# A Risk Forecasting Framework for Nanomaterials

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US-EU Collaborations in NanoEHS
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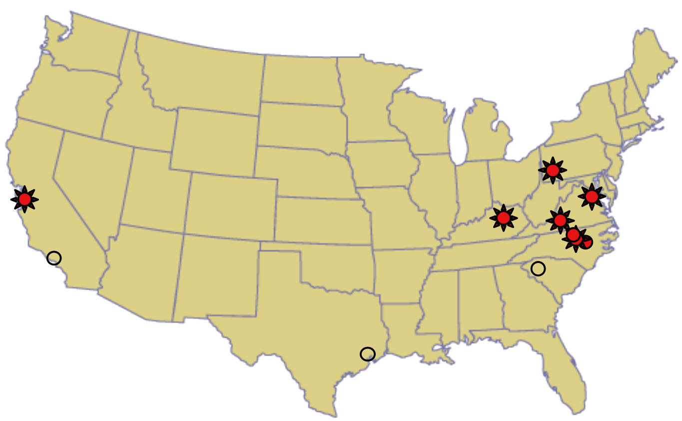
Duke University

CEINT

# 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)*



ICEINT
International Consortium for the Environmental Implications of Nano Technology

ENPRA
Risk Assessment of Engineered NanoParticles

SEVENTH FRAMEWORK PROGRAMME

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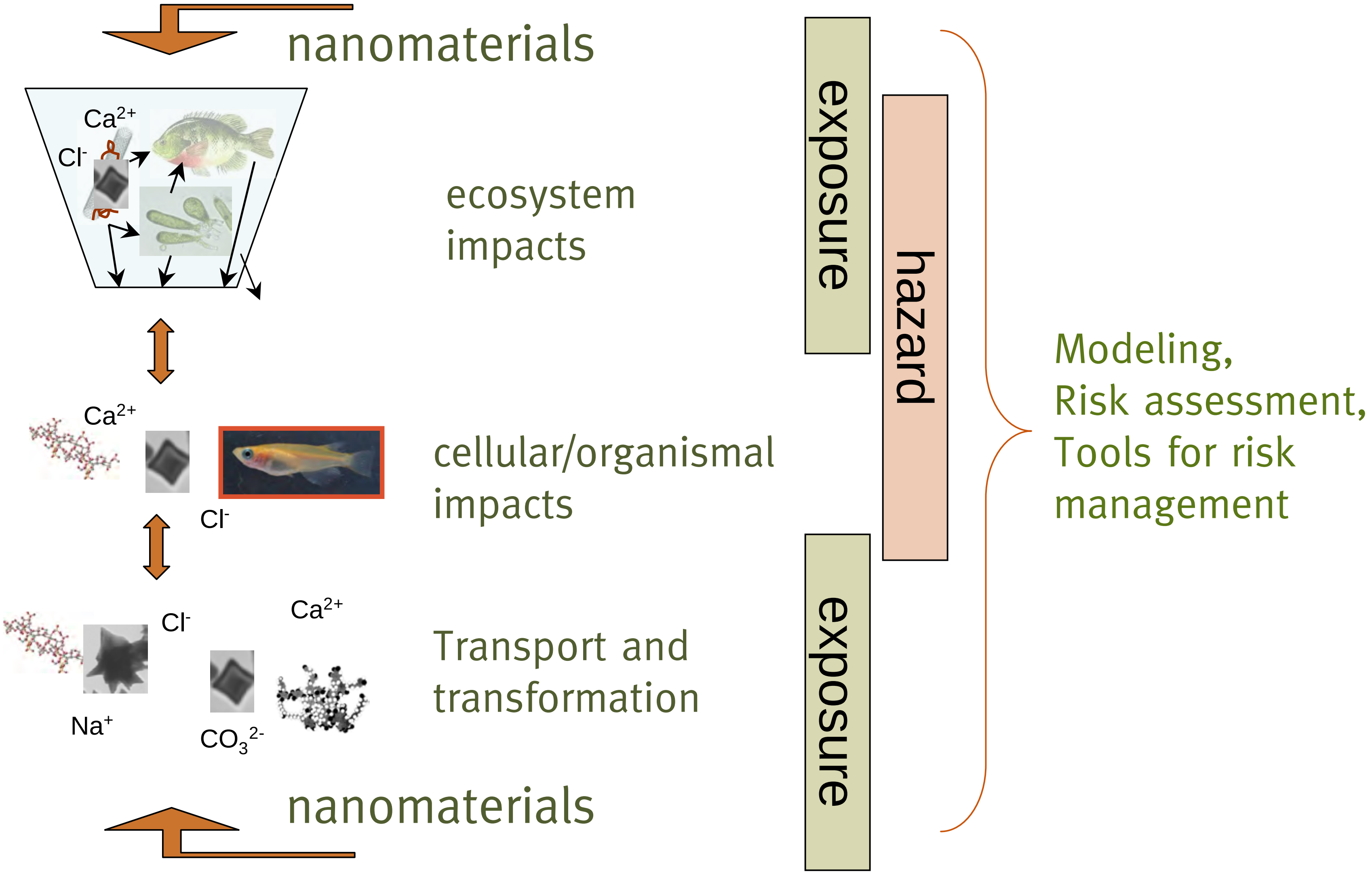
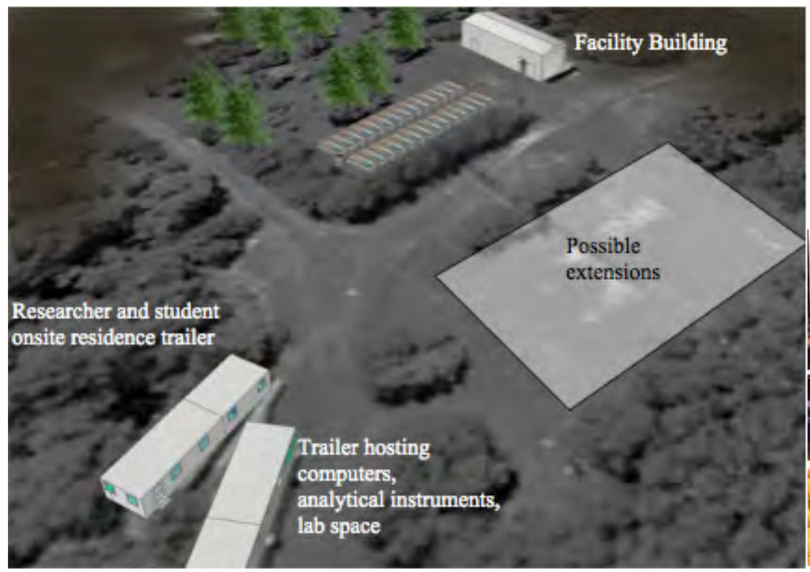
# Research Themes



