Nanomaterial Exposure:
A Framework for considering Uncertainty and Complexity

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CEINT

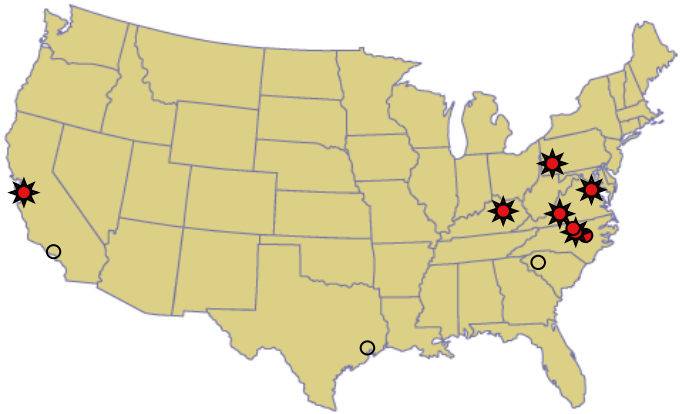
Center for the Environmental Implications of NanoTechnology

www.ceint.duke.edu

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

Duke UNIVERSITY

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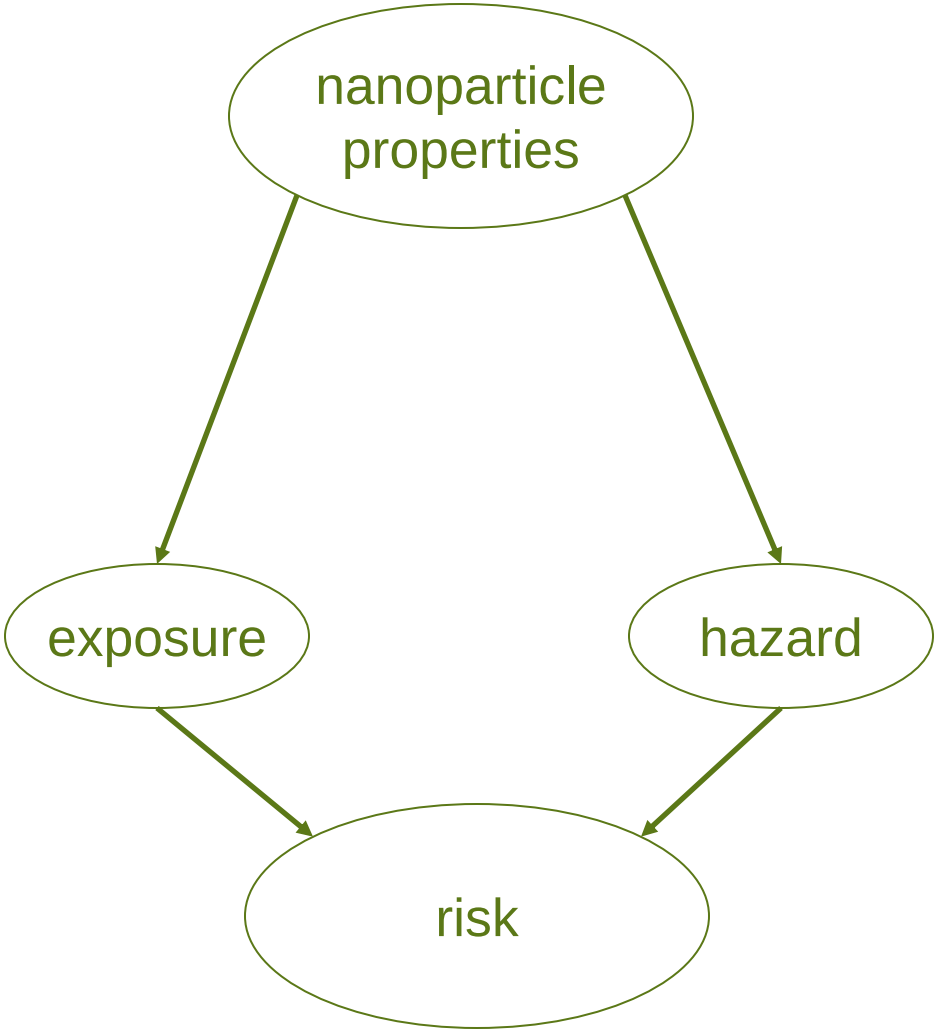
Elucidate general principles that determine nanomaterial behavior and translate this knowledge into the language of risk assessment



