Exposure modeling of engineered nanoparticles

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ABSTRACT

An elementary step towards a quantitative assessment of the risks of new compounds to the environment is to calculate their predicted environmental concentrations (PEC). The aim of this study was to use a life-cycle perspective to model the quantities of engineered nanoparticles released into the environment. The quantification was based on a substance flow analysis from products to air, soil and water. The following parameters were used as model inputs: estimated worldwide production volume, allocation of the production volume to product categories, particle release from products and flow coefficients within the environmental compartments. The method was applied to the engineered nanoparticles titanium dioxide, silver, and carbon nanotubes. The PEC-values were then compared to the predicted no effect concentrations (PNEC) derived from the literature to estimate a possible risk. The results of this study make it possible for the first time to carry out a quantitative risk assessment of nanoparticles in the environment and suggest further detailed studies of nano-titanium dioxide.

Keywords: exposure, modeling, nanoparticles, risk asessment

1 INTRODUCTION

The increase in the use of engineered nanoparticles (NP) makes exposure of the natural environment to these compounds more and more likely (Nowack and Bucheli, 2007). The environmental risks of NP are determined by their potential hazards (such as toxicity), as well as by the extent the material will come into contact with an organism (Helland et al., 2007; Koehler et al., 2008). The basis for a sound risk assessment of a possibly hazardous substance is thus a comparison between the exposure (concentration in the environment) and the toxic effects of the substance So far, no measurements of engineered NP in the environment have been available due to the absence of analytical methods able to quantify trace concentrations of NP. A recent study reports the identification of engineered nanosized TiO_2 particles in river water originating from facade run-off (Kaegi et al., 2008).

Usually the concentration of a new substance in the environment is not known at the time of the assessment. Therefore expected concentrations have to be modeled with the help of extrapolations and analogies. The value derived from such modeling, the PEC (predicted environmental concentration), is compared to the PNEC (predicted no effect concentration), which extrapolates the concentration at which no adverse effect on organisms is to be expected. An ingredient is judged to be environmentally compatible if the PEC/PNEC ratio is smaller than one.

The goal of this study was to model the expected concentrations of nano-Ag, nano-TiO_2 and CNT in the environment (Mueller and Nowack, 2008). The risk assessment was carried out for the three environmental compartments water, air and soil for Switzerland. Based on this model, a first assessment of the potential risk posed by the three mentioned NP was conducted by comparing the PEC to the PNEC.

2 MATERIALS AND METHODS

The modeling was based on established methods to assess the exposure of chemicals to the environment (ECB, 2003). A realistic and a high exposure scenario (RE- and HE scenario) were developed due to the high uncertainty of the data. The RE-scenario was based on the most realistic information received. The worst-case scenario relied on estimations that would lead to higher concentrations in the environment.

The calculation of the predicted environmental concentration (PEC) was based on a substance flow analysis. The flows of the NP from the products to the environment, waste incineration plants (WIP), landfills and/or sewage treatment plants (STP) were quantified. The predicted no observed effect concentration (PNEC) was derived from ecotoxicological data.

The detailed method description can be found in (Mueller and Nowack, 2008).

3 RESULTS

Figures 1 show the NP-flows from the products to the environmental compartments, sewage treatment plants (STP), waste incineration plants (WIP) and the landfill for the HE-scenario. In the case of nano-Ag and nano-TiO_2, the most prominent flows are between the products and the STP (3.27 t/a, 249.22 t/a), the STP and the WIP (2.65 t/a, 201.87 t/a) and the WIP to the landfill (3.26 t/a, 230.91 t/a) for the RE and the HE scenario. Unlike nano-Ag and nano-TiO_2, the most prominent flow for CNT is between the products and the WIP (1.75 t/a) and from the WIP to the landfill (1.30 t/a). The reason is that CNT-containing material staying in Switzerland ends almost exclusively in the WIP if not recycled.

The modeling suggests that currently nano-Ag poses little or no risk to soil organisms (Table 1). The RQ water is less than one thousandth. Also in the HE-scenario, the modeling suggests that currently little or no risk is to be expected from nano-Ag in the soil compartment and the water in general.

The modeling suggests that nano-TiO_2 may pose a risk to water organisms with a RQ of 0.7 (Table 1). By contrast, the RQ air is smaller than one thousandth. Also in the HE-scenario, the expected concentration of nano-TiO_2 in water is critical (RQ >16) whereas the RQ air is very small (0.004).

The calculation indicates that currently CNT most probably pose little to no risk to air and water organisms. The RQ water and air are both very small. Also in the HE-scenario, the expected concentration of CNT in water and air are small. Ecotoxicological data on soil organisms are scarce and an evaluation is not yet possible.

