Modeling Metal Rapid Removal Experiments for Hazard Classification

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Workshop on Progressing the Rapid Removal Concept for Metals Classification/Hazard Identification

ECHA
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Introduction

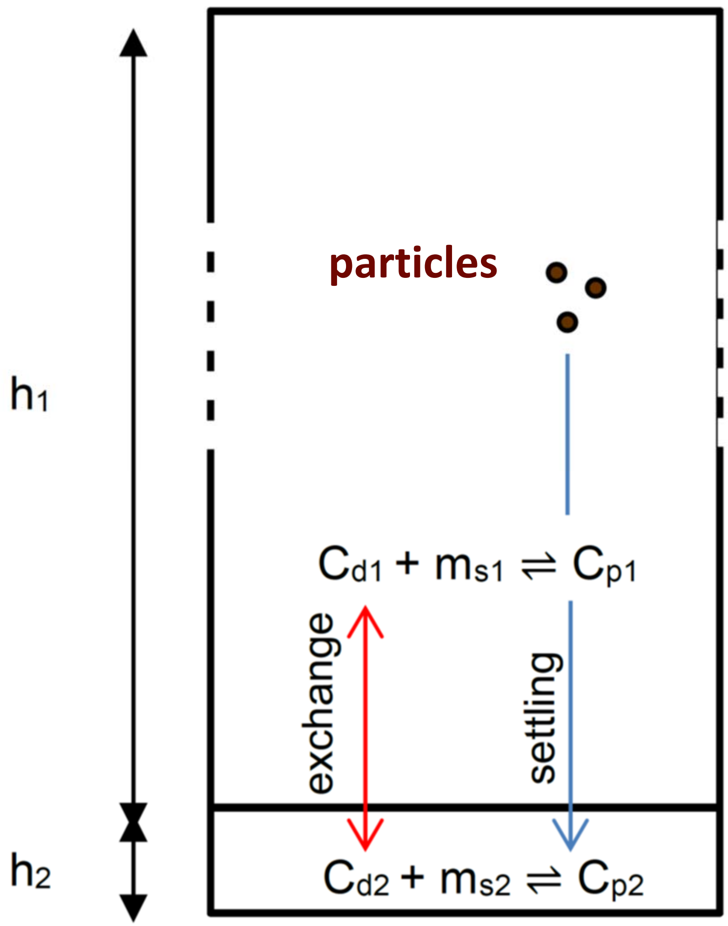
- A Weight of Evidence (WoE) approach has been developed to assess rapid removal of metals from the water column
  - Action item: Develop extension of T/D P that can be used as a standardized approach for hazard classification
- Goal of modeling task: Provide mechanistic insight into important processes controlling metal removal from the water column in T/DP-E experiments performed by CanmetMINING and University of Michigan

Materials and Methods

- CanmetMINING OECD 29 T/DP-E (part 1) experiments
  - 4-days and 28-days in duration
  - pH 6 metal solutions, spike with single addition of 10 g/L of low binding substrate, mix and let settle, collect samples at various times
- Mass balance equations describing mechanisms of metal removal in the T/DP-E experimental systems were developed and solved with a computer program

2-Layer Model

Two-Layer Model



Example Model Equations for Layer 1

Dissolved Metal:

$$\frac{dC_{d1}}{dt} = -\frac{k_{ads}}{\sigma}\left(\frac{C_{d1}}{\phi_1}(m_{s1}\sigma - C_{s1}) - \frac{C_{p1}\sigma}{K_d}\right) + \frac{k_f}{h_1}\left(\frac{C_{d2}}{\phi_2} - \frac{C_{d1}}{\phi_1}\right)$$

Kinetic Adsorption/ Desorption — Dissolved Phase Bulk Exchange

Particulate Metal:

$$\frac{dC_{p1}}{dt} = \frac{k_{ads}}{\sigma}\left(\frac{C_{d1}}{\phi_1}(m_{s1}\sigma - C_{s1}) - \frac{C_{p1}\sigma}{K_d}\right) - \frac{w_s}{h_1}C_{p1}$$

