PFAS in Soil: Considering Leaching to Groundwater

NEWMOA Webinar

July 29, 2020

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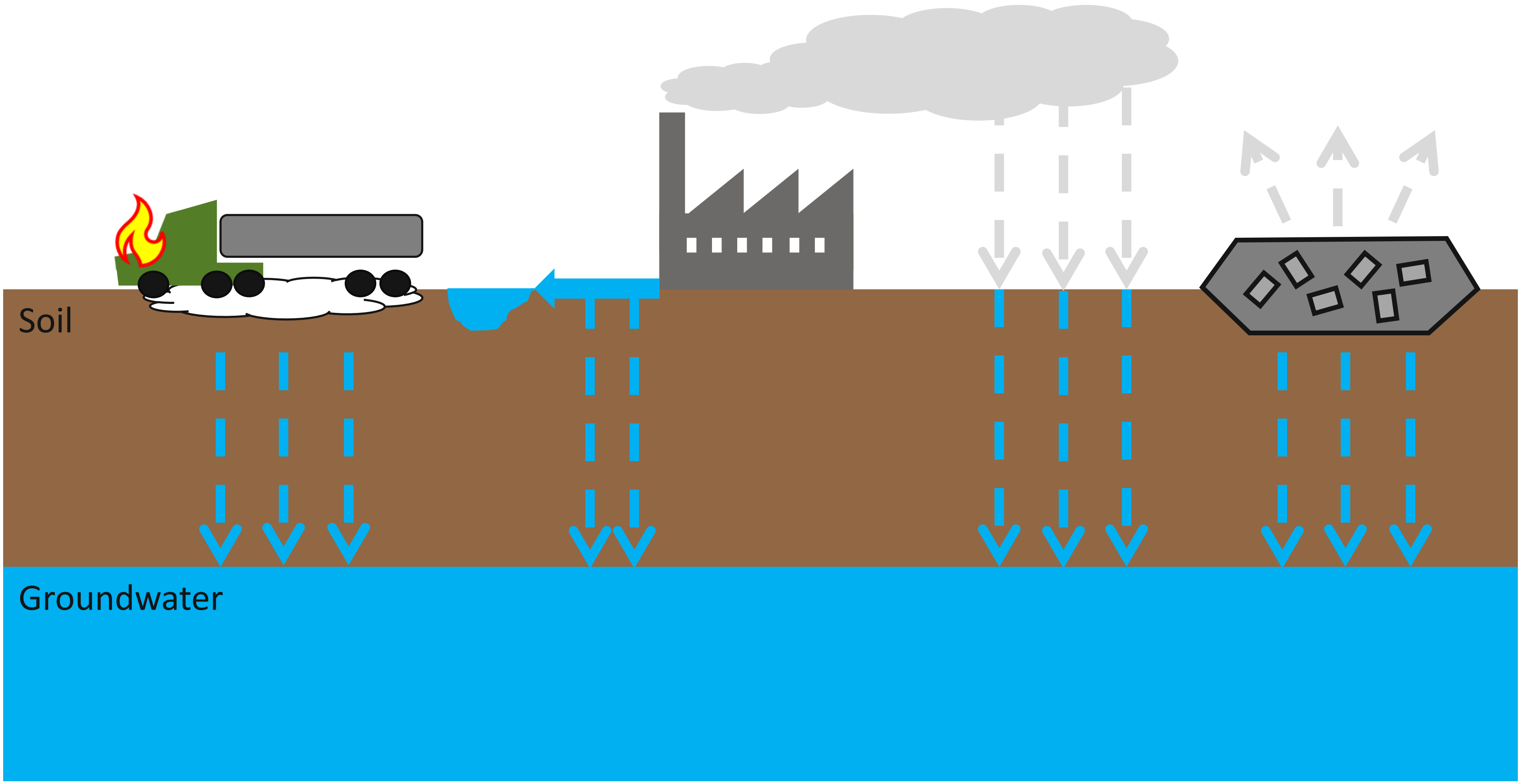
Outline

- Fundamentals and background
- Leaching-based screening values
- Anthropogenic background
- Screening approaches

The focus of this presentation is on PFOA and PFOS. PFAS, including precursors to PFOA and PFOS, have widely ranging chemistries and properties.

