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Simulating the fate and transport of nanomaterials in surface waters

Quantifying Exposure to Engineered Nanomaterials From Manufactured Products – Workshop
Arlington, VA July 7 – 8, 2015

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Overview

- Processes of nanomaterials in surface waters
- The WASP model
- Preliminary Study
- Current Development
    - Redesign of WASP Architecture for nanomaterials

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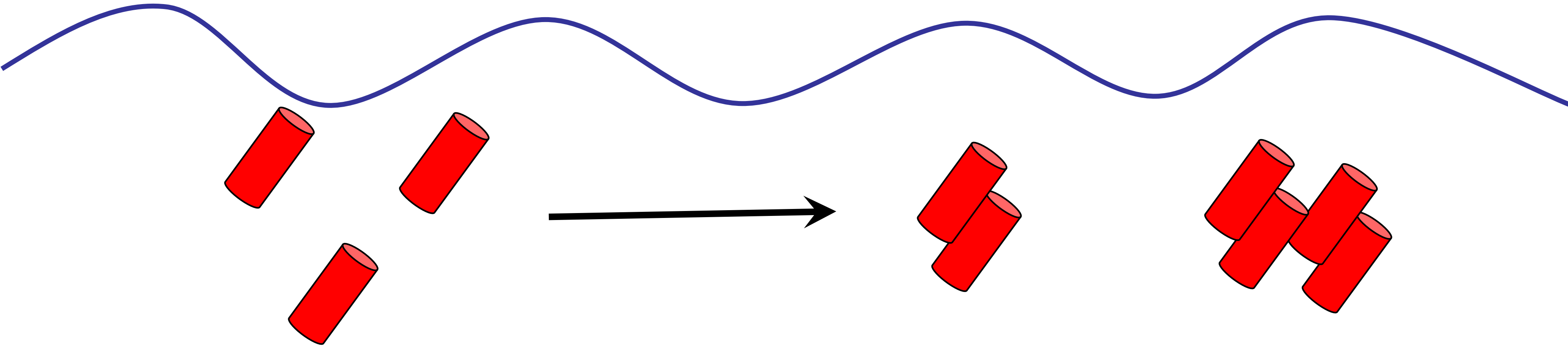
Nanomaterial Processes: Homo-aggregation