# Mesocosms

- 26 mesocosms constructed, planted
- Probes, data acquisition, and web-based data monitorin
- Webcam
- Preliminary experiment started Oct ‘09
- First duplicated experiment with Ag NPs to begin May- June 2010
- $CeO_2$, SWCNTs, $TiO_2$ (single mc)




# Example: TiO2 exposure via wastewater discharge

exposure
*organismal impacts
*ecosystem impacts

vector describing nanoparticle characteristics

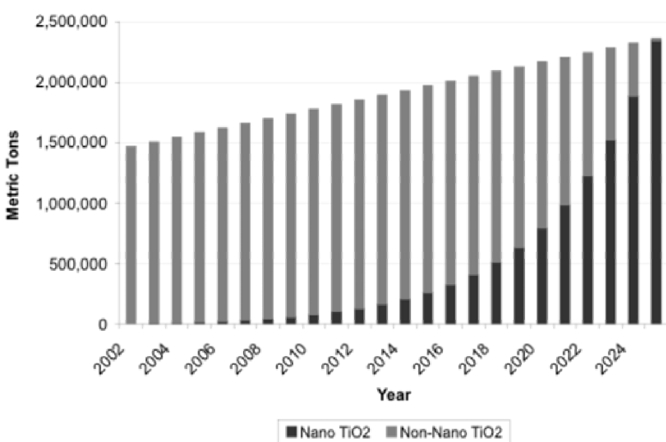
vector describing system (wastewater treatment plant, mesocosm)

$$C_{TiO2,sludge} = \left(S_{TiO2}\right) f_{TiO2,ww} \cdot P_{sludge}\left(\vec{\lambda}_{TiO2}, \vec{\gamma}_{ww}\right) / \left[Q_{ww} r\right]$$

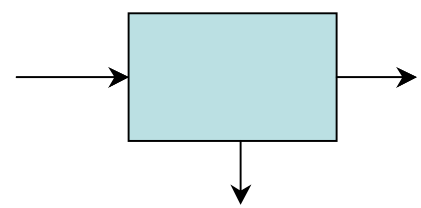
Source inventory (per time)
commercialization trends

usage profile
*social science
*engineering

Partitioning transfer function
*physical chemical properties
*transport
*microbiology