Soil is a key media for many releases



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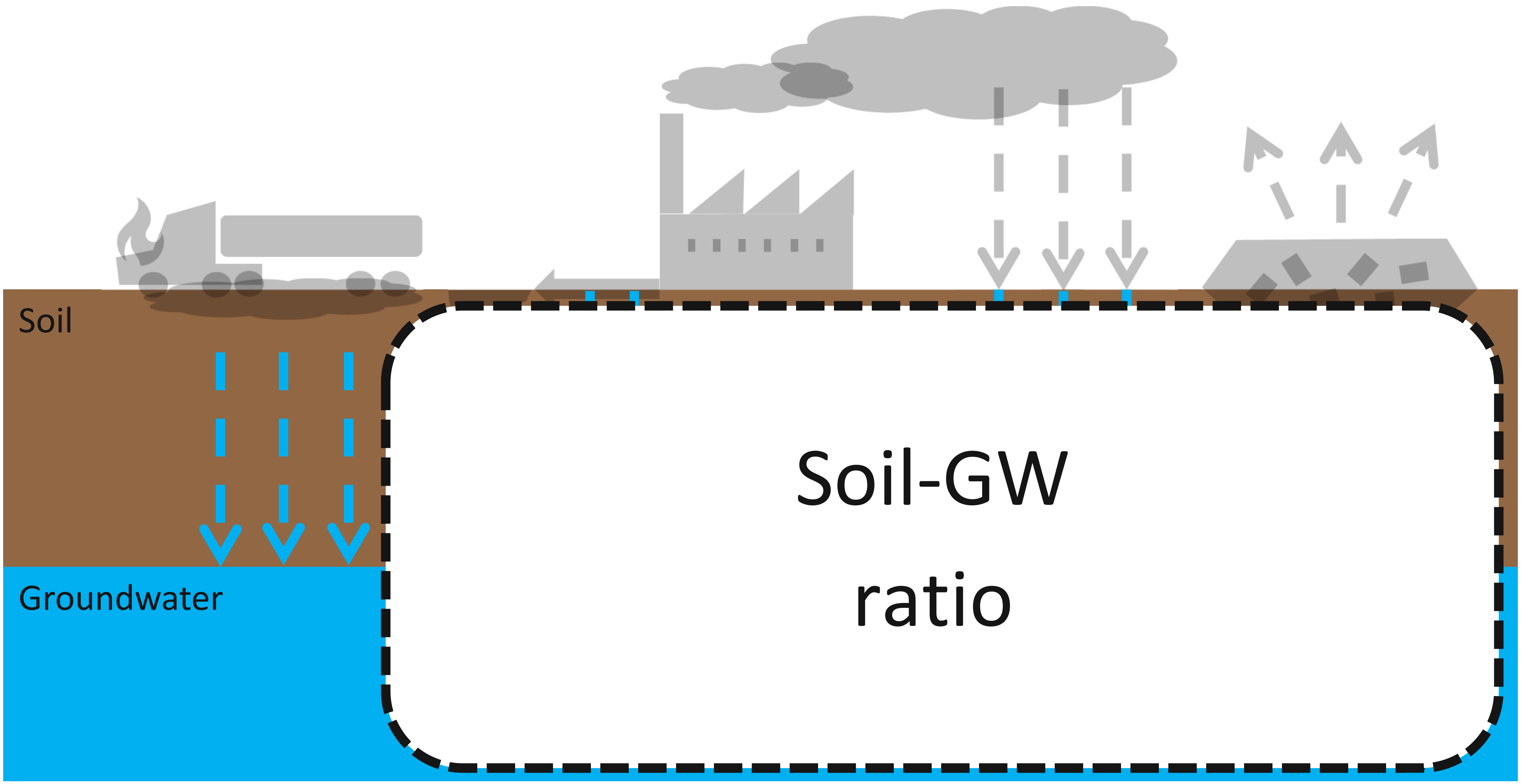

