The Environmental Implications of Nanotechnology

Fate, Transport and Removal of Nanomaterials in Aquatic Environments

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Introduction - Novelty

• Unusual physicochemical properties
  o Small size, surface structure, chemical composition, bulk vs. nano
  o May be a dry powder suspended in a gas (nanoaerosol), suspended in liquid (nanohydrosol), or embedded in a matrix (nanocomposite)

• Applications
  o Medicine
  o Energy
  o Electronics
  o Consumer products
  o Environmental applications
Quantum Dots

Simultaneous excitation at 365 nm

Size-dependent emission

Fluorescence

Wavelength, (nm)
TiO$_2$

Quantum dot

Fullerene (Bucky ball)

Carbon Nanotube

Introduction - Toxicity

• Evidence of toxicity
  
  
  o Fullerene “bucky balls” toxic to fish and humans (Wiesner et. al, *ES&T* 2006)
  
  o Quantum dots (Cd) and nanosilver (Ag) toxic due to metal release (Mahendra et. al, *ES&T*, 2008; Benn and Westerhoff, *ES&T* 2008)
Growth of Nanotechnology

**FIGURE 3.** Forecasted nano-TiO$_2$ production as a portion of total U.S. TiO$_2$ production.
Growth of Nanotechnology
Framing the Research Strategy

Risk Assessment Process

1. Identify Hazard
2. Assess Magnitude of Exposure
3. Assess Dose Response Relationship
4. Characterize Risk
2011 NNI Environment, Health, and Safety Research Strategy

- Nanomaterials Synthesis and Use Potential Release & Disposal
- Research to Understand and Manage Risk
  - Measurement
  - Human Exposure
  - Human Health
  - Environment
- Risk Assessment
- Predictive Modeling
- Risk Management
  - Product life cycle
  - Regulatory decision-making
  - Public outreach
  - Research planning

www.nano.gov
Integrated Research Framework

Product Life Cycle Stages

- Raw Materials
- Research, Design and Development
- Production
- Commercialization Consumer Use
- Disposal or Recycling

Environmental Pathways
- Air
- Water
- Soil
- Wastewater/landfills

Transport & Transformation
- Environmental conditions
- Biological conditions
- Primary & secondary contaminants

Exposure (Biota)
- Aquatic
- Terrestrial

Exposure (Human)

Effects
- Ecosystems
- Humans

Risk Assessment Paradigm

Exposure Assessment
Transport/Transform Concentration in Env. External Dose

Hazard ID Internal Dose & Response
Life Cycle Stages

Adapted from UC CEIN
Traditional Toxicological Approach

Failure to address Industrial Chemical Toxicology at the scale of production

- 50,000 + chemicals registered for commercial use in the US
- < 1,000 have undergone toxicity testing

Overwhelming of resources: each test
- $2-$4 million (for in vivo studies)
- > 3 years to complete
Mission of the UC Center for the Environmental Implications of Nanotechnology (UC CEIN)

The mission of the UC CEIN is to insure that nanotechnology is introduced and implemented in a responsible and environmentally-compatible manner to allow the US and the International community to leverage the benefits of nanotechnology for global economic and social benefit.
Objectives of the UC CEIN

- Develop a library of reference NMs
- Understand the impacts of different types of NMs on organisms and ecological systems
- Develop a predictive model of toxicology and environmental impacts of NMs
- Develop guidelines and decision tools for safe design and use of NMs
Collaborations with Institutions Worldwide

Image Courtesy of GoogleMaps
Shared Facilities

**Synthesis & Characterization**
- Molecular Foundry (LBNL)
- CNSI (UCLA & UCSB)
- Center for Accel Mass Spec (LLNL)
- CNSE (UCR)
- I/UCRC (Columbia U)
- FIMS (Bremen U)
- NYU (Singapore)

**Fate & Transport**
- Nano-Bio Interfacial Forces Lab (UCLA)
- Fate & Transport Labs (UCR, UCSB)
- Water Quality Research Lab (UCLA)
- Somasundaran’s Lab (Columbia U)

**UC CEIN Central Facilities**
- High Throughput Screening
- Shareable Database
- Modeling Framework
- NCEAS infrastructure

**Ecotox**
- Micro-Environ Imaging Facility (UCSB)
- Bodega Bay Marine Lab (UC Davis)
- Sandia Biocharacterization lab
- Subcell to Organism In Vivo Imaging
- Ecotox Lab at UCSB
- New shared lab space at UCSB
Research has a Goal.....