•Simulation
•Bayesian networks

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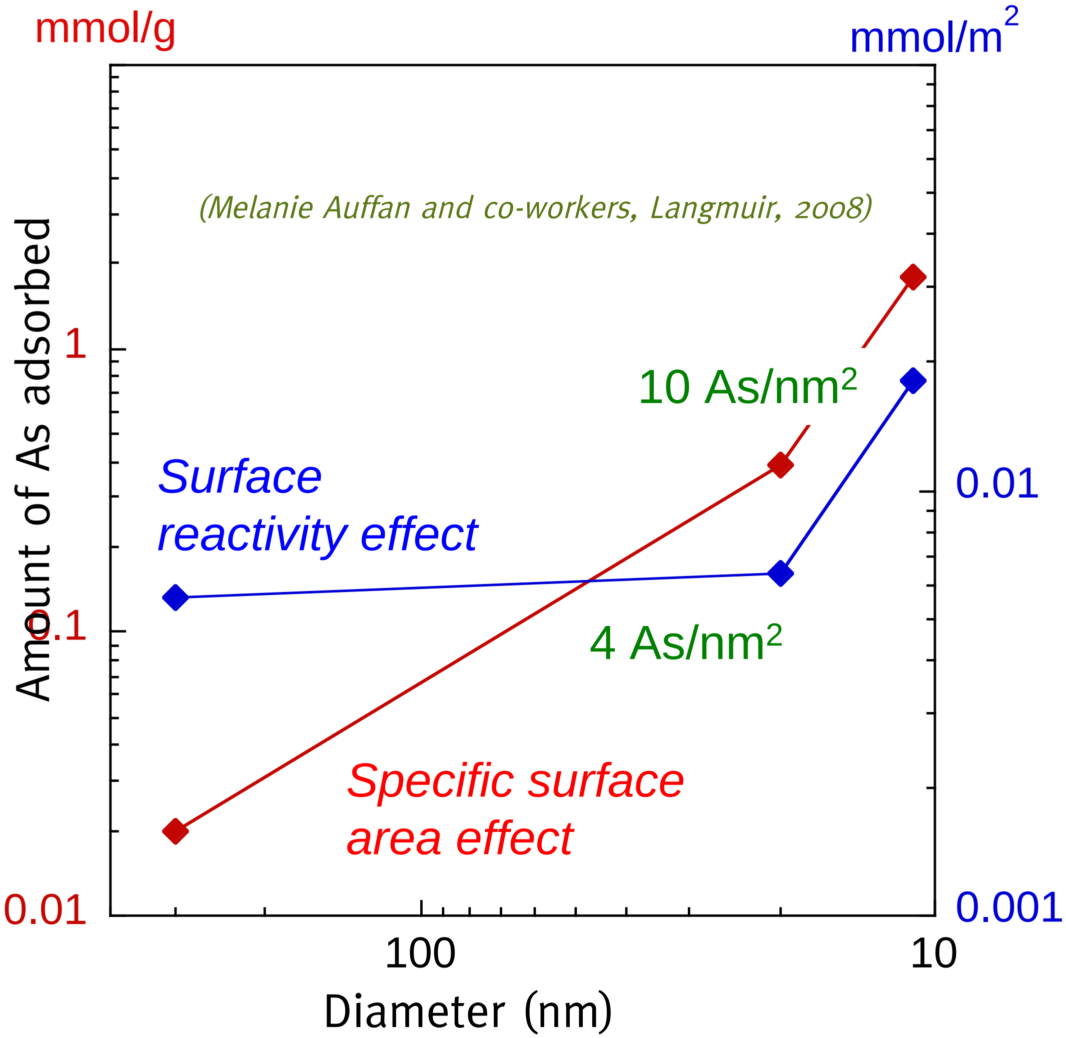
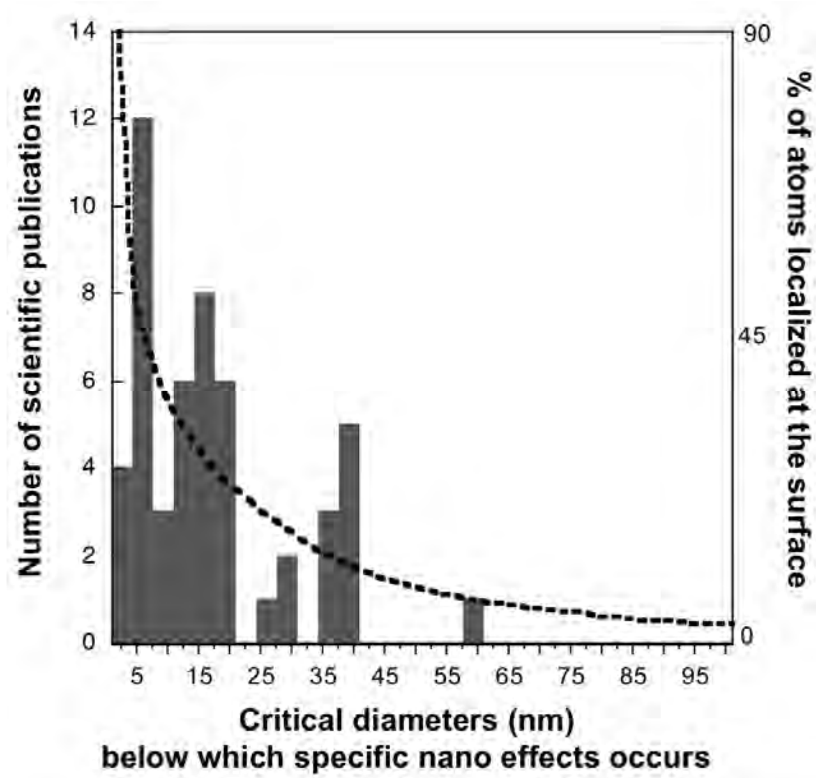
# A nanoparticle is:
# 1) small 2) has novel properties




*Nature Nanotechnology* 2009

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# 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