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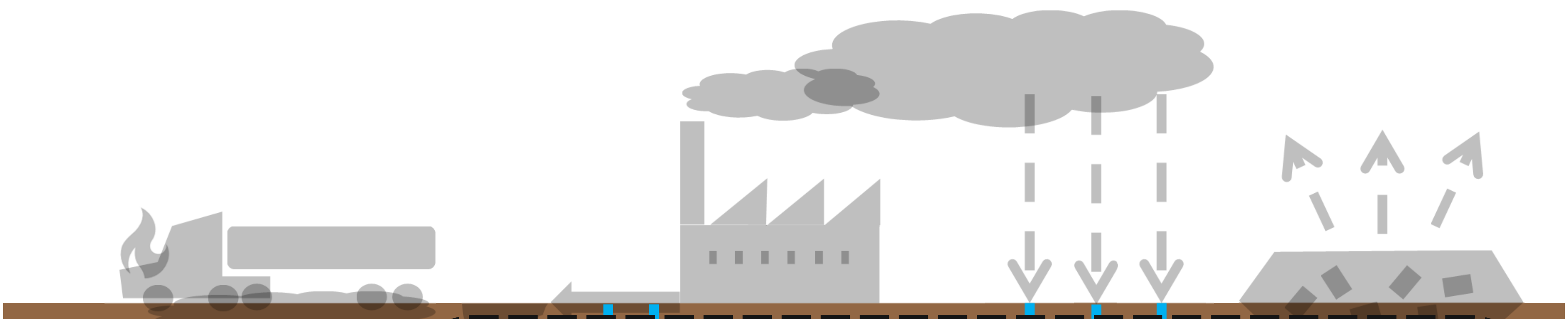
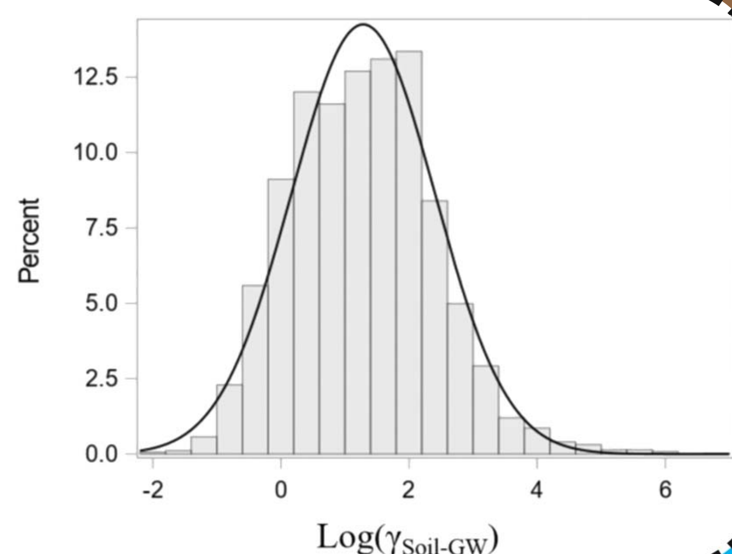


U.S. Air Force sites histogram of Soil-GW Ratios[1]

- 324 AFFF sites
- Source-zone soil and GW
- 8 orders of magnitude variation



1. *Anderson, Adamson, and Stroo. (2019). Journal of Contaminant Hydrology, 220 59-65: https://doi.org/10.1016/j.jconhyd.2018.11.011*