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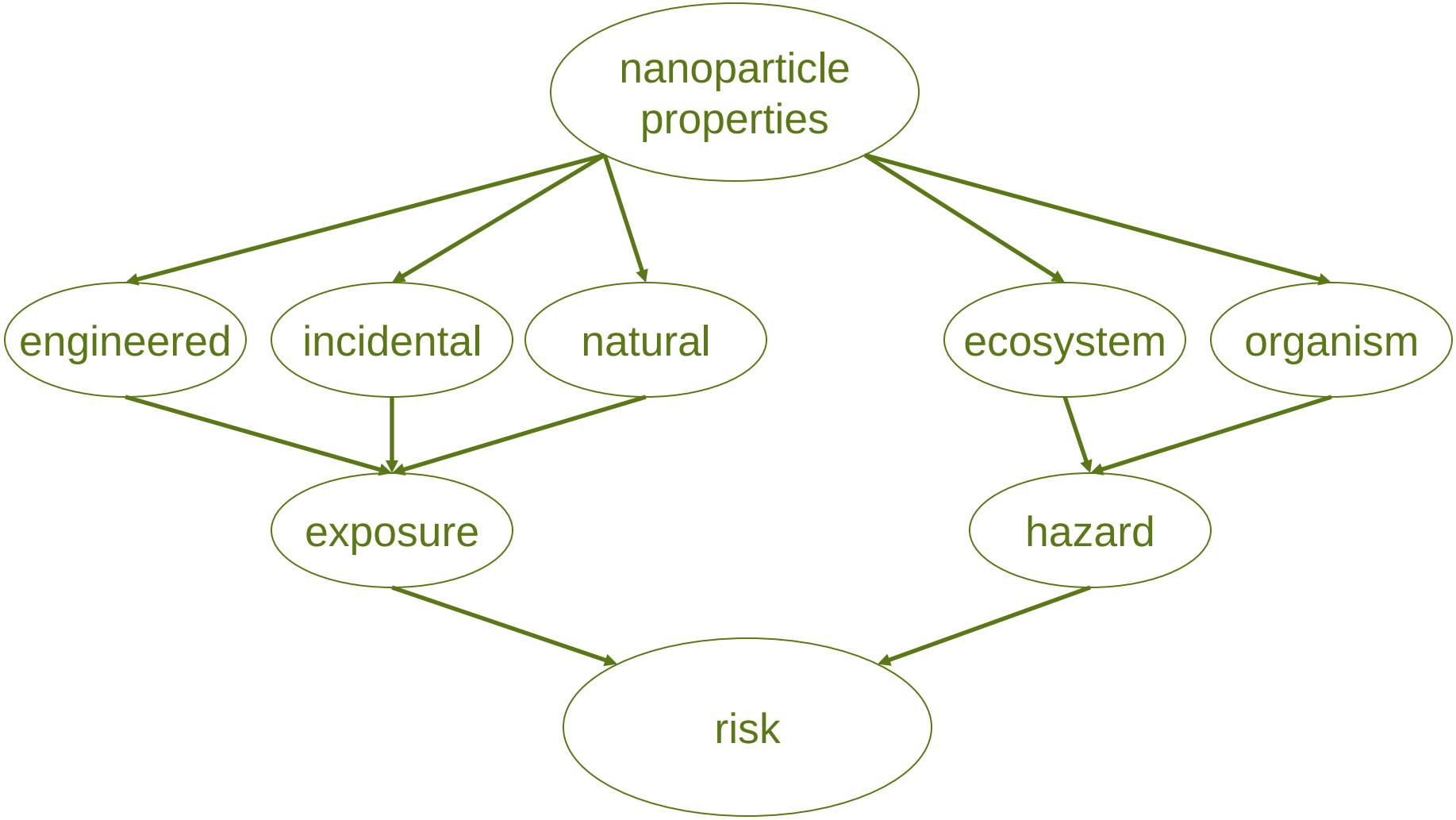