Table 1: Calculation of the risk quotient (PEC/PNEC) for water, air and soil. Data are from (Mueller and Nowack, 2008).

	nano-Ag		**nano-TiO2**		**CNT**	
	RE	HE	RE	HE	RE	HE
Air	nd	nd	0.0015	0.004	1.5*10-5	2.3*10-5
Water	0.0008	0.002	>0.7	>16	0.005	0.008
Soil	nd	nd	nd	nd	nd	nd

nd: not determined due to lack of ecotoxicological data
RE: realistic scenario
HE: high emission scenario

4 DISCUSSION

When comparing the substance flow charts of nano-Ag and nano-TiO_2, it is obvious that the main particle flow takes place from the products to the STP, from there to the WIP and finally to the landfill (for nano-Ag around two thirds and for nano-TiO_2 around three quarters of the total particle volume). The particle flow from the WIP to the landfill turned out to be the predominant flow of all three substances due to the relatively high filtering efficiency of the wastewater treatment and the waste incineration plants. Leachate from landfills was neglected in this modeling, as the standard of landfills in Switzerland is high. But as the identified flows of NP to landfills are important, it will be necessary to study the possibility of leachate from landfills more closely.

It can be noticed that the PEC values for CNT are the lowest of the three NP in all environmental compartments. It has been stated that currently very little of these very expensive materials will find their way to contaminate the outdoor environment. It has to be expected, though, that in the future - when the price of CNT falls and CNT application in consumer products becomes more widespread – the concentration in the environment will increase considerably. The system flow chart of CNT shows no particle flow to the STP (and the water compartment). In the current situation for Switzerland the particles are almost exclusively exported (leaving the system boundary) or transported to the WIP. Because CNT are partially burned in the WIP, the percentage of CNT in the landfill is lower than with the other two substances (one fifth to about half of total particle volume). However, with an increasing variety of products that contain CNT, the CNT flows may change considerably.

The current lack of studies on the ecotoxicity of all substances in all compartments makes it difficult to evaluate the risks to organisms. Almost no studies for organisms in the soil compartment exist to date and the PNEC-values found in the literature vary substantially. The NOEC-values found for nano-TiO_2 differ, for example, by up to a factor of 1000, highlighting the fact that the methods/materials applied in the studies are not comparable and further research with standardized tests are needed.