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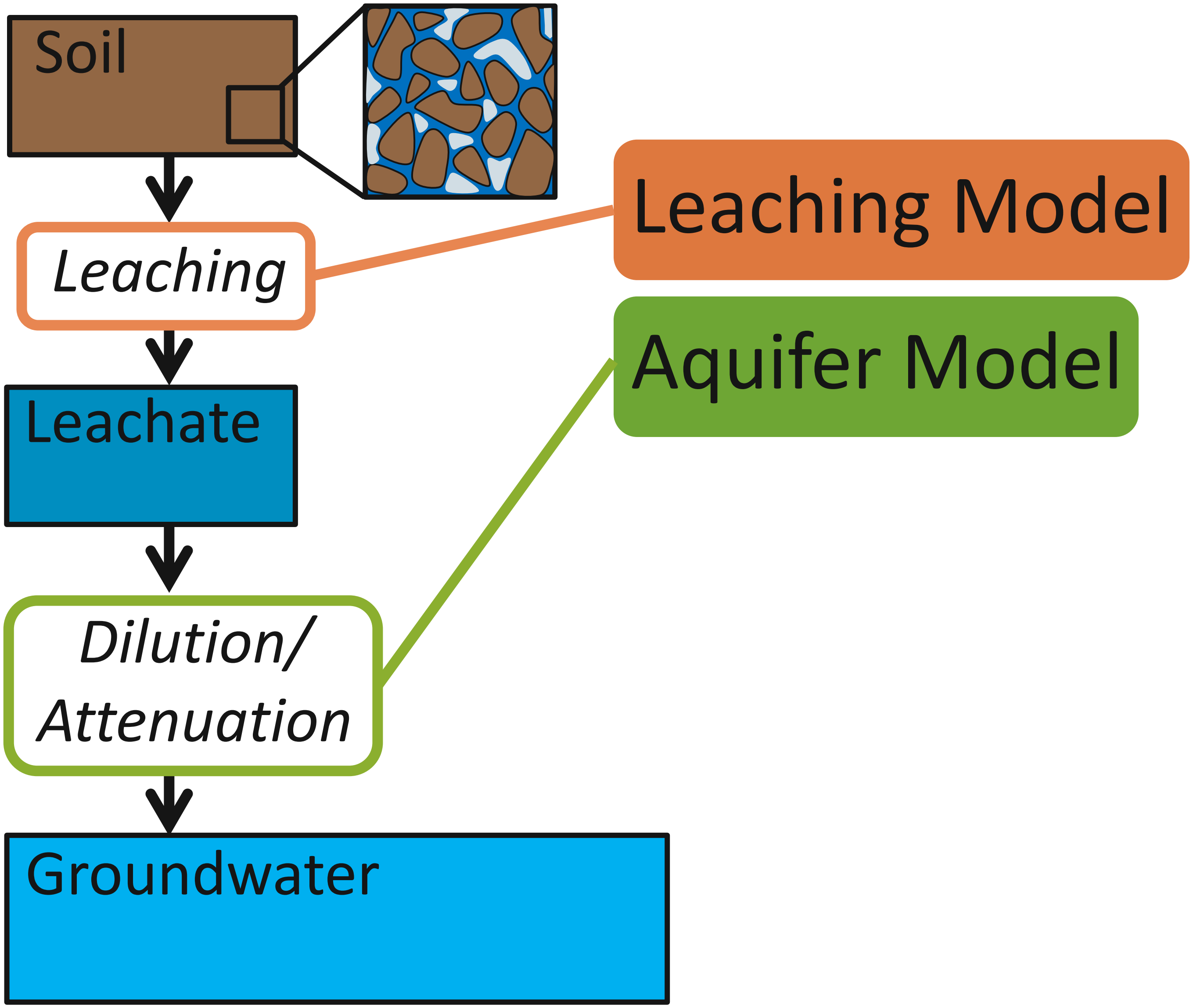
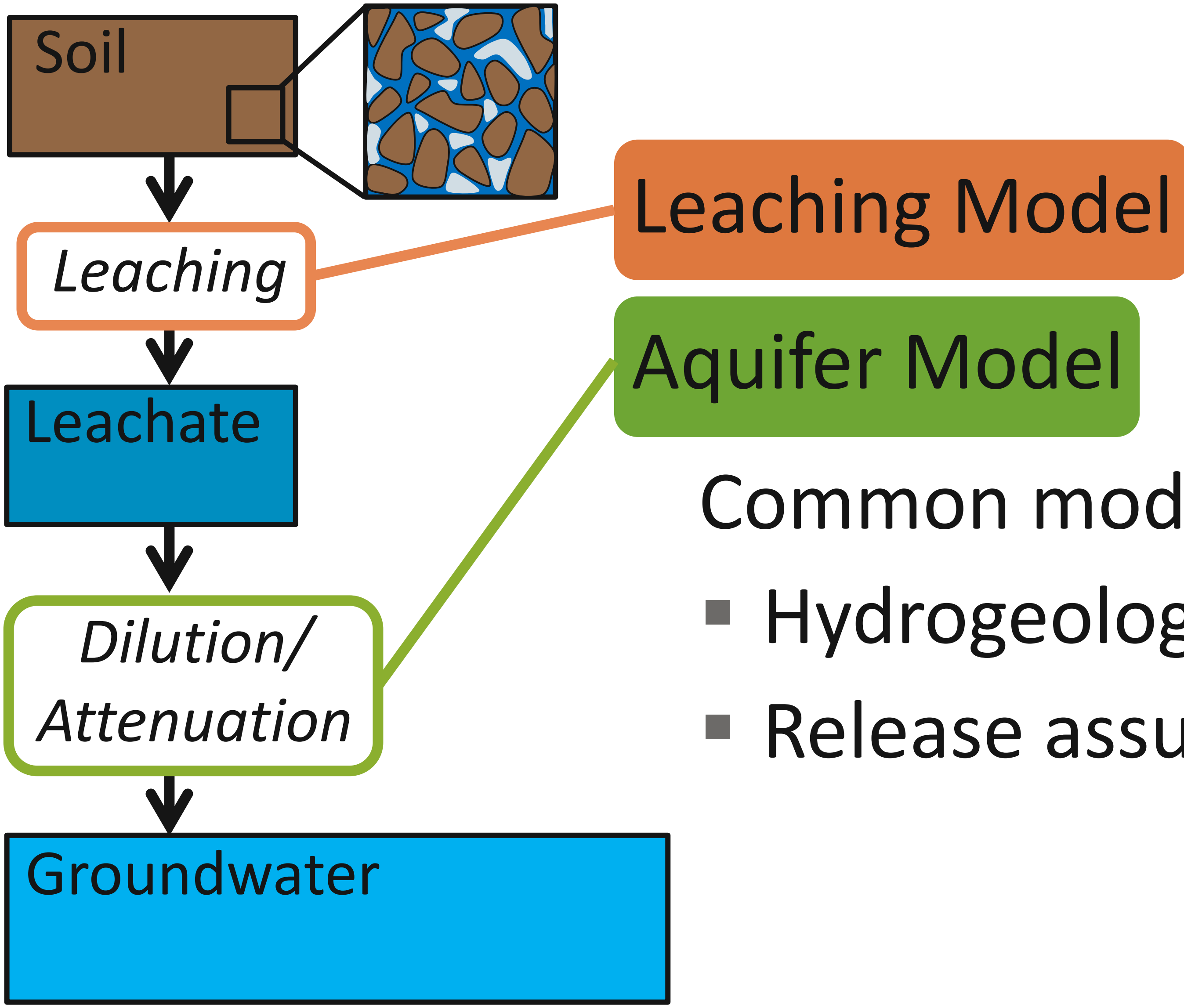
Leaching Models



