Modeled Environmental Concentrations of Engineered Nanomaterials (ENM) for different regions and at different resolutions

Fadri Gottschalk, Tobias Sonderer, Christoph Ort, Roland W. Scholz, Bernd Nowack

Environmental Risk Assessment and Management Group (ERAM)
Empa - Swiss Federal Laboratories for Materials Testing and Research
St. Gallen, Switzerland

Natural and Social Science Interface (NSSI), Department of Environmental Sciences, ETH Zurich
Outline

- Aim, concept and method of the material flow modeling
- Results of the engineered nanomaterial flow simulation studies (regional)
- Engineered nanomaterial concentrations in rivers at local resolution
- Conclusions
What’s the problem?

- Engineered nanomaterials (ENM) are released to the environment.
  - Synthetic TiO$_2$ nanoparticle emissions from exterior facades into the aquatic environment (*Kaegi et al.* 2008).
  - Nanoparticle silver emissions into water from commercially available sock fabrics (beaker glass) (*Benn and Westerhoff*, 2008).
  - Release of nanosilver from textiles during washing (washing machine) (*Geranio et al.*, 2009).

- Some data on environmental behavior and ecotoxicology of engineered nanomaterials are available.

- Analytical methods are not (yet) available for quantitative nanomaterial detection in the environment.
Aim, concept and method of the environmental exposure modeling
Basic concept: transfer coefficients modeled as contaminant specific values

\[ m = m_{\text{compound}} = m_{\text{product}} \cdot c^{(i)} \]

\[ TC_{js} = \frac{m_{js}}{\sum_r m_{rj}} \]
Why probabilistic/stochastic modeling?

PMFA*

- Central statistics
- Information from industry
- Stored amounts and flows in articles and goods
- Emission factors
- Intervals for emission to different media
- Phys-chem properties
- Environmental data
- Background inflow
- PECs
- Intermedia transport
- Residence time/persistence
- Collection of field data
- Correlation with measured data
- Revision of model parameters

*PMFA: Probabilistic Material Flow Analysis

Adapted from Föredragshallare, 2009
Results of the simulation studies (Switzerland, EU, USA)
Worldwide production volumes from different sources in tons/year (year of estimation)

<table>
<thead>
<tr>
<th>TiO₂</th>
<th>Ag</th>
<th>ZnO</th>
<th>CNT</th>
<th>Fullerenes</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>500 (2006)</td>
</tr>
</tbody>
</table>
Material-flow model for nano-TiO$_2$ for the US (mode values in tons/year)
Material-flow model for CNT for the US (mode values in tons/year)
Modeled concentrations in waters for the EU (mode and 15 and 85% quantiles in ng/L)

<table>
<thead>
<tr>
<th></th>
<th>TiO₂</th>
<th>Ag</th>
<th>ZnO</th>
<th>CNT</th>
<th>fullerenes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface water</td>
<td>15</td>
<td>0.76</td>
<td>10</td>
<td>0.004</td>
<td>&lt;0.0005</td>
</tr>
<tr>
<td></td>
<td>(12-57)</td>
<td>(0.59-2.16)</td>
<td>(8-55)</td>
<td>(0.0035-0.02)</td>
<td>(&lt;0.0005-0.2)</td>
</tr>
<tr>
<td>Treated wastewater</td>
<td>3'470</td>
<td>43</td>
<td>432</td>
<td>15</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>(2'500-10’800)</td>
<td>(33-111)</td>
<td>(340-1’420)</td>
<td>(11-32)</td>
<td>(4-26)</td>
</tr>
</tbody>
</table>
Concentrations in sludge treated soil in the US between 2001 and 2012
## Risk evaluation: $\text{PEC}_{\text{modal}}/\text{PNEC}$ (for Europe)

<table>
<thead>
<tr>
<th></th>
<th>TiO$_2$</th>
<th>Ag</th>
<th>ZnO</th>
<th>CNT</th>
<th>fullerenes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface water</td>
<td>0.02</td>
<td>1</td>
<td>0.3</td>
<td>&lt;0.0005</td>
<td>&lt;0.0005</td>
</tr>
<tr>
<td>Cleaned wastewater</td>
<td>4</td>
<td>61</td>
<td>11</td>
<td>&lt;0.0005</td>
<td>0.02</td>
</tr>
<tr>
<td>Sediment</td>
<td>na</td>
<td>na</td>
<td>na</td>
<td>&lt;0.0005</td>
<td>na</td>
</tr>
<tr>
<td>Soil</td>
<td>0.004</td>
<td>na</td>
<td>na</td>
<td>&lt;0.0005</td>
<td>&lt;0.0005</td>
</tr>
<tr>
<td>Sludge treated soil</td>
<td>0.3</td>
<td>na</td>
<td>na</td>
<td>&lt;0.0005</td>
<td>&lt;0.0005</td>
</tr>
</tbody>
</table>

PEC: Predicted environmental concentrations
PNEC: Predicted no effect concentrations

Assessment factor 1000
na: not available
Modeled engineered nanomaterial concentrations in rivers at local resolution
PECs in Swiss rivers at water levels reached or exceeded in 95% of the time (modal ENM emission)

without sedimentation with sedimentation

Modal PEC of nano-Ag at baseflow $Q_{347}$ [ng L$^{-1}$], current PNEC 0.7 ng L$^{-1}$

- < 0.028
- 0.028 - 0.14
- 0.14 - 0.7
- 0.7 - 3.5
- 3.5 - 17.5
- > 17.5

○ discharge to lake or no $Q_{347}$ available
PECs and exceedances of PECs above predicted no effect concentrations (PNECs) for nano-Ag (0.7 ng L$^{-1}$)

Gray box diagram: scenario with sedimentation

River section: Courroux (Délemont)
PECs and exceedances of PECs above predicted no effect concentrations (PNECs) for nano-Ag (0.7 ng L\(^{-1}\))

Gray box diagram: scenario with sedimentation

River section: Seyon-Valangin
Open points

- Better data on production and use needed
- Release from products: only few studies available
- Different forms and functionalizations of nanomaterial
- Geographical and time-dependent differentiation
- Lack of ecotoxicological data for some environmental compartments and nanomaterials
Acknowledgement

- PD Dr. Bernd Nowack, Prof. Dr. Roland W. Scholz, Tobias Sonderer, Dr. Christoph Ort
- Federal Office for the Environment (FOEN), Empa (Group B. Nowack), ETH (Professorship R.W. Scholz).

Sources