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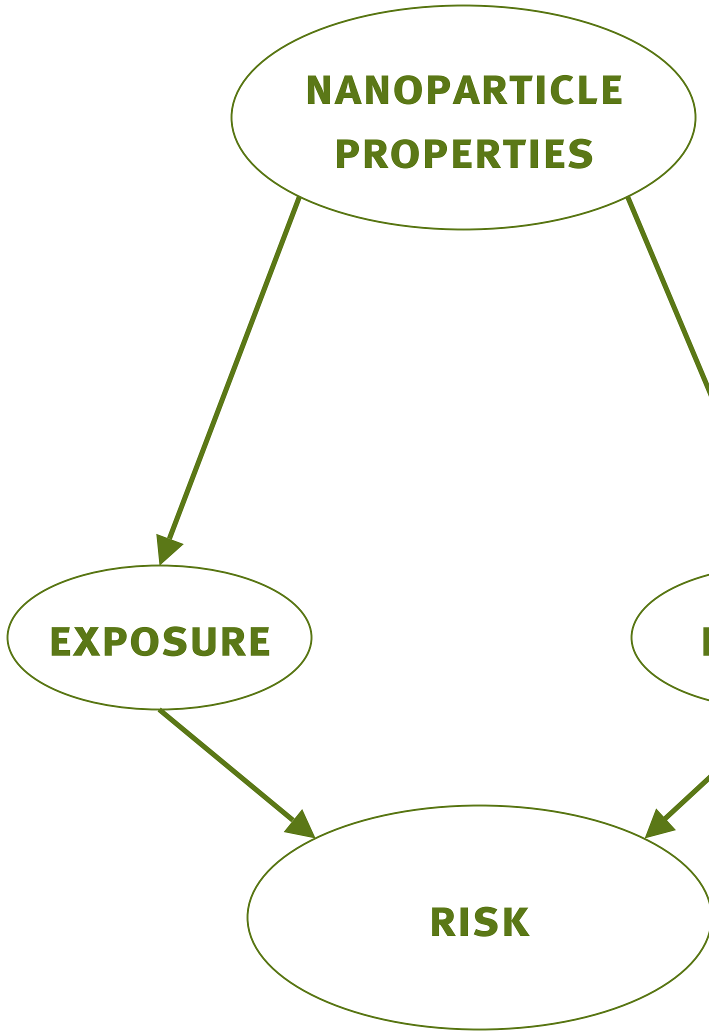
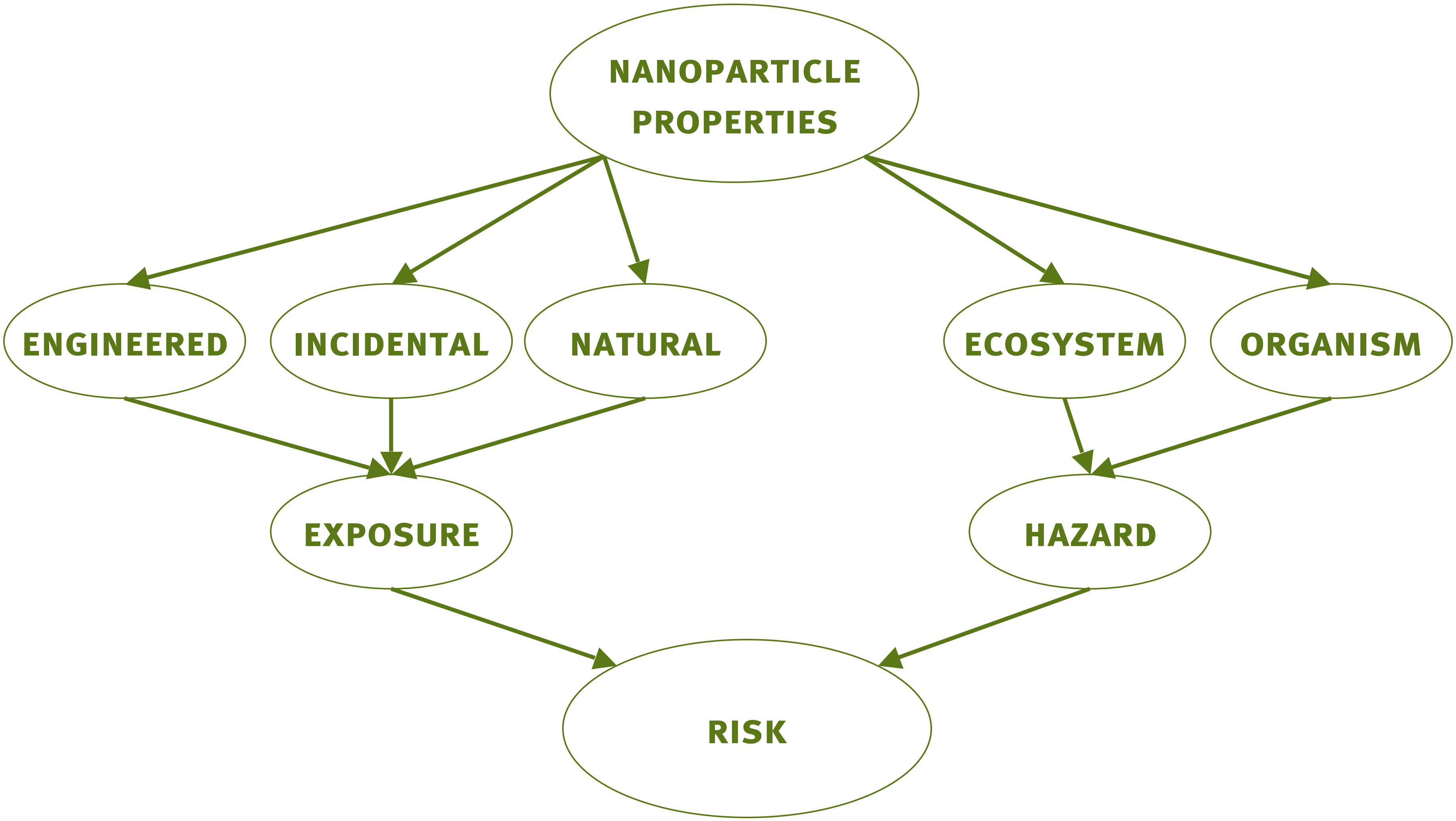
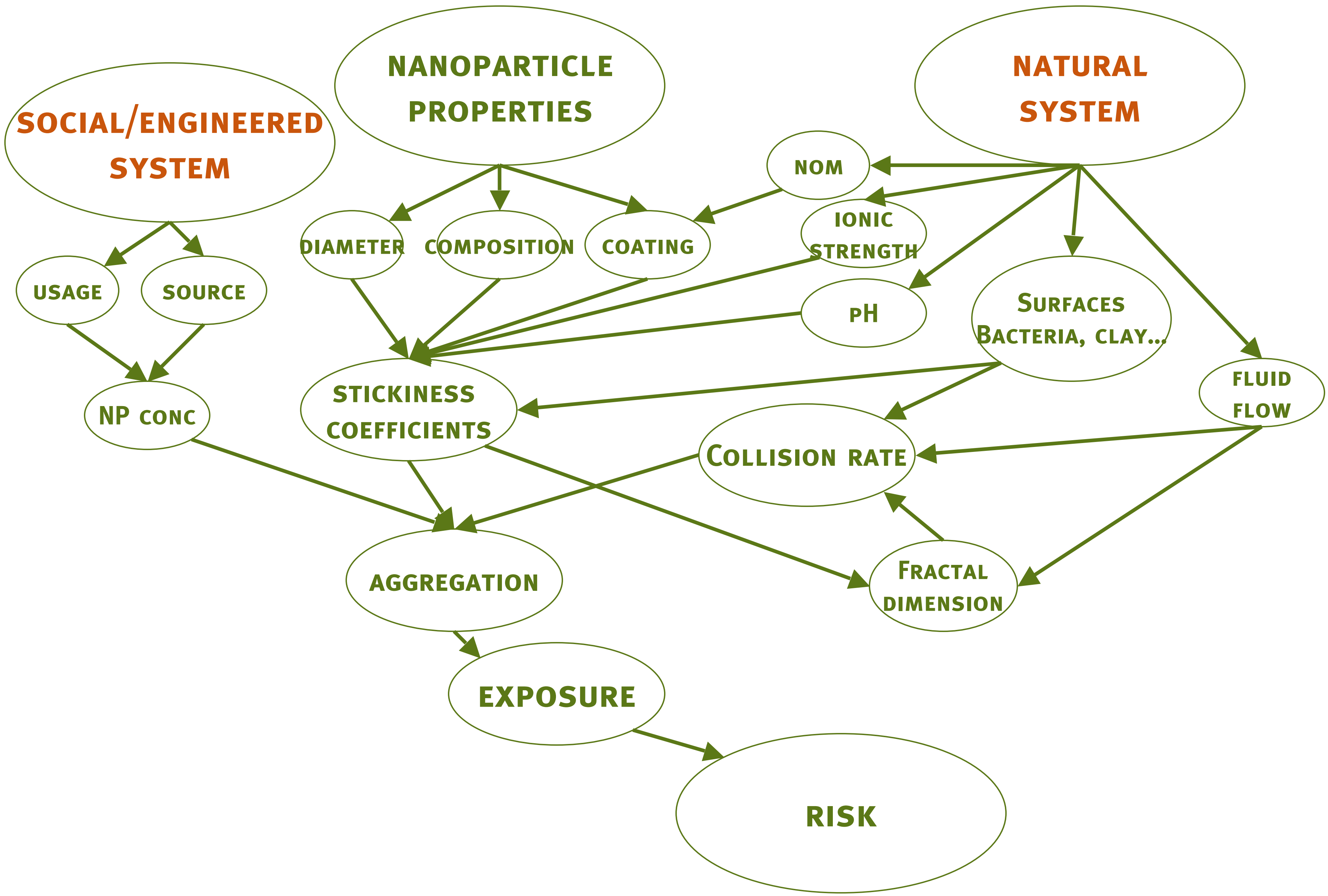
# Risk Assessment Framework