Leaching Models



Common model inputs

- Hydrogeology
- Release assumptions

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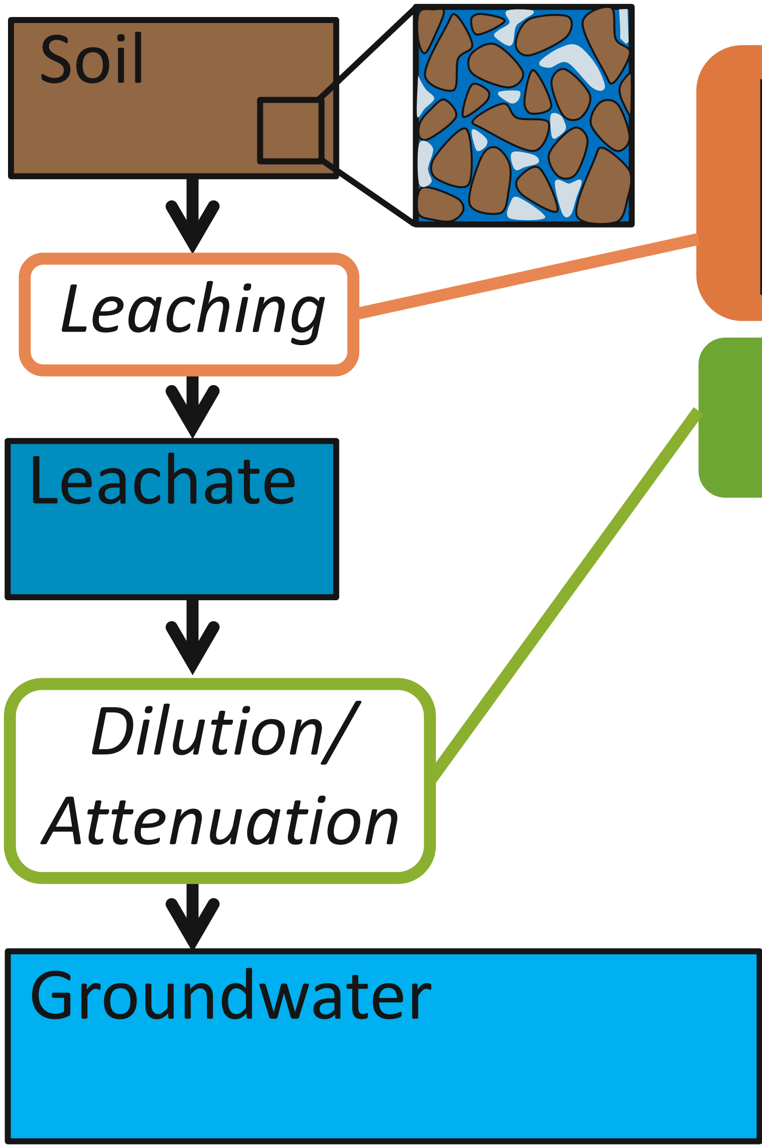
USEPA Soil Screening Level