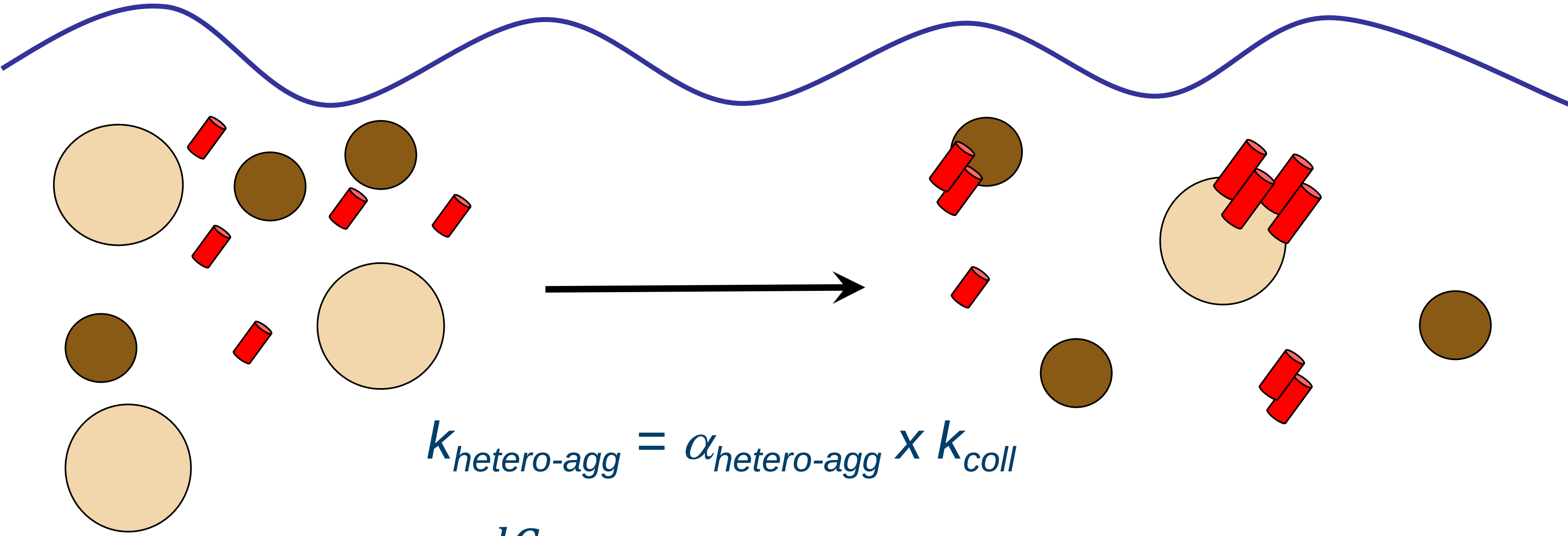


$$k_{homo\text{-}agg} = \alpha_{homo\text{-}agg} \; x \; k_{coll}$$

$$\frac{dC}{dt} = -k_{homo-agg}C$$

Given that the environmental concentration of nanomaterials will be small, we assume homo-aggregation to be negligible

Nanomaterial Processes: Hetero-aggregation



$$k_{hetero\text{-}agg} = \alpha_{hetero\text{-}agg} \times k_{coll}$$

$$\frac{dC}{dt} = -k_{hetero-agg} S$$

Each nanomaterial can associate with each particle

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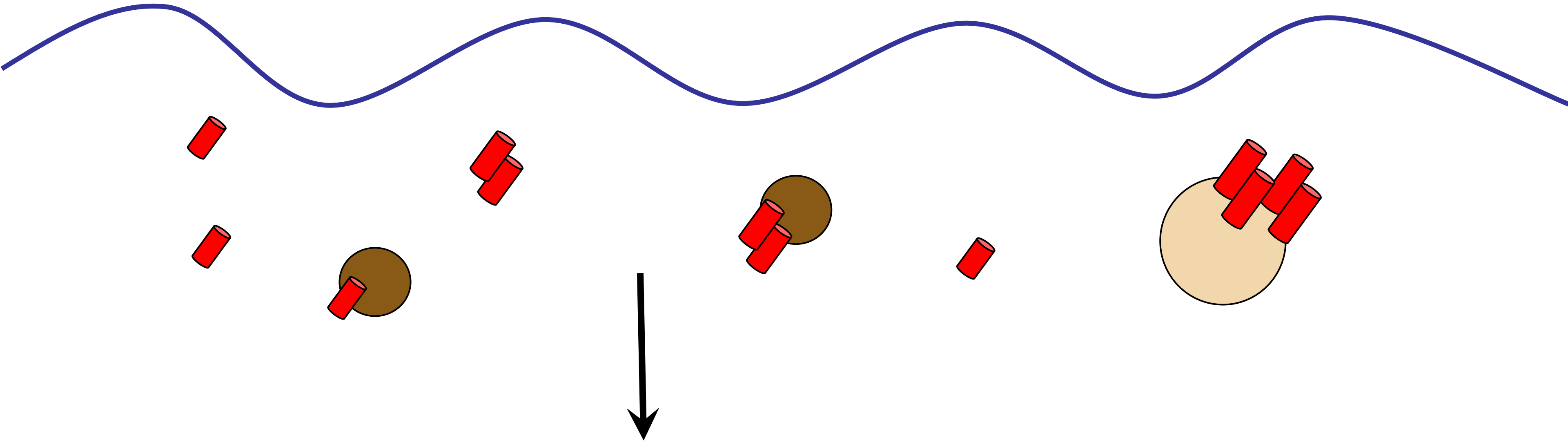
Nanomaterial Processes: Settling