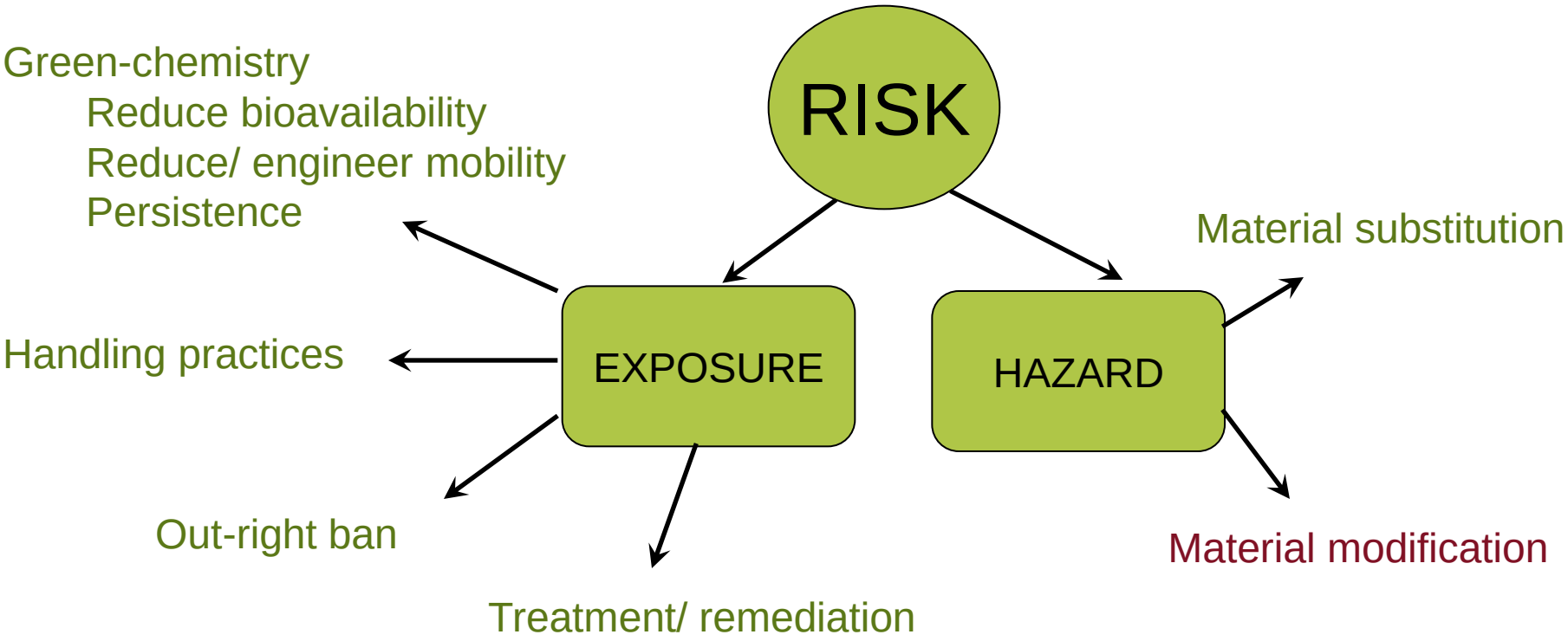
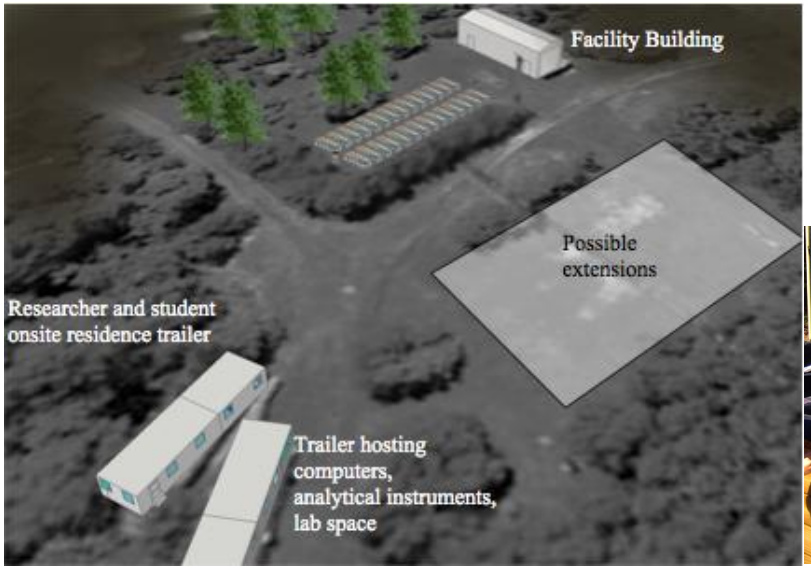


