A Risk Forecasting Framework for Nanomaterials

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Center for the Environmental Implications of NanoTechnology (CEINT)

1. Elucidate general principles that determine environmental behavior of nanomaterials
2. Provide guidance in assessing existing and future concerns
3. Educate students and the general public regarding nanotechnology, nanoscale science, and the environment

Core Institutions: Duke (headquarters), CMU, Howard, Virginia Tech, U Kentucky, Stanford

- 36 faculty, 76 undergraduate and graduate students
- Collaborating US universities & government entities
- ICEINT- International partners (France) supported by CNRS and CEA
- TINE (UK- Rothamsted, Cranfield, Lancaster, NERC CEH), ENPRA (IOM)
Research Themes

nanomaterials

ecosystem impacts

cellular/organismal impacts

Transport and transformation

Modeling, Risk assessment, Tools for risk management

Duke UNIVERSITY
**Mesocosms**

- 26 mesocosms constructed, planted
- Probes, data acquisition, and web-based data monitor
- Webcam
- Preliminary experiment started Oct ‘09
- First duplicated experiment with Ag NPs to begin May-June 2010
- CeO₂, SWCNTs, TiO₂ (single mc)
**Example: TiO2 Exposure via Wastewater Discharge**

\[
C_{TiO2,sludge} = (S_{TiO2}) f_{TiO2,ww} \cdot P_{sludge} \left( \lambda_{TiO2}, \gamma_{ww} \right) / [Q_{ww} r]
\]

- Exposure
  - *organismal impacts*
  - *ecosystem impacts*

- Vector describing nanoparticle characteristics
- Vector describing system (wastewater treatment plant, mesocosm)

- Source inventory (per time)
- Commercialization trends

- Usage profile
  - *social science*
  - *engineering*

- Partitioning transfer function
  - *physical chemical properties*
  - *transport*
  - *microbiology*

- Simulation
- Bayesian networks

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**Source:** Duke University

**Institute:** CEINT
A nanoparticle is:
1) SMALL 2) HAS NOVEL PROPERTIES

(Melanie Auffan and co-workers, Langmuir, 2008)

Nature Nanotechnology 2009
**Desirable Elements of a Risk Forecasting Framework**

1) **Generates forecasts and associated levels of uncertainty for questions of immediate concern**

2) **Incorporates fundamental properties of nanomaterials with goal of forecasting risk for new materials**

3) **Considers all pertinent sources of nanomaterials**

4) **Includes life-cycle and ecosystem-level impacts**

5) **Ability to adapt and update risk forecasts as new information becomes available**

6) **Feedback to improve information gathering**

7) **Feedback to improve nanomaterial design**
Risk Assessment Framework

Nanoparticle Properties

Exposure

Hazard

Risk
Multiple sources, multi-scale impacts

Nanoparticle Properties

- Engineered
- Incidental
- Natural

Exposure

- Ecosystem
- Organism

Risk

- Hazard
AGGREGATION MAY OCCUR BETWEEN MANY COMPONENTS
Transfer function

$V_{\text{porous}} / \Delta \log q_k (\mu m^3)$

Porous diameter (\mu m)

Time = 0 days
Source of NM S

Intermediate Product

\( I_{j,i=1 \to n} \)

Nano-Enabled Product

\( P_{j,i=1 \to m} \)

- Air
- WWTP
- Storage /Use
- Landfill
- Sludge
- Effluent
- Natural Waters
- Agricultural Land
## Nanomaterial Fabrication Estimates

<table>
<thead>
<tr>
<th>Product</th>
<th>Lower bound (tpy)</th>
<th>Upper bound (tpy)</th>
</tr>
</thead>
<tbody>
<tr>
<td>nano-TiO₂</td>
<td>7,800</td>
<td>38,000</td>
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<tr>
<td>nano-Ag</td>
<td>2.8</td>
<td>20</td>
</tr>
<tr>
<td>nano-CeO₂</td>
<td>35</td>
<td>700</td>
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<tr>
<td>CNT</td>
<td>55</td>
<td>1101</td>
</tr>
<tr>
<td>Fullerences</td>
<td>2</td>
<td>80</td>
</tr>
</tbody>
</table>

*C. Hendren, Wiesner and co-workers, in review*
Partitioning experiments
MONTE CARLO CALCULATIONS OF SLUDGE CONCENTRATIONS
Thank You

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