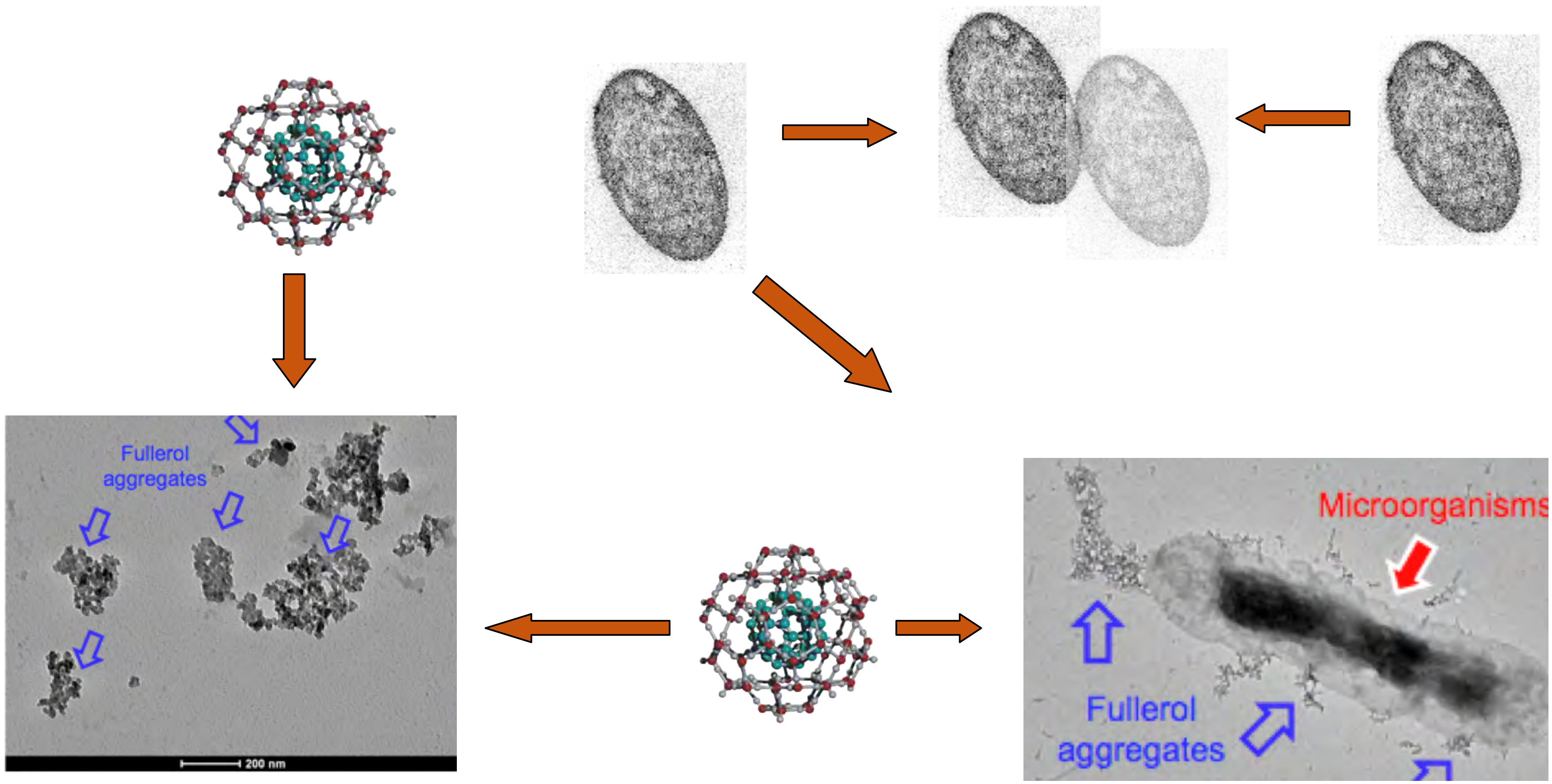
# Multiple sources, multi-scale impacts



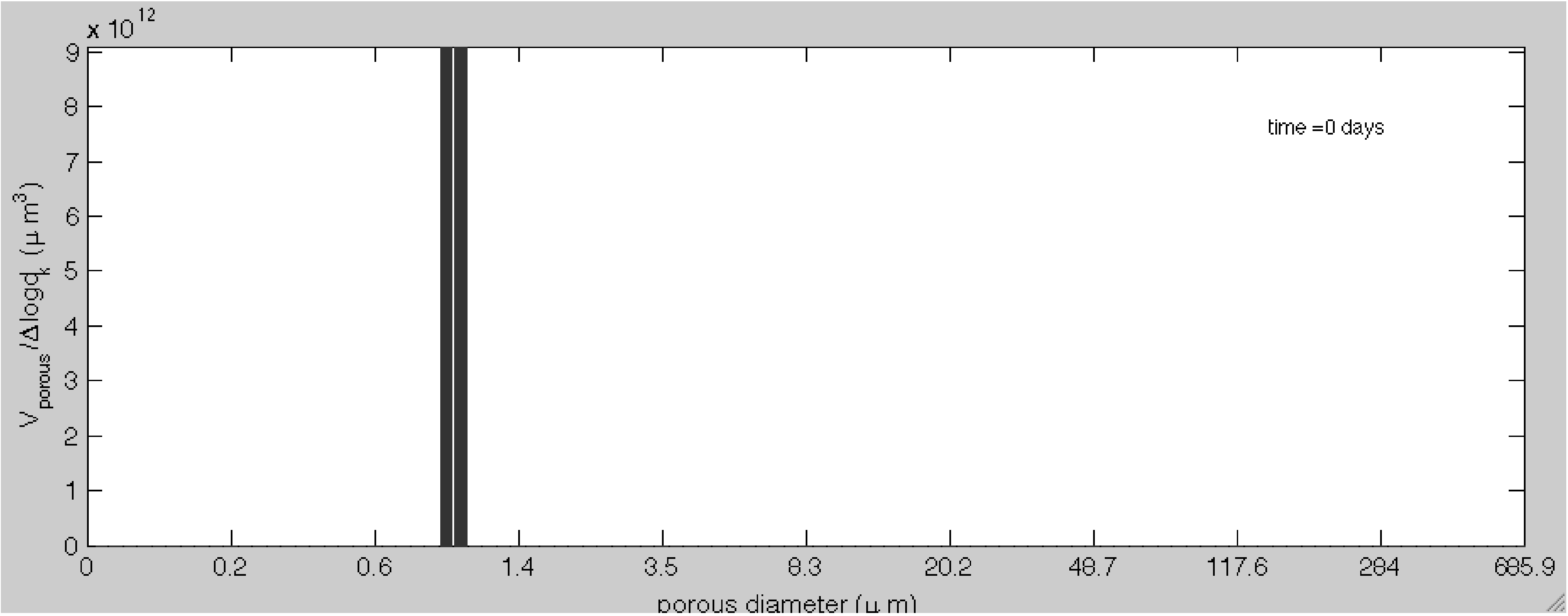


Social/Engineered System
Nanoparticle Properties
Natural System
NOM
Ionic strength
Diameter
Composition
Coating
pH
Usage
Source
Surfaces
Bacteria, clay…