$$\left[K_d + \frac{\theta_W + \theta_a H'}{\rho_b}\right]^*$$

$$DAF$$

Variables

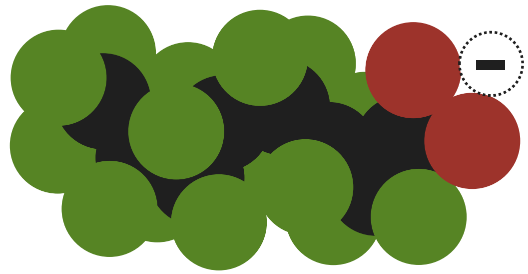
- **Chemical-specific K_d**
- Henry's Law H'
- Water-filled soil porosity
- Dry soil bulk density
- Dilution/attenuation factor

*Simplified by assuming nonionizing compound. Details: https://semspub.epa.gov/work/HQ/175232.pdf

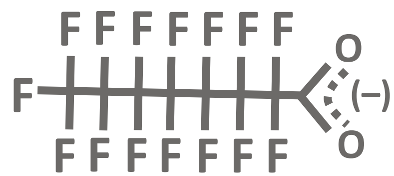
PFOA Chemical Structure

Fluorocarbon tail

- Hydrophobic
- Lipophobic

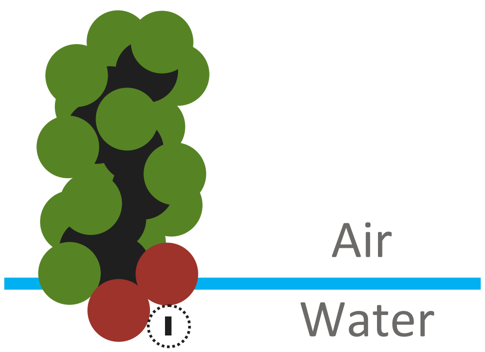


Ionic skeletal and 3D models



Functional group

- Hydrophilic
  - High solubility
  - Low volatility



Surfactant

Branched isomer models

Throughout the presentation, PFOA molecules are illustrated. These illustrations are not to scale, and numerous other details are not shown, including counterions, water molecules, and solids molecules.

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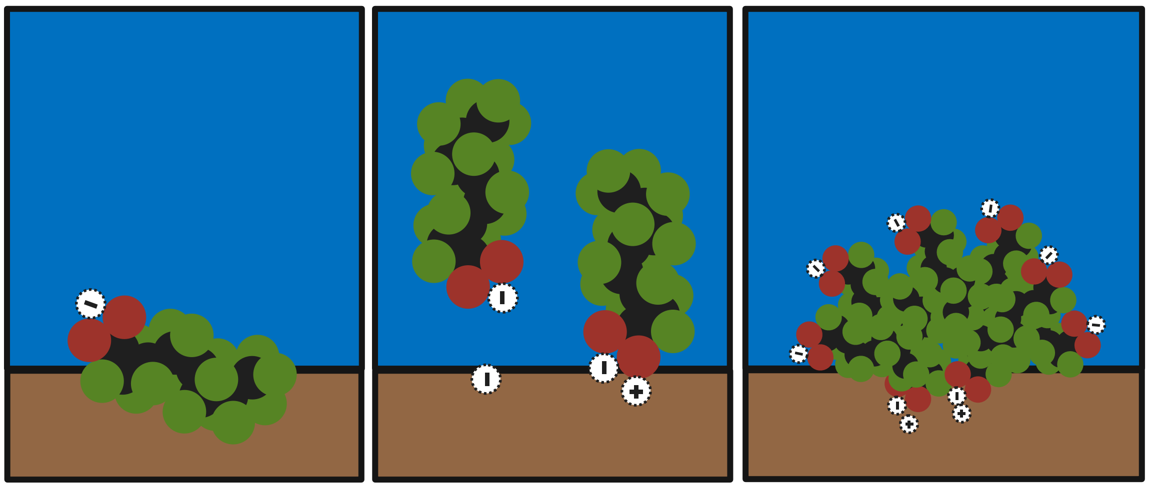
General Phase Partitioning