Kinetic Adsorption/ Desorption — Settling

σ, w_s, k_f - Sediment and/or setup specific

k_{ads}, K_d - Metal specific

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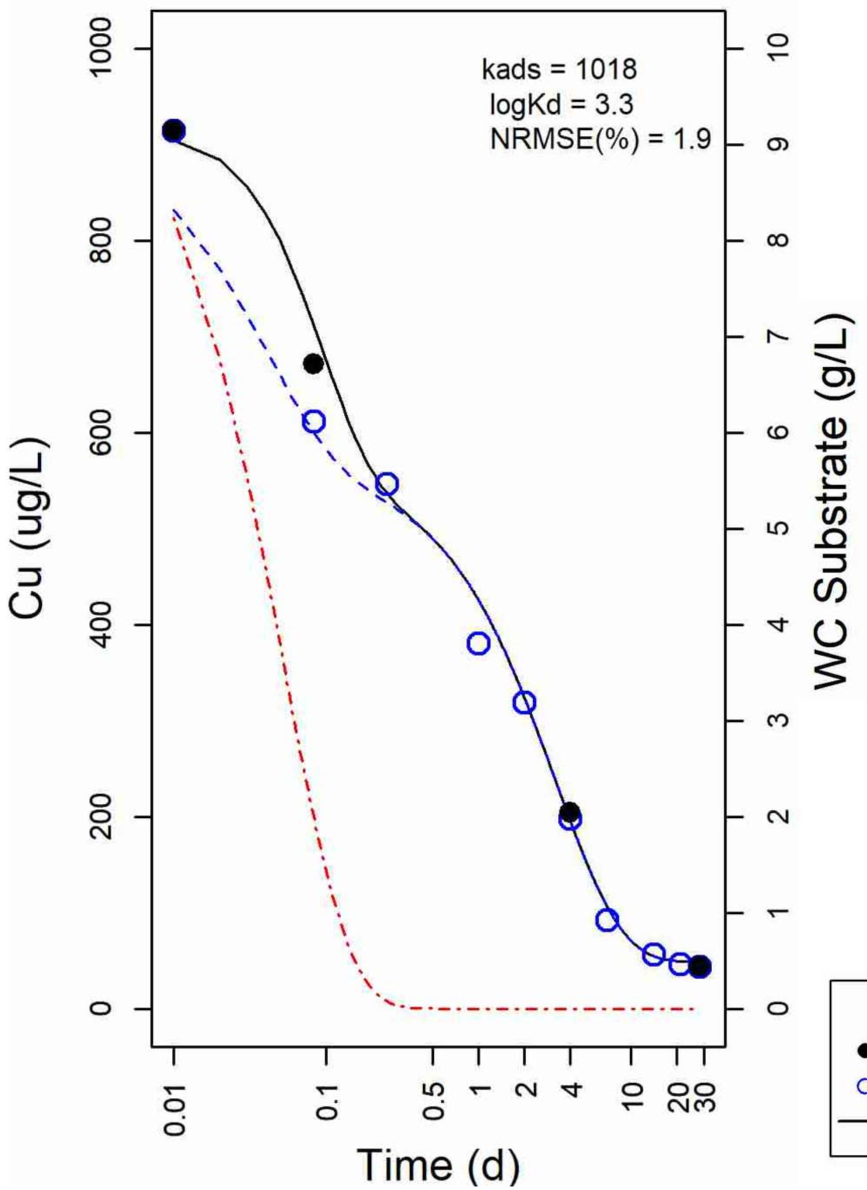
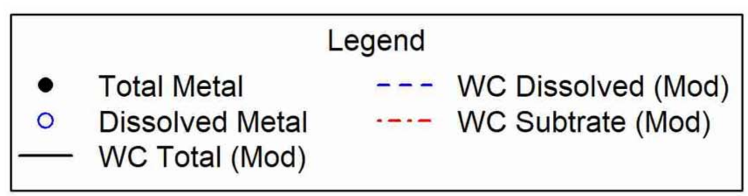
2-Layer Model Results: Copper



- Added substrate particles settle rapidly
- Some metal in the water column adsorbs to particles and settles with them
- Once particles have settled from the water column, dissolved and total metal merge → all water column metal is dissolved
- Metal removal from the water column continues via transport to and direct adsorption by the settled substrate particles