Fluid flow
NP conc
Stickiness coefficients
Collision rate
Aggregation
Fractal dimension
Exposure
Risk

# Aggregation may occur between many components



# Transfer function

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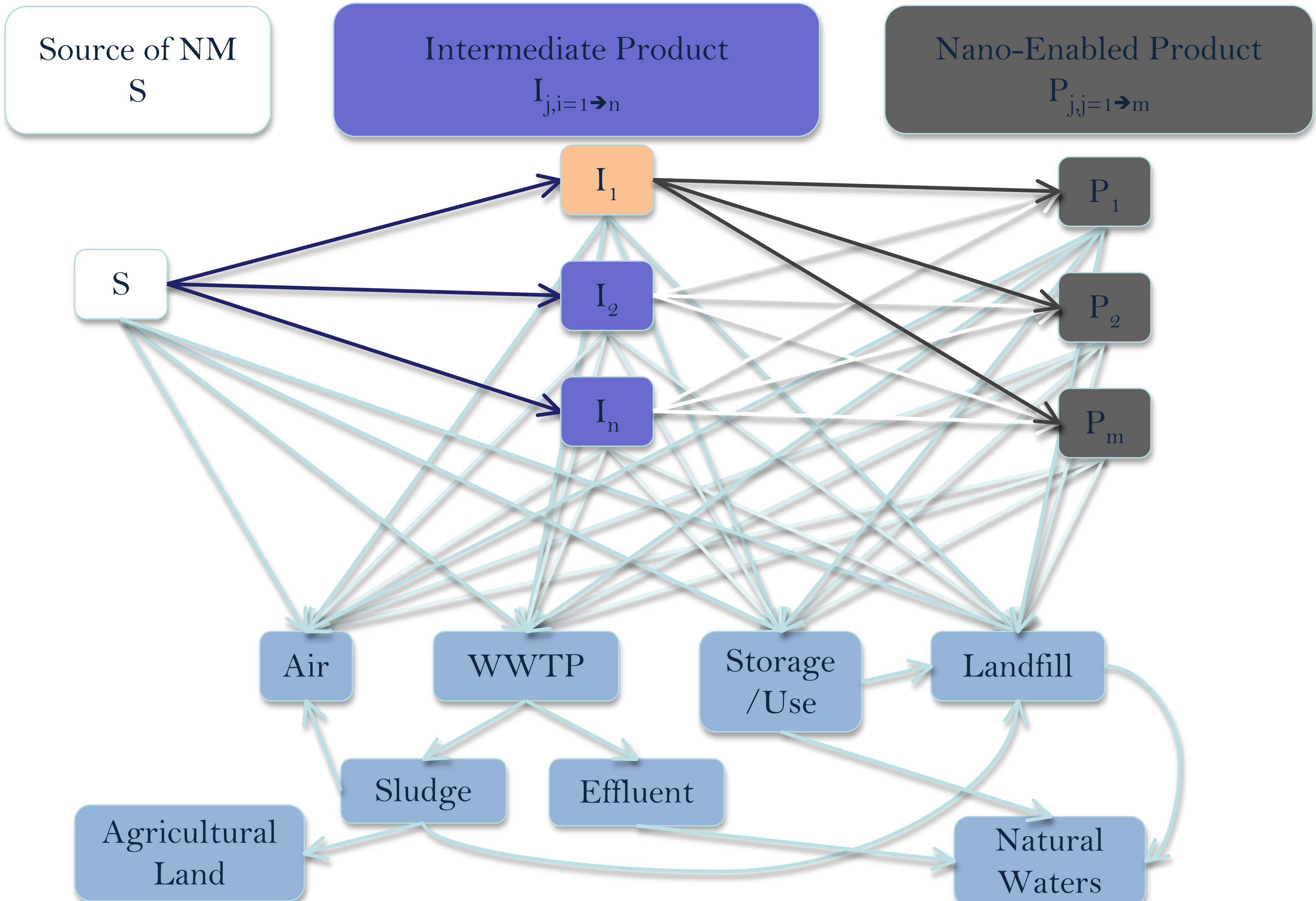