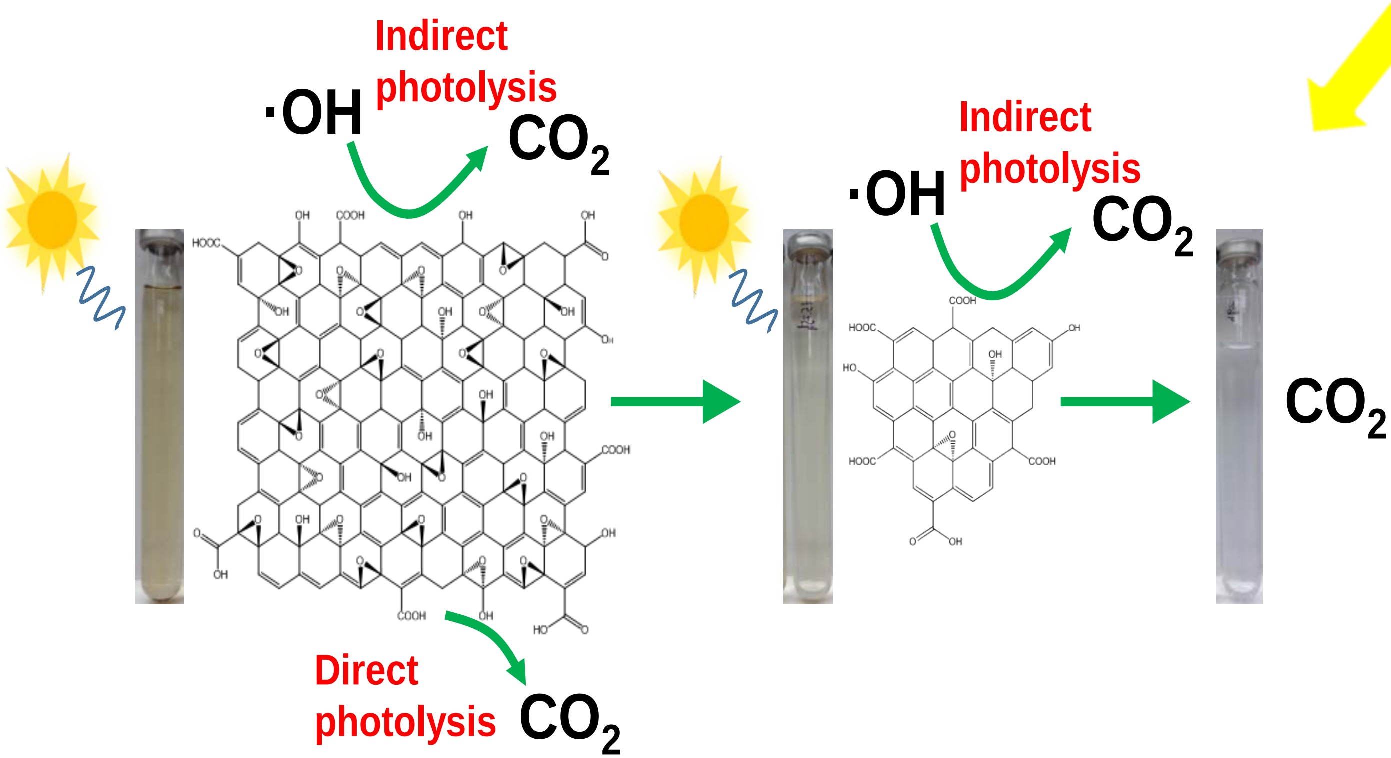


Stoke's Law: $v_{settling} = \frac{2}{9}\frac{(\rho_b - \rho_f)}{\mu} g R^2$

Each particle settles at a different velocity depending on size

Nanomaterial Processes: Transformations

$$I = I_o e^{-kx}$$



(Hou et al., ES&T 2015, 49, 3435-3443)