IF NANOMATERIALS POSE A RISK WHAT ARE THE OPTIONS FOR MANAGING RISK?



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
- CeO2, SWCNTs, TiO2 (single mc)



Example: TiO2 exposure via wastewater discharge

exposure
*organismal impacts
*ecosystem impacts

vector describing nanoparticle characteristics

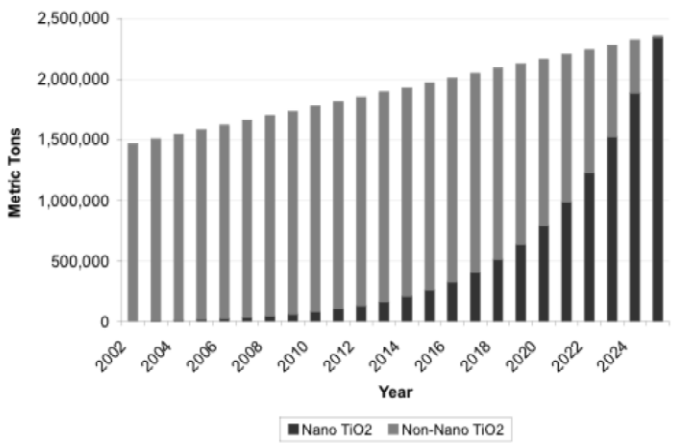
vector describing system (wastewater treatment plant, mesocosm)

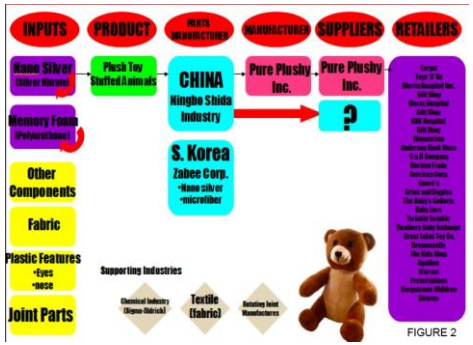
$$C_{TiO2,sludge} = (S_{TiO2}) f_{TiO2,ww} \cdot P_{sludge}\left(\vec{\lambda}_{TiO2}, \overrightarrow{\gamma_{ww}}\right) / [Q_{ww} r]$$

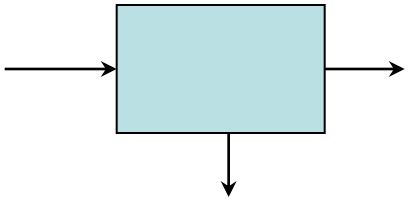
Source inventory (per time)
commercialization trends

usage profile
*social science
*engineering

Partitioning transfer function
*physical chemical properties
*transport
*microbiology