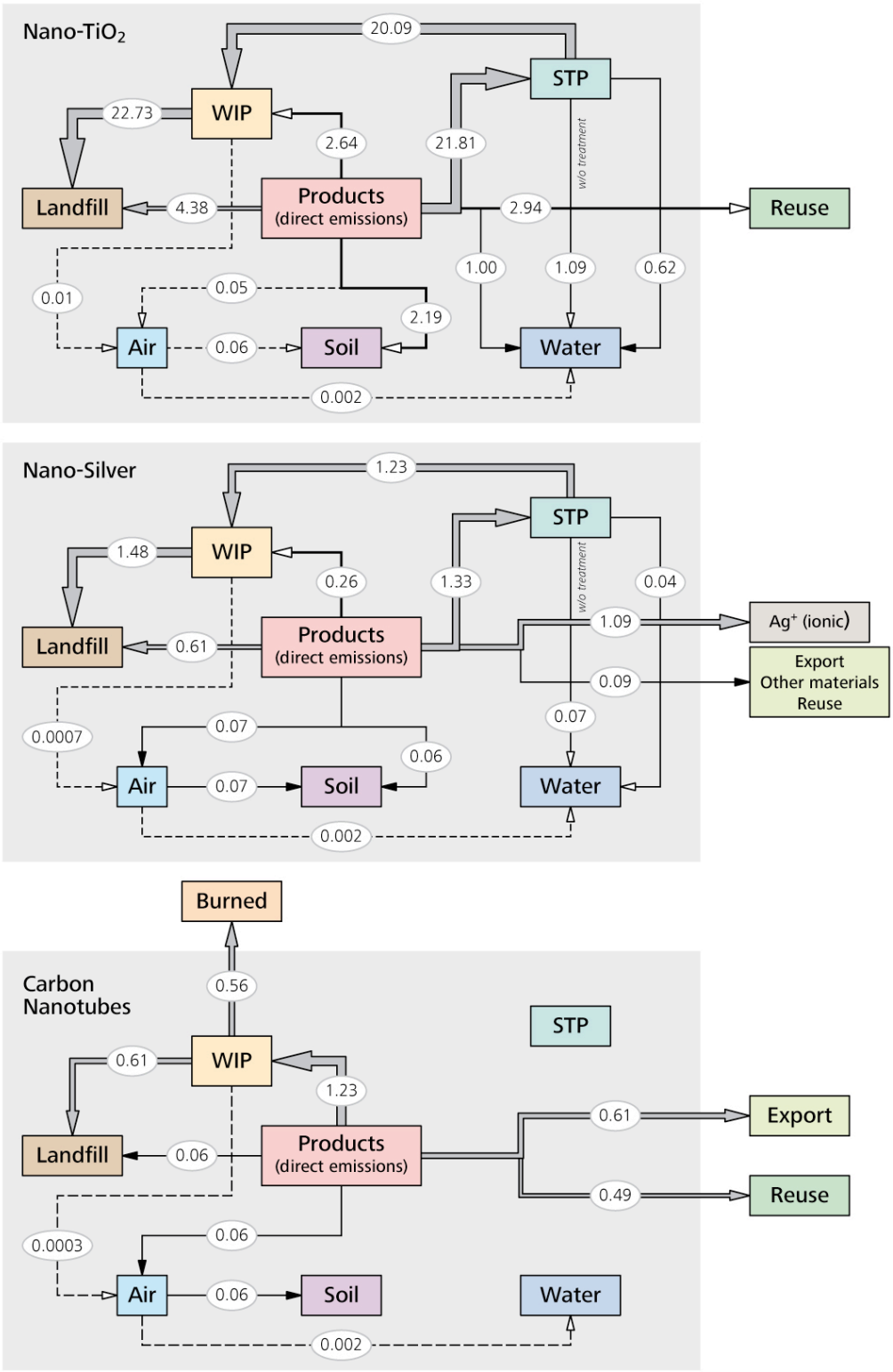

Figure 1: nano-Ag , nano-TiO_2 and CNT flows from the products to the different environmental compartments, WIP, STP and landfill (HE-scenario). All flows are in tons/year. The thickness of the arrows is proportional to the amount of silver flowing between the compartments. The figure has been adapted from (Mueller and Nowack, 2008).

The wide range of values observed is mainly due to a difference in the methods applied and in the material used. Differences in size, shape, modification and purity may considerably influence the result. A precise characterization of the particles used is thus necessary. In this study, it was not possible to consider particle differences due to the patchy base data, neither for the substance flow modeling nor for the toxicological evaluation. When analyzing the results, it should therefore be kept in mind that the size and the functionalization of NP will have a great influence on their effects. However, this has been partially taken into account.

Based on the PEC-values received in this study, it is now possible to make a first estimation as to what substances and compartments may pose the highest risk. This evaluation, however, needs to be very critically examined and should only provide a rough approximation. A low risk quotient does not necessarily mean that this compartment is risk-free; instead further detailed experimental and modeling studies should focus on all aspects. The modeling shows that the concentration of nano-TiO_2 in water may pose a risk to aquatic life (risk quotient >0.73 and >16 in the RE- and HE-scenario, respectively). The behavior and ecotoxicity of nano-TiO_2 in water and especially wastewater should therefore be studied more closely.

The expected concentrations of CNT and nano-Ag probably pose little risk based on the data presently known. Assuming that the PNEC-values are accurate and the ways of release stay the same, the production volume of nano-Ag would need to increase 100 times in order for the risk quotient to rise to about 1. Please note that this calculation does not include the risk emanating from ionic silver. In the case of CNT the paths of release will change with an increasing variety of products that contain CNT. An extrapolation of the RQ(CNT) to the future is thus not possible. It has also to be considered that this study did not include emissions from production sites, and it assumed well mixed environmental compartments, which denotes that much higher concentrations could be found locally e.g. around production sites.

REFERENCES

ECB, 2003. Technical Guidance Document on Risk Assessment. European Chemicals Bureau.

Helland, A., Wick, P., Koehler, A., Schmid, K., Som, C., 2007. Reviewing the environmental and human health knowledge base of carbon nanotubes. Environ. Health Perspect. 115, 1125-1131.

Kaegi, R., Ulrich, A., Sinnet, B., Vonbank, R., Wichser, A., Zuleeg, S., Simmler, H., Brunner, S., Vonmont, H., Burkhardt, M., Boller, M., 2008. Synthetic TiO2 nanoparticle emission from exterior facades into the aquatic environment. Environ. Pollut. 156, 233-239.

Koehler, A., Som, C., Helland, A., Gottschalk, F., 2008. Studying the potential release of carbon nanotubes throughout the application life cycle. J. Cleaner Produc. 16, 927-937.

Mueller, N.C., Nowack, B., 2008. Exposure modeling of engineered nanoparticles in the environment. Environ. Sci. Technol. 42, 4447–4453.

Nowack, B., Bucheli, T.D., 2007. Occurrence, behavior and effects of nanoparticles in the environment Environ. Pollut. 150, 5-22.