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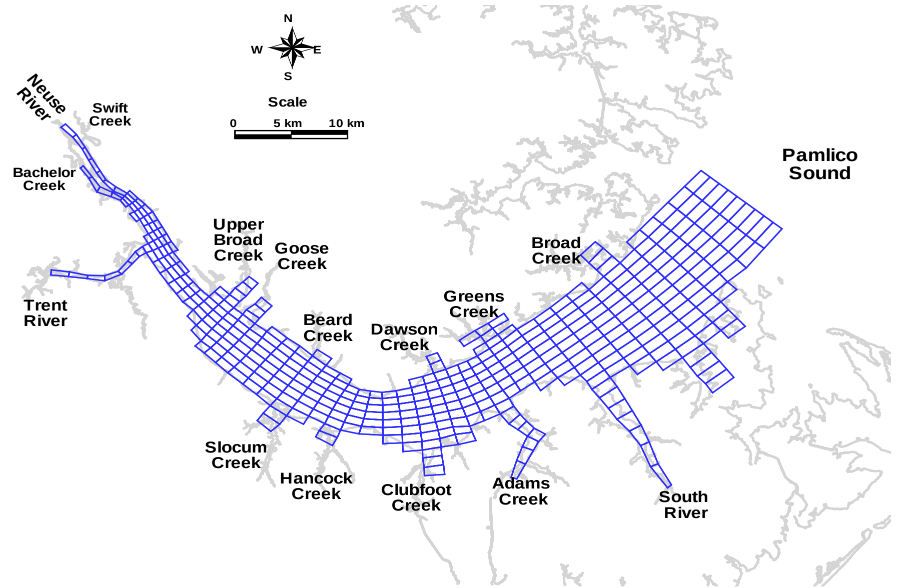
WASP Background

- Originally developed in the 1980s
  (Di Toro et al., 1983; Connolly and Winfield, 1984; Ambrose, R.B. et al., 1988)
- Currently WASP version 7
- One of the most widely used water quality models in the US and the world
- WASP is a ***general, flexible modeling system*** that allows users to develop a model specific to their system and for their contaminants
- Simulates concentrations over time and space

Aquatic Ecosystems

- Applied to a wide range of aquatic ecosystems
    - Tampa Bay, FL
    - Lake Okeechobee, FL
    - Neuse River Estuary, NC
    - Great Lakes
    - Potomac Estuary
    - Lake Waccamaw, NC
    - Delaware River Estuary
    - Sudbury River, MA
    - Brier Creek, GA

Dimension	System
0D	Ponds
1D	Lakes, Streams
2D	Rivers
3D	Estuaries, large lakes



Contaminants

Module	Contaminants
Heat	Temperature, Salinity, Alkalinity
Eutrophication	Dissolved Oxygen, Nitrogen (Nitrate, Ammonia), Orthophosphate, Algae
Toxicants	PAHs, PCBs, pesticides, metals
Mercury	Elemental mercury (Hg^0), Divalent Mercury (Hg^{2+}), Methylmercury (MeHg)

Brier Creek, Georgia

Brier Creek, GA
Coastal Plain River
66 miles long

8 segment WASP model was developed for Hg TMDL and for benefits assessment of Clean Air Mercury Rule