•Simulation
•Bayesian networks

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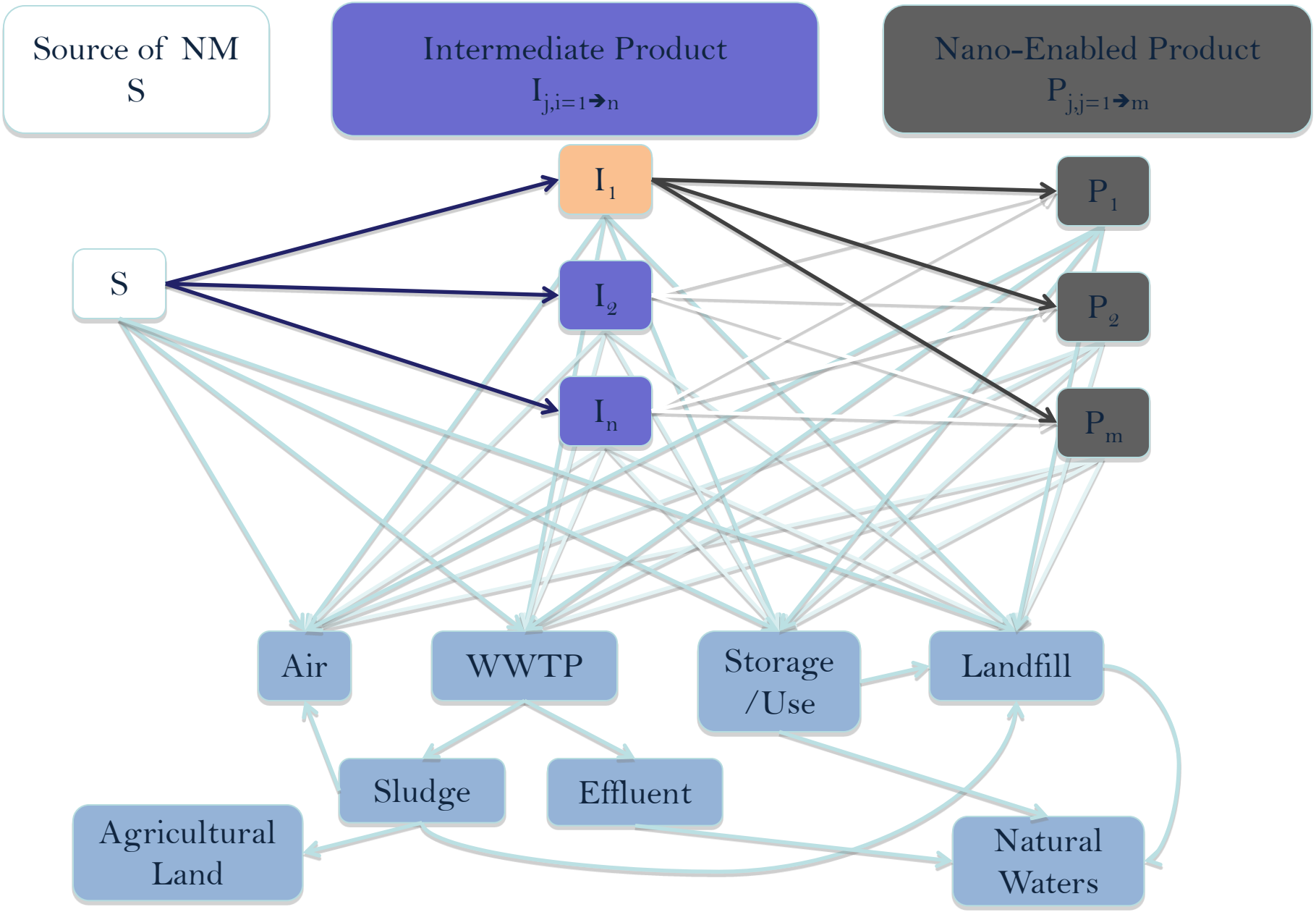

Source of NM
S
Intermediate Product
$I_{j,i=1 \rightarrow n}$
Nano-Enabled Product
$P_{j,j=1 \rightarrow m}$
S
I_1
I_2
I_n
P_1
P_2
P_m
Air
WWTP
Storage /Use
Landfill
Sludge
Effluent
Agricultural Land
Natural Waters

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

Aggregation considered as a two step process

surface chemistry (coatings, composition of surfaces)

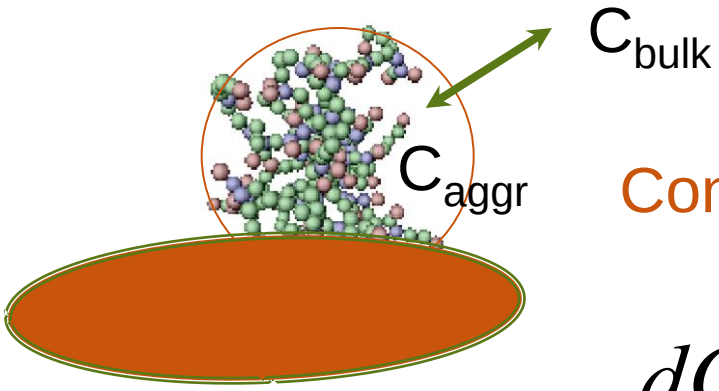
Transport + Attachment ⇒ Aggregation

Physics
(fluid flow)