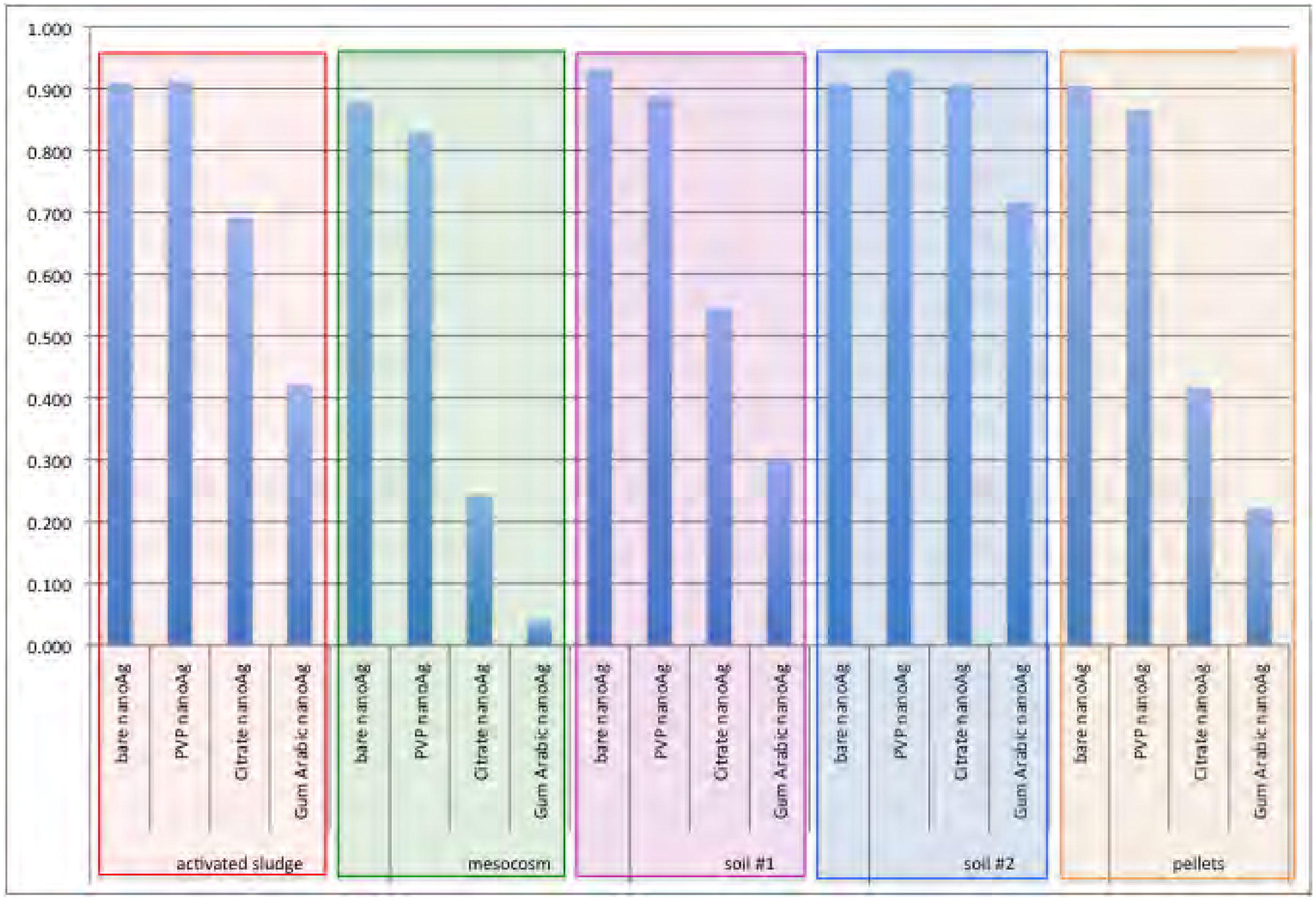
Source of NM
S
Intermediate Product
$I_{j,i=1 \rightarrow n}$
Nano-Enabled Product
$P_{j,j=1 \rightarrow m}$
$I_1$
S
$I_2$
$I_n$
$P_1$
$P_2$
$P_m$
Air
WWTP
Storage /Use
Landfill
Sludge
Effluent
Agricultural Land
Natural Waters