- **Knowledge Education Outreach**
  - IRG1: NM characterization
  - IRG2: Interactions at molecular, cellular, organ and systemic levels
  - IRG3: Organismal & community ecotoxicology
  - IRG4: NM fate & transport
  - IRG5: HT screening (Data generation for NM QSARs)
  - IRG6: Modeling of the Environmental Multimedia NM Distribution & Toxicity
  - IRG7: Risk perception

- **Academia**
- **Industry**
- **Government**
- **Public**
High Throughput Screening and Data Mining based on QSAR relationships that can be used to rank NM for risk and priority *in vivo* testing

Prioritize *in vivo* testing

High Throughput Cellular or Molecular Screening
Predictive Mechanism-based Toxicological Approach

In vitro testing:
• Mechanisms/pathways
• Material Libraries
• Bacteria/Cells/Embryos
• High content or HTS

Representative in vivo testing:
• different trophic levels
• Food webs
• DEB Modeling etc

Transport & Fate:
• Material Libraries
• Phys chem features
• Sources
• Life cycle

Hazard Identification & scoring

Advanced computational modeling and expert system

Risk Reduction & Prediction
• Safe Design
• Limit exposure

Emerging patterns

Hazard
Predictive Mechanism-based Toxicological Approach

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Risk Reduction & Prediction
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• Limit exposure

• Probabilistic Risak Modeling
• Risk Perception
Transport and Fate of Nanomaterials in Aquatic Environment

Source: UC CEIN (modified)
Objectives

Goal: To shed a light on fundamental mechanisms governing fate, transport and removal of engineered nanomaterials in both natural and engineered environment

Objective 1:
Development of standard handling approach for consistent nanoparticle dispersion: Effects of sonication, NP type and concentration

Objective 2:
Determination of fundamental mechanisms in transport and removal of nanoparticle: Role of nanoparticle concentration, solution chemistry, and hydrodynamic effects

Objective 3:
Evaluation of influence of natural organic matter and bacteria in transport and removal of nanoparticle
Experimental Approach - Transport

System 1: Packed-Bed Column

System 2: Radial Stagnation Point Flow

System 3: Parallel Plate Flow

$k_d = - \frac{u}{\epsilon L} \ln \left( \frac{C}{C_0} \right)$
Experimental Approach - Characterization

- Transmission Electron Microscopy (TEM)
- Electrokinetic Characterization (ZetaPALS)
- Potentiometric Titration
- Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-AES)
- Thermogravimetric analysis
- Stability
  - Aggregation (Dynamic Light Scattering)
  - Sedimentation (Absorbance)
• NP transport in soils depends on groundwater constituents
• Transport reduced in the presence of Ca\(^{2+}\)
• Humic acid (NOM) is important when K\(^+\) present, less for Ca\(^{2+}\)
• Parallel plate setup can produce rapid results that correlate with soil column studies
Overall Summary and Ongoing Work

• Microscope-based transport approach is promising to understand fundamental mechanisms

• Overall, transport and removal of nanomaterials is a function of several parameters including NP type, NP concentration, solution chemistry (pH, IS, valence) and presence of organic matter

• NOM, pH, and aggregation of NP seem to be the most significant parameters for transport of metal oxide nanomaterials

• In future, influence of primary particle size and bacteria on NP transport will be investigated.
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Thank you
Carbon Nanotubes

Structure of a single-walled carbon nanotube (SWCN)

Structure of a multi-walled carbon nanotube (MWCN)