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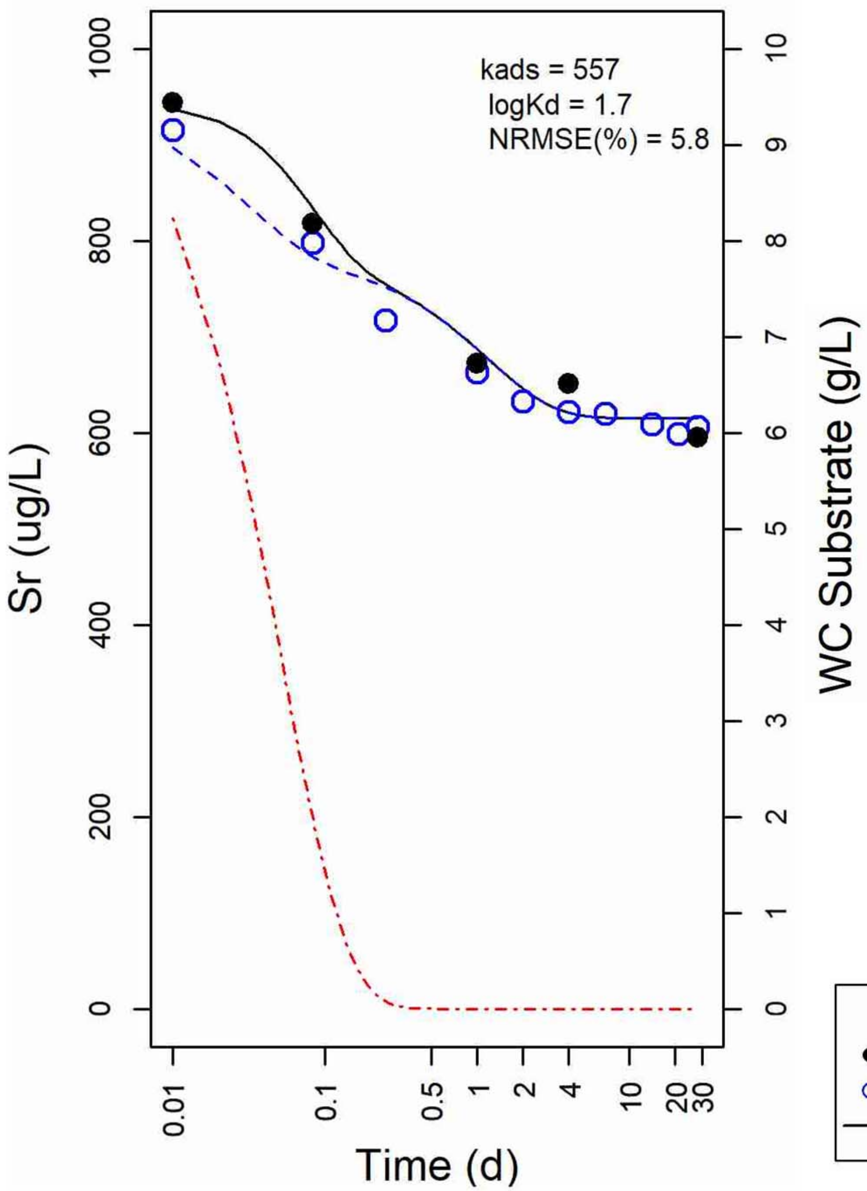
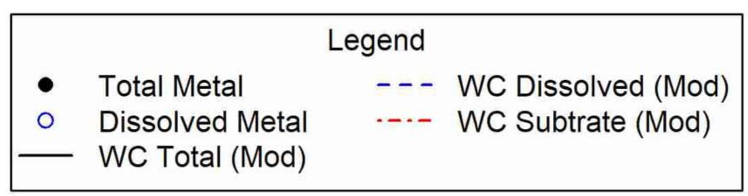
2-Layer Model Results: Strontium



- Same mechanisms described for copper are at play for strontium
- Because of slower adsorption (lower k_{ads}) and lower affinity for the particulate phase (lower K_d), the overall extent of strontium removal is less than copper



