





# CONSIDERATIONS OF NANOMATERIALS ENVIRONMENTAL FATE TO SUPPORT GROUPING AND ENVIRONMENTAL RISK PREDICTION

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#### Introduction & objectives

Large varieties of nanomaterials (NMs) are used in many products and can be released into the environment. Grouping of NMs is discussed as approach to reduce the environmental fate testing effort. Basically, environmental fate grouping of NMs is performed on the basis of their physico-chemical (PC) properties.

In this project, a fate grouping approach has been developed and verified / adjusted by testing of 15 different NMs.

## **Grouping Scheme for Fate Prediction**

 NM properties, first thresholds, and the influence of these properties on environmental behavior, i.e. transformation (by dissolution, chemical), agglomeration and mobility is determined. The latter is expressed in binary form ("YES" / "NO") (Fig. 1).

surface potential		polarity		1	primary particle size			particle shape		
ZP negative ≤ -15 mV	ZP neutral /positive >- 15 mV	hydrophobic	hydrophilic		< 40 nm	> 40 nm		spherical	tubes / wires	
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transformation (by dissolution, chemical),		transformation (by dissolution, chemical),			transformation (by dissolution, chemical),					
agglomeration		agglomeration			agglomeration in water					
mobility in soil*		mobility in soil*			mobility in soil*			mobility in soil*		
NO	YES	NO	YES		NO	YES				
YES*	NO*	YES*	NO*		YES*	NO*		YES*	NO*	

Fig. 1: Results for grouping

- "YES / NO"-groups are allocated to the figures "0" and "1". This allows for further aggregation to result in one figure each (= group) for transformation and mobility in water and soil, respectively (Fig. 2).
- Transformation and mobility groups are further combined into a fate group (see also poster TH085).



Fig. 2: Grouping of mobility in soil for NM220 and NM212. Dots without edging → grouping based on experimental data; dots with edging → grouping based on literature data and expert judgement.

 Grouping results obtained from data based on literature and on experiments are compared for transformation, agglomeration and mobility. This step is to verify / falsify the hypotheses.

# Procedure

- Proposition of hypotheses about the influence of NM properties on transformation, agglomeration and mobility in water and soil.
- Development of a fate grouping approach.
- Systematic testing of agglomeration in air and water, transformation in water and soil and mobility in soils using a broad set of NMs differing in their PC-properties.
- Comparison of grouping based on literature data / expert knowledge and on experimental results.
- Experimental results for mobility in soil type Dystric Cambisol (column leaching) are presented exemplarily for NM220 (BaSO4) and NM212 (CeO2) (Fig. 3).



Fig. 3: Results for mobility experiments for NM220 (BaSO<sub>4</sub>) and NM 212 (CeO<sub>2</sub>) differing in their zeta potential. Presented are the ICP MS- Analysis results of different soil segments of the soil columns. The mobility experiments based on the OECD TG 312, NM suspension were applied, after sonication using a Cup Horn (BRANSON -10 min, interval 0.2/0.8 sec).

### Conclusions

- For transformation and agglomeration in water the investigated properties seem to be not sufficient for a grouping and further properties need to be considered.
- The primary particle size is not identified as influencing property for the agglomeration in water whereas the zeta potential has an influence. Agglomeration potential increases with increasing zeta potential independent on the algebraic sign.
- In soils the investigated properties can be used for NMs grouping regarding transformation and mobility.
- → Further experiments need to be conducted to verify the results with other NMs and to derive quantitative threshold values for the identified parameters.

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# Considerations of nanomaterial's environmental fate to support grouping and environmental risk prediction

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Engineered nanomaterials (ENM) are used in different products with the consequence that they can be released into the environment during their life cycle. Given the large varieties of ENM, the effort for an individual investigation and assessment would be enormous. Therefore grouping of ENM and read across between different materials is a major target for future risk assessment. In this poster we present practicable approaches that can support the discussion on grouping of ENM regarding their environmental fate for a subsequent risk prediction.

In our project we focused on the behaviour of the pristine ENM in aquatic and terrestrial compartments. The transformation (chemical transformation and dissolution) and the transport (mobility and agglomeration) of an ENM in the environment was studied. To predict the exposure potential for the environmental compartments both pieces of information were combined to result in a number code (from 1 for low to 3 for high) for a so called "fate bond" which will be included in a matrix of ENM grouped regarding their potential environmental risk. For example, if the transformation via dissolution and chemical transformation is low in the environmental compartment, the transformation potential of the ENM is low. If the mobility is low and the agglomeration potential is high, the transport is also low. Low transformation and low transport means high ENM exposure potential in the considered compartment and leads to a number value of "3" in the fate bond. For simplification, in this project water phase and sediment phase are considered as one compartment (water compartment) and therefore transport and mobility effected by e.g. agglomeration and sedimentation are not needed to be considered in the presented approach. In contrast, for soil systems the mobility was analysed in detail, as important factor for the exposure concentration. For an environmental risk prediction the fate information (fate bond) is combined with the (ecotoxicological) hazard properties (ecotox bond; presentat at an additional poster) of an ENM. In this poster, the concept to support discussion on grouping and risk prediction will be presented and discussed by using various ENMs as examples.

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