Nanoparticles tend to aggregate

Nanoparticles aggregate

Conditions in aggregate ≠ bulk



Concentration factor ~ 10^3 to 10^5

$$\frac{dC}{dt} \propto n^{\frac{4}{D}-2}$$

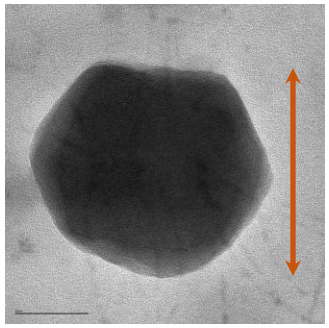
$$\frac{\frac{dC}{dt}_{D=2}}{\frac{dC}{dt}_{D=3}} = 2x10^3{}_{n=10^5}$$

Aggregation defined by:

n= number of nanoparticles per aggregate

Structural descriptor (fractal dimension, density…)

Ordered packing D= 3



$n \sim 10^6$

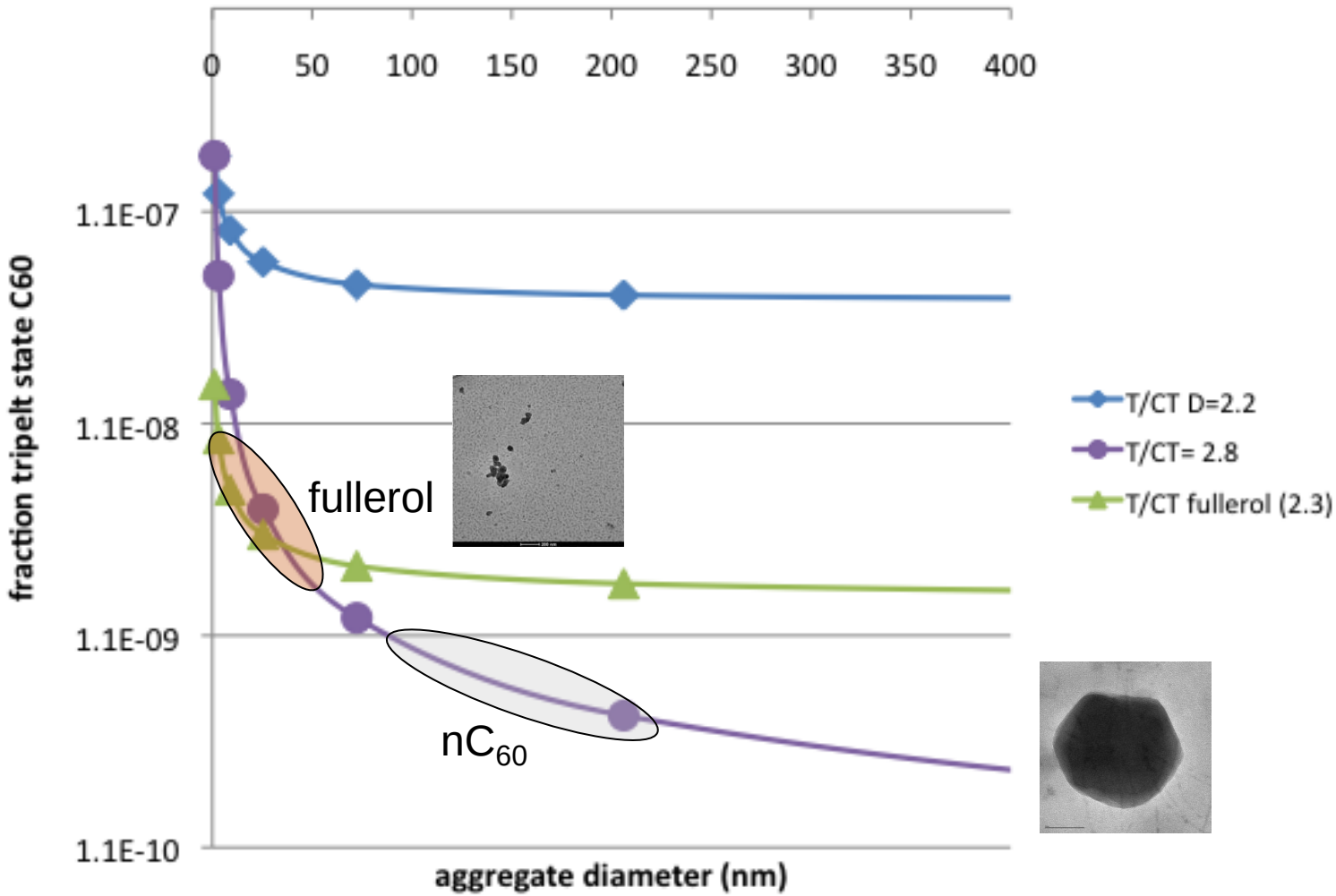
$d_{aggr} \sim 200$ nm

Fractal D = 2.3

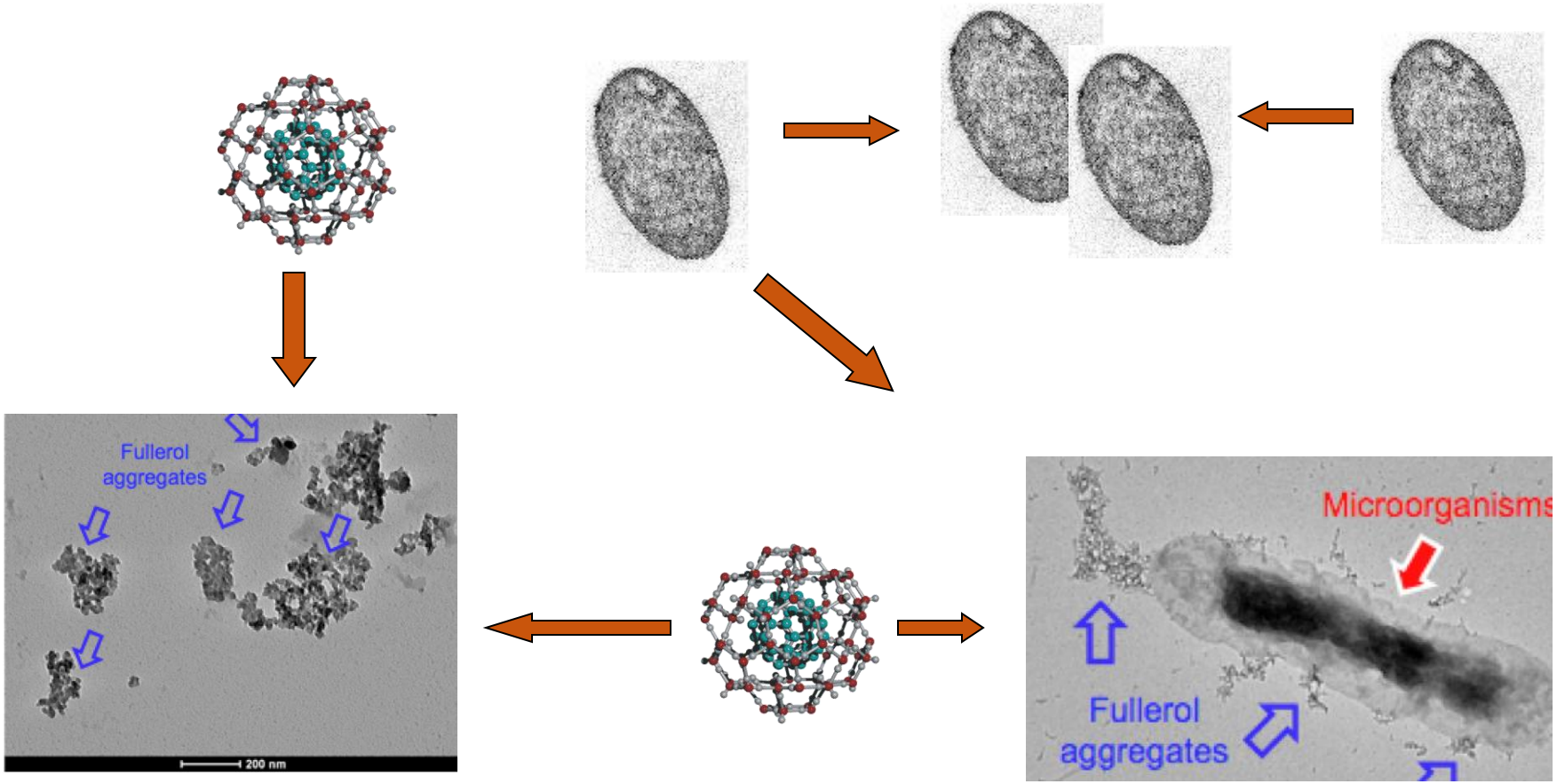
$n \sim 10^3$

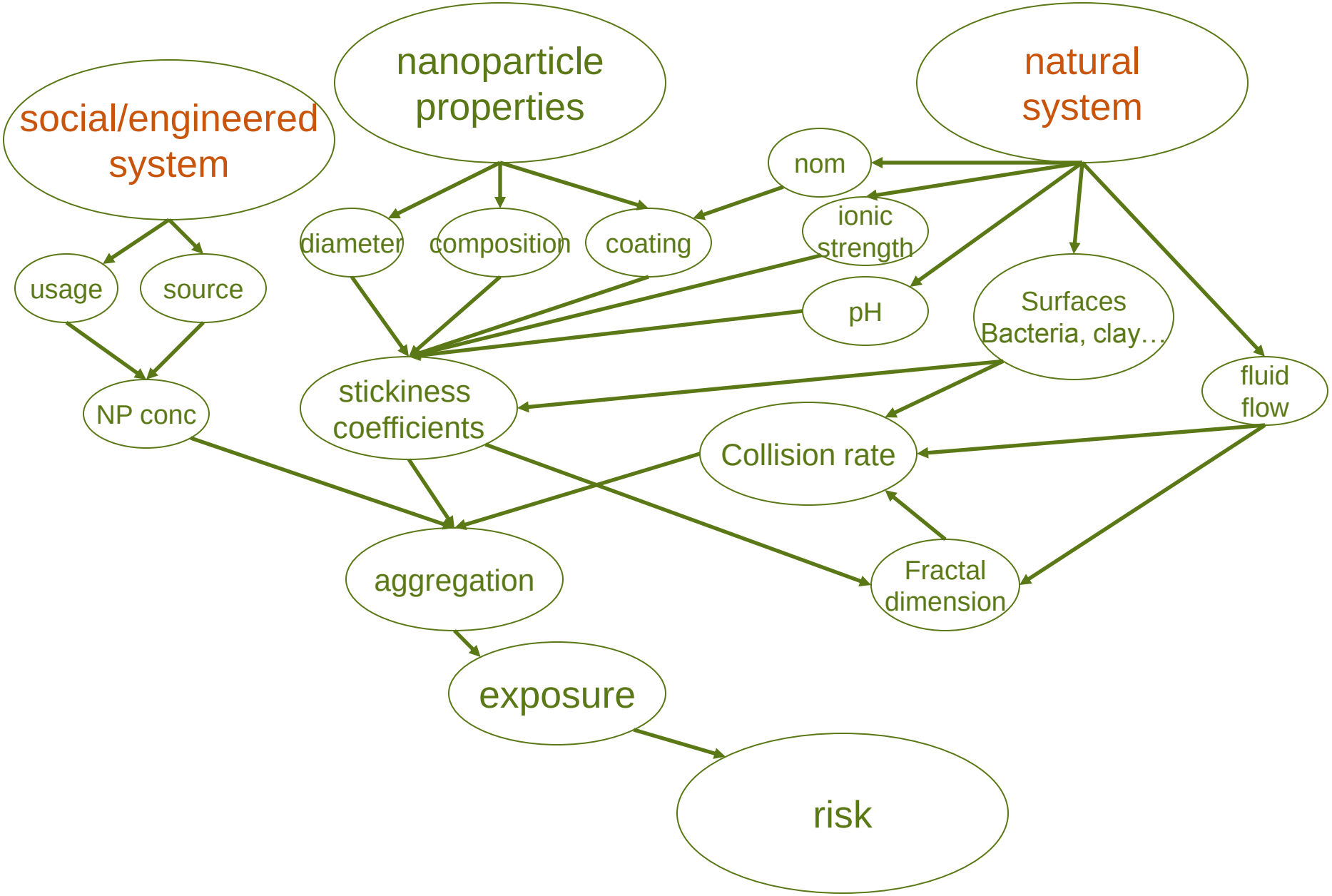
$d_{aggr} \sim 20$ nm

Aggregate structure resolves the ROS paradox



Aggregation may occur between many components




social/engineered system
nanoparticle properties
natural system
usage
source
diameter
composition
coating
nom
ionic strength
pH
Surfaces Bacteria, clay…
fluid flow
NP conc
stickiness coefficients
Collision rate
aggregation
Fractal dimension
exposure
risk

Transfer function

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Thank You

ICEIN 2011

May 9- 11

Duke University

Durham, NC

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