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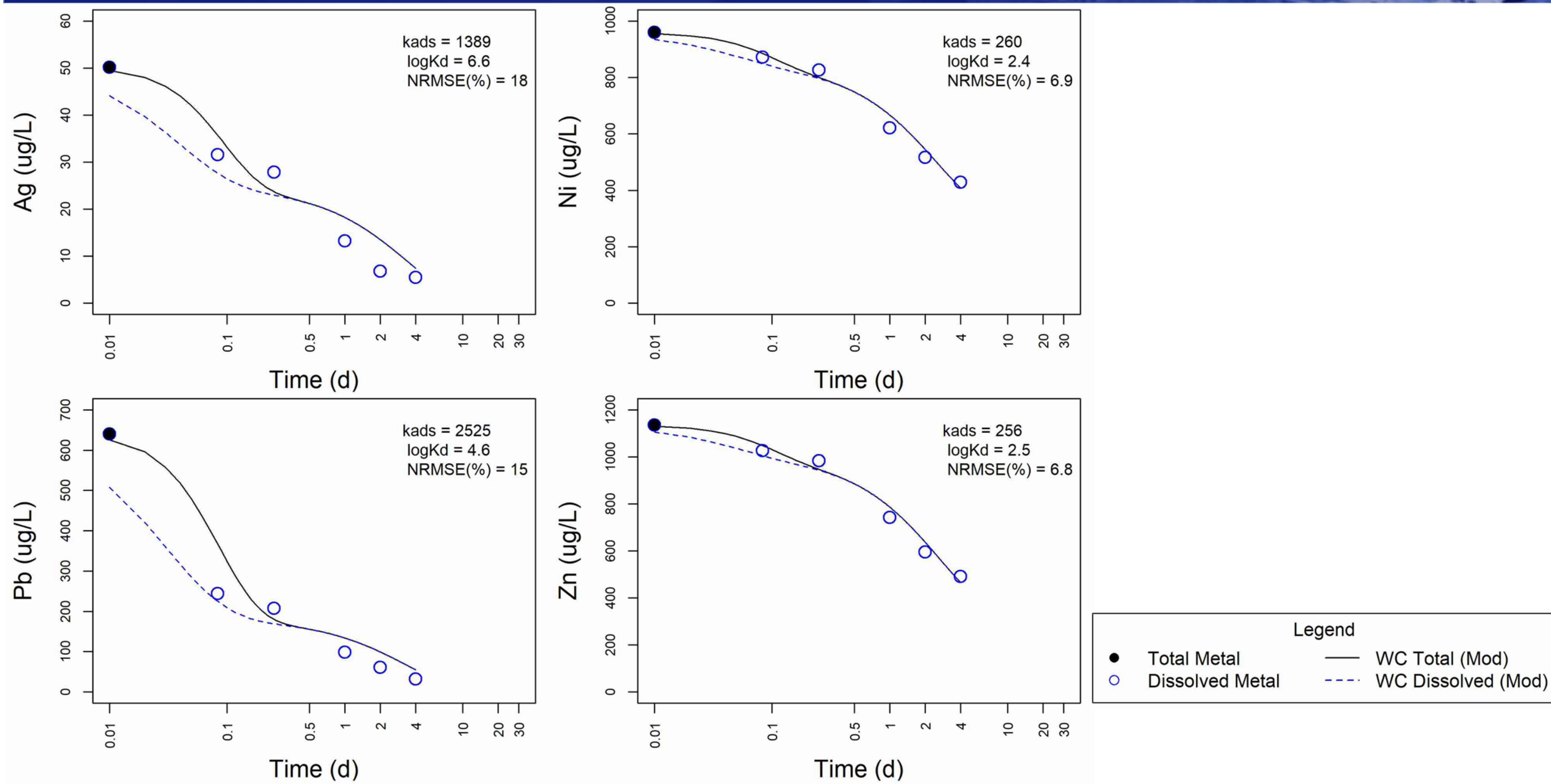
2-Layer Model Results: Other Metals



- The model was able to fit data for Ag, Pb, Ni, and Zn using same settling velocity and bulk exchange coefficient as for Cu and Sr
  - Only metal-specific k_{ads} and K_d parameters were varied to fit data