Simplified model

- Three soil phases
- Described with partition coefficients
- Steady-state, equilibrium

constant for known or assumed conditions

PFOA/PFOS Phase Partitioning



Hydrophobic sorption

Electrostatic interactions

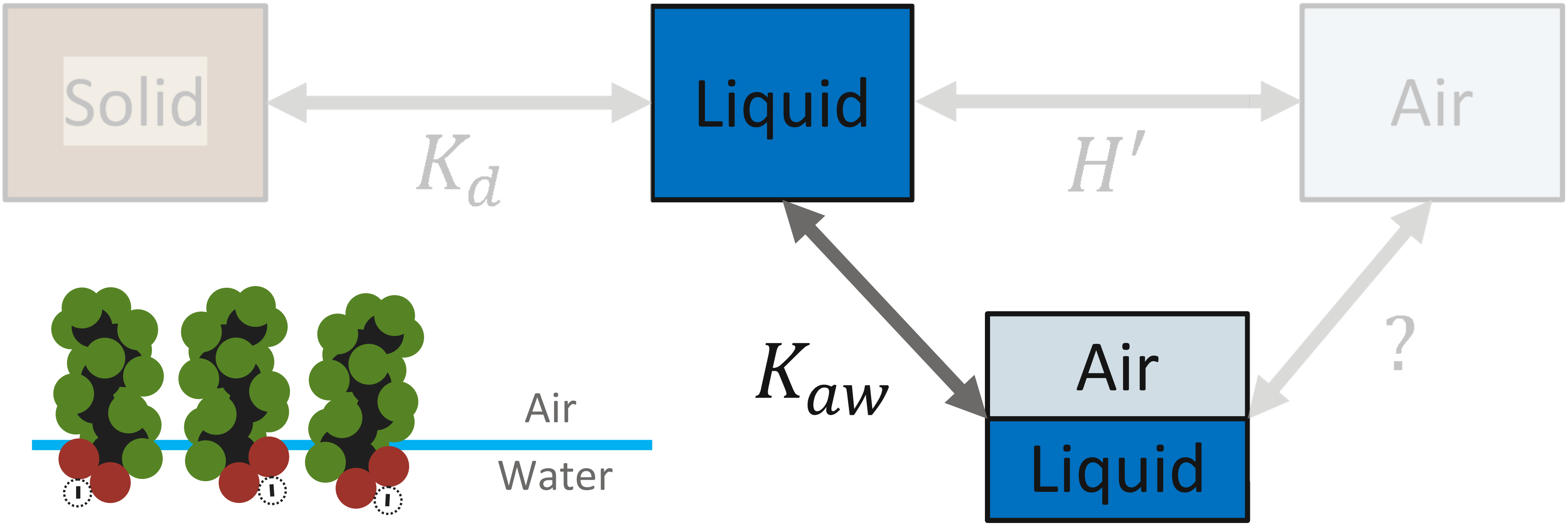
Surfactant behavior (at higher conc.)

Li et al. (2018)[1]

- Not just $K_d = K_{oc} \times f_{oc}$

1. Li, Oliver, and Kookana. (2018). Science of the Total Environment, 628-629 110-120: https://doi.org/10.1016/j.scitotenv.2018.01.167

PFOA/PFOS Phase Partitioning



Brusseau et al. (2019)[1] and Guo et al. (2020)[2]

- >80% total retention
- Greater retention in sand vs. finer-grains

Dr. Linda Abriola SERDP/ESTCP air-water and NAPL-water interface partitioning presentation: https://www.youtube.com/user/SERDPESTCP

1. *Brusseau, Yan, Van Glubt, Wang, Chen, Lyu, Dungan, Carroll, Holguin. (2019). Water Research, 148 41-50: https://doi.org/10.1016/j.watres.2018.10.035*
2. *Guo, Zeng, and Brusseau. (2020). Water Resources Research, 57: https://doi.org/10.1029/2019WR026667*

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