Brier Creek, Georgia

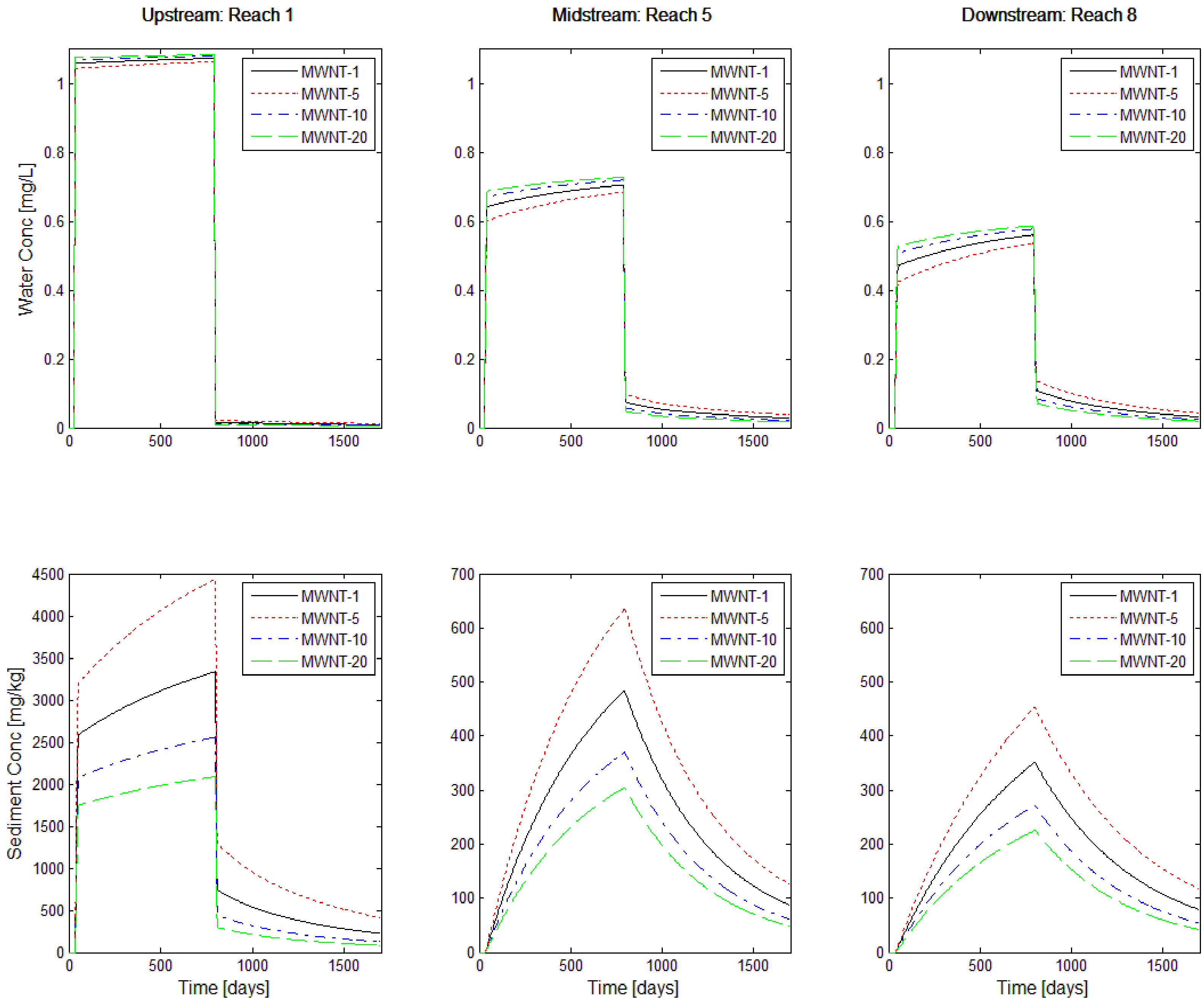
Adapted to investigate release of MWNT and OH-MWNT into upstream segment assuming instantaneous sorption as baseline for future work.

Range of ionic strengths:

1, 5, 10, 20 mM NaCl

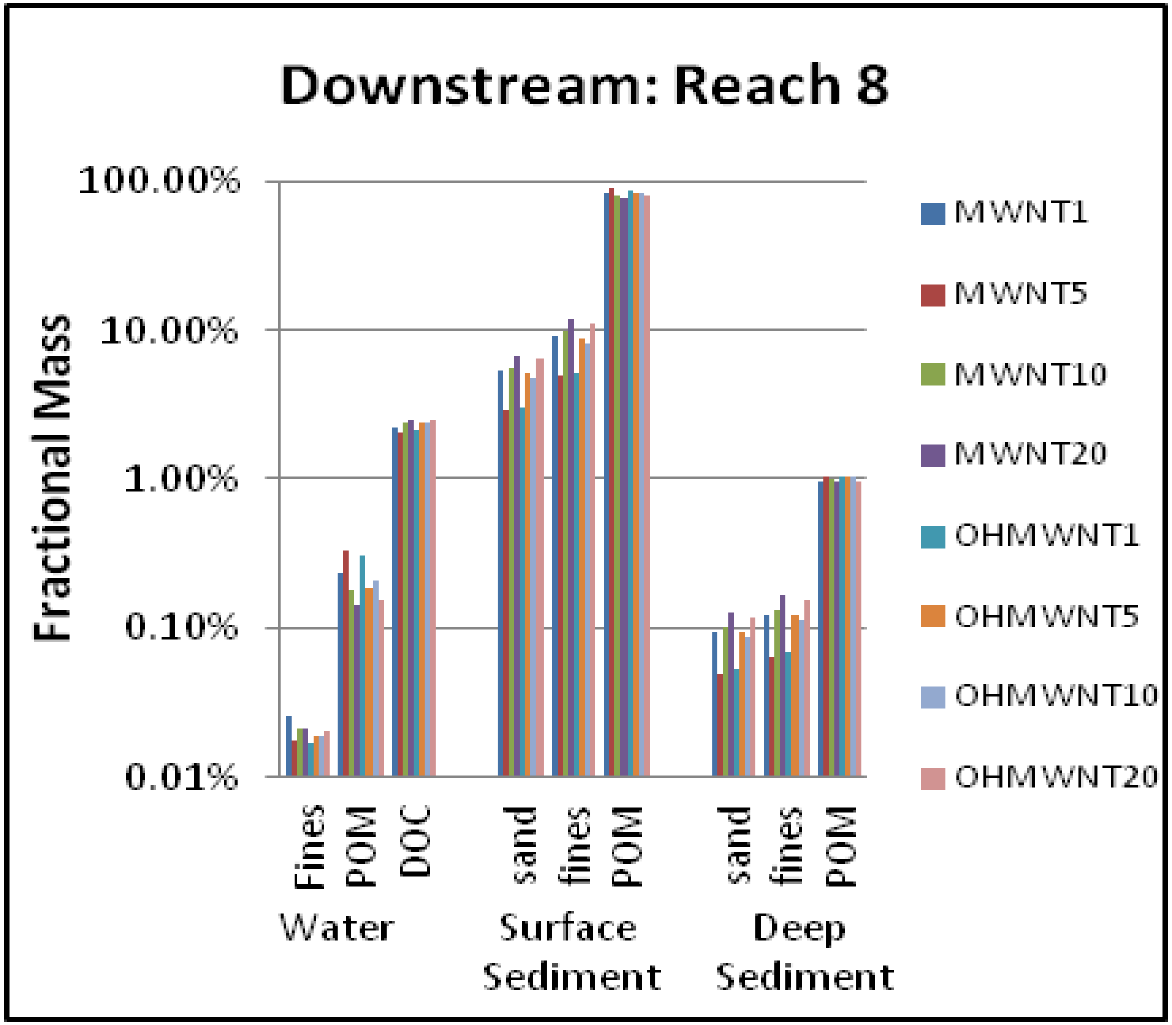
Four surfaces:

sand, fines, POM, DOC



Upstream: Reach 1
Midstream: Reach 5
Downstream: Reach 8
Water Conc [mg/L]
Sediment Conc [mg/kg]
MWNT-1
MWNT-5
MWNT-10
MWNT-20
Time [days]

Distribution across media



WASP 8 Development

- Fortran 95
- Dynamic allocation, 0 to *n* of each state variable
- More state variables
    - Chemicals
    - Solids
    - DOC
    - Nanomaterials
- Nano-specific processes (e.g., hetero-aggregation)

Future Work

- Use lab and field data to parameterize nanomaterial processes in WASP
  - Simulate nanomaterial concentrations
    - Over time and length of river
    - Both in surface water and sediments
  - Distribution across media
    - DOC, silt, clay, POM, aqueous
- Model sensitivity
  - Compare K_d to $k_{het\text{-}agg}$
  - Range of α's
- Explore different aquatic ecosystems
  - Streams, Lakes, Rivers, Ponds