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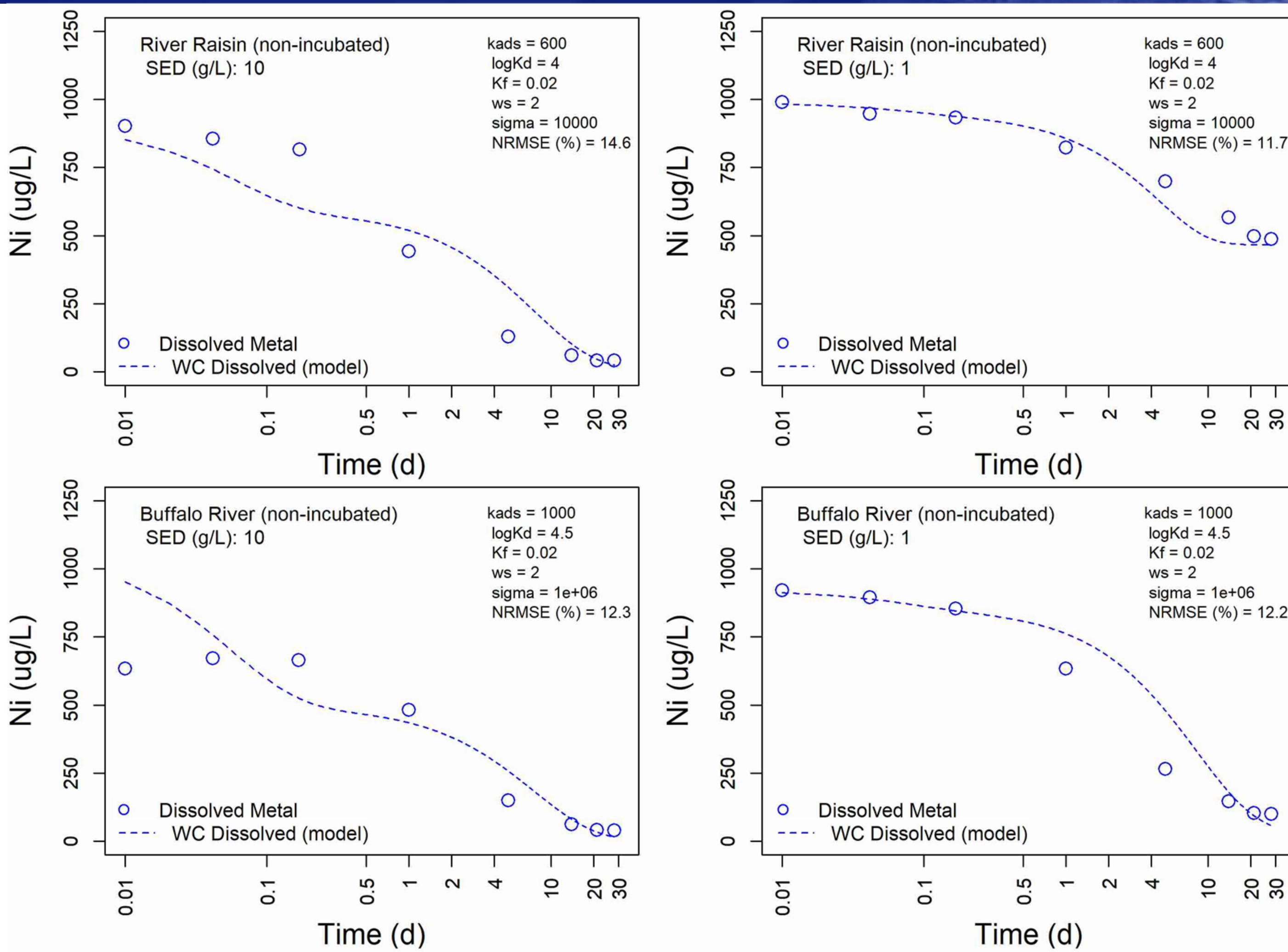
2-Layer Model Results: University of Michigan T/DP-E Experiments with Ni



The model was able to fit T/DP-E data from a different laboratory with different substrate types/loadings