# Nanomaterial fabrication estimates

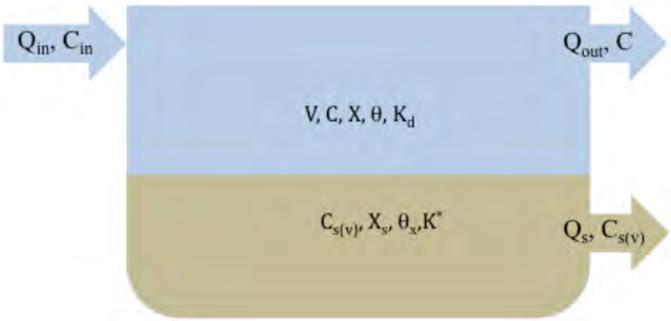
| Product | Lower bound (tpy) | Upper bound (tpy) |
|---|---|---|
| nano-$TiO_2$ | 7,800 | 38,000 |
| nano-Ag | 2.8 | 20 |
| nano-$CeO_2$ | 35 | 700 |
| CNT | 55 | 1101 |
| Fullerenes | 2 | 80 |

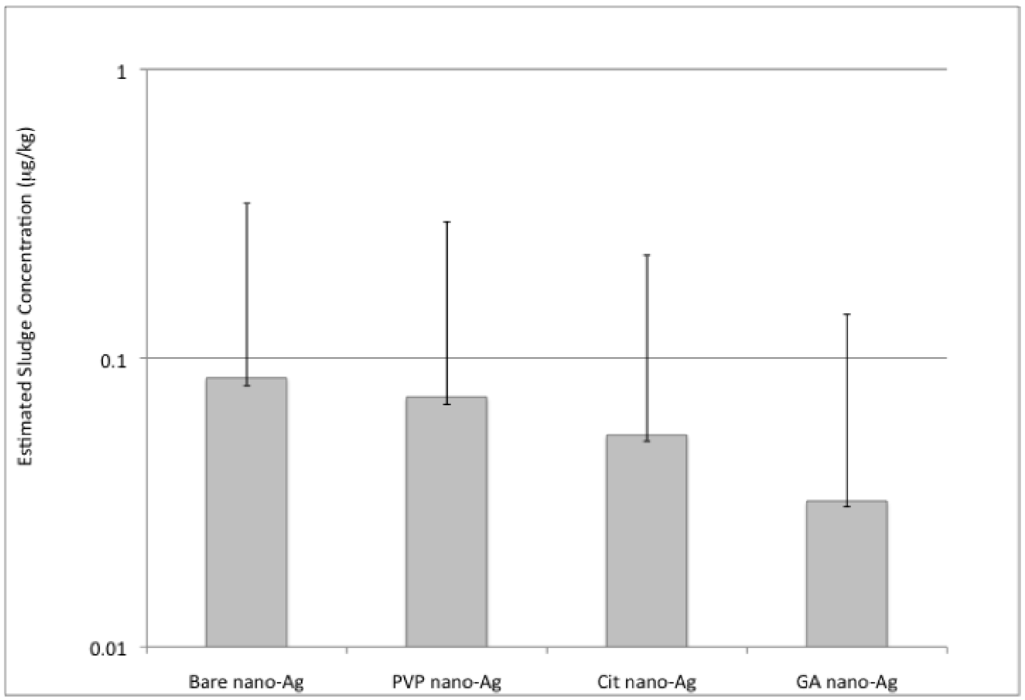
*C. Hendren, Wiesner and co-workers, in review*

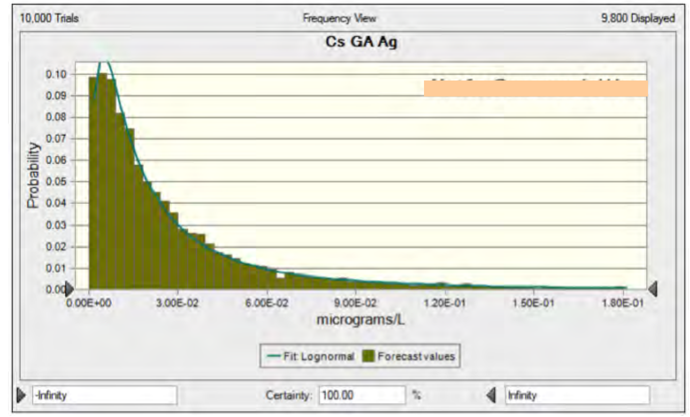
# Partitioning experiments

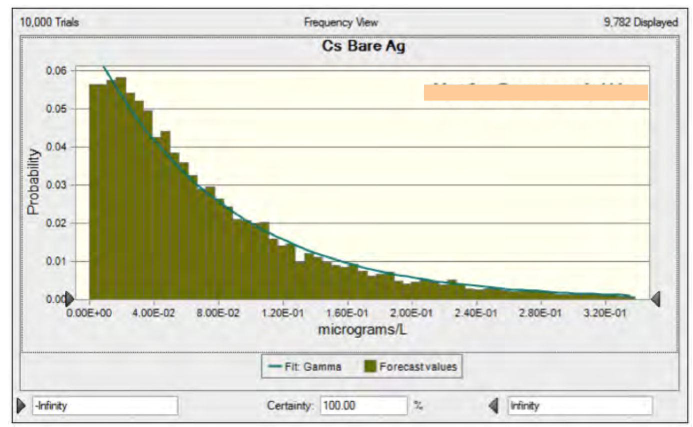


# MONTE CARLO CALCULATIONS OF SLUDGE CONCENTRATIONS

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# THANK YOU

*ICEIN 2011*

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