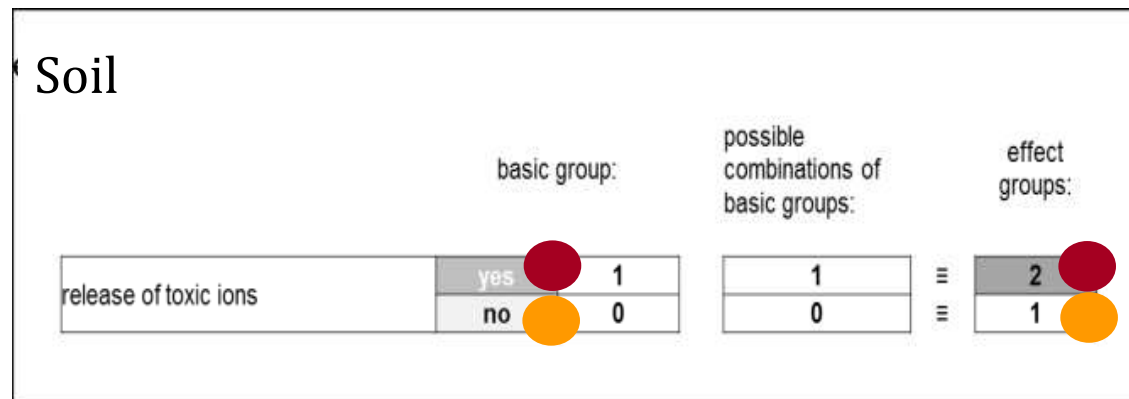
plausibility check of assumptions used for release grouping

ATEG4nano - case study hazard grouping



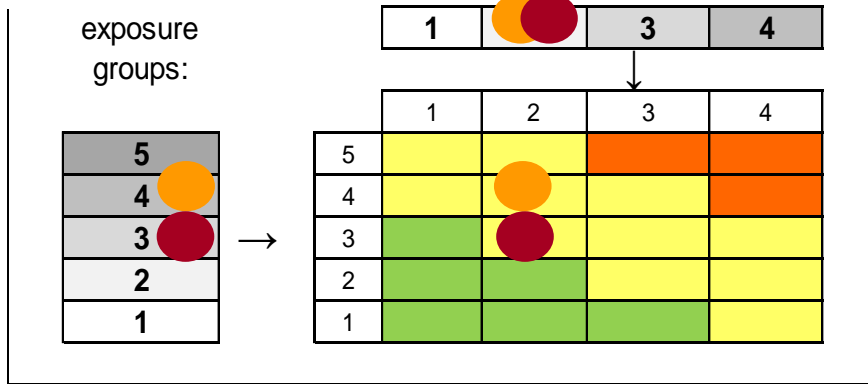
● TiO₂

● ZnO



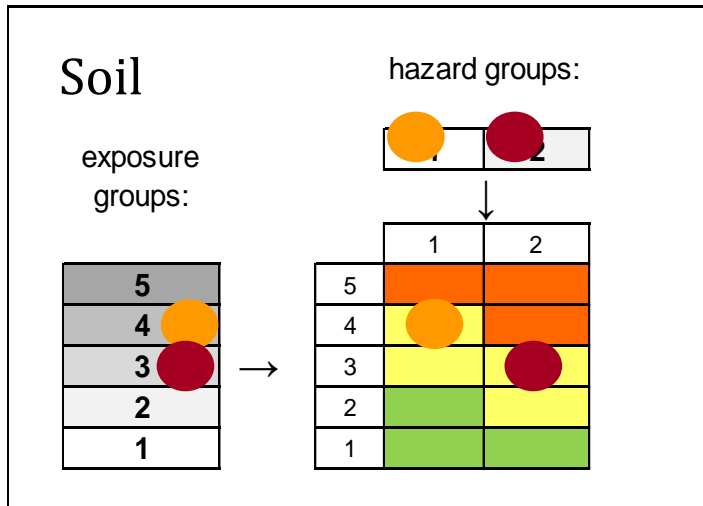
AEG4nano – case study risk grouping

Surface water
/sediment



● TiO₂
● ZnO

Soil



Yellow: plausibility check of grouping
 Release grouping: no reliable information
 Hazard grouping provisional (unknown PC parameter)

Summary - AEG4nano

Aim: grouping of ENMs regarding their risk to the **aquatic** and **terrestrial** environment

- Combines exposure (release, fate) with hazard groups into a risk matrix -> highly aggregated
- Grouping of ENM regarding their environmental exposure (release, fate) and effects seems to be possible
- Visualisation of results facilitates priority setting

Summary & Conclusion

- Sophisticated approach regarding hazard/read across (-> **SEG4nano**): transfer of results
- Highly aggregated approach for risk grouping (-> **ATEG4nano**): priority setting
- Hazard grouping: distinct types of NM group according to their actual hazard as determined in standard ecotoxicity tests
- Risk matrix approach was shown to be suitable to distinguish the risks of different types of nanomaterials for environmental risk assessment

“Grouping concept for metal and metal oxide nanomaterials with regard to their ecotoxicological effects on algae, daphnids and fish embryos” K. Hund-Rinke, K. Schlich, D. Kühnel, B. Hellack, H. Kaminski, C. Nickel. (2018) NanoImpact, 9, 52-60.

Next steps

- Specify release (AEG4nano)
- Specify trigger values (SEG4nano, AEG4nano)
- Consideration of further PC and biological parameters (TiO_2 and ZnO)
- Additional testing to describe environmental processes (fate) is still required
- Extension for carbon based or organic ENM

} METHODS!

Thank you!

“Grouping concept for metal and metal oxide nanomaterials with regard to their ecotoxicological effects on algae, daphnids and fish embryos” K. Hund-Rinke, K. Schlich, D. Kühnel, B. Hellack, H. Kaminski, C. Nickel. (2018) NanoImpact, 9, 52-60.

“Grouping of nanomaterials regarding their fate and effects in the environment” Dana Kühnel, Carmen Nickel, Esther van der Zalm, Boris Meisterjahn, Monika Herrchen, Kerstin Hund-Rinke, in prep.

“Grouping of nanomaterials with regard to their environmental risk – the risk matrix” K. Hund-Rinke, D. Kühnel, C. Nickel, M. Herrchen, in prep.



nano**GRAVUR**