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Impact of Substrate Loading

- CANMET - OECD 29 T/DP-E (part 1) used a single addition of substrate at 10 g/L
  - Questions were raised whether substrate loading affected removal
- Goal: Use calibrated model to assess additional substrate loading scenarios including 10 additions of 1 g/L (instead of 1 addition of 10 g/L)
  - Alternate loading yields same substrate concentration in Layer 2 at day 28

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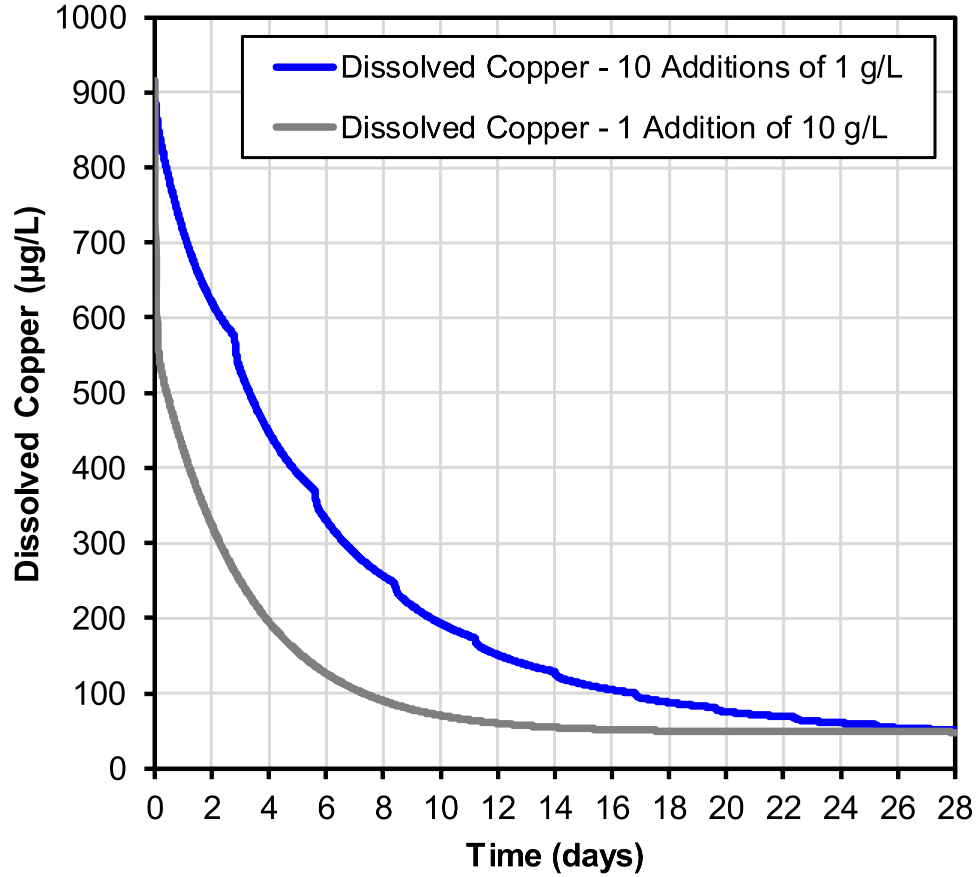
Substrate Loading Results: Copper

1 addition of 10 g/L

- Removal via sedimentation followed by removal via transport to and direct adsorption by settled substrate particles

10 additions of 1 g/L

- Removal by sedimentation is limited; direct adsorption by settled substrate still important



Slower removal but same overall removal extent at day 28

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Concluding Remarks

- The OECD 29 T/DP-E (part 1) experimental data could be successfully modeled
- The mechanistic model highlights important processes occurring in the T/DP-E including:
  1. kinetic adsorption of dissolved metals to substrate particles;
  2. settling of particles with adsorbed metals; and
  3. dissolved metal transport to and direct adsorption by the settled particles

Concluding Remarks

- Calibrated metal-specific parameters (e.g., Kd) follow expected trends based on intrinsic properties of the individual metals
  - e.g., Cu compared to Sr
- Alternative substrate loading scenarios: ***rate*** of removal was impacted but overall ***extent*** of removal was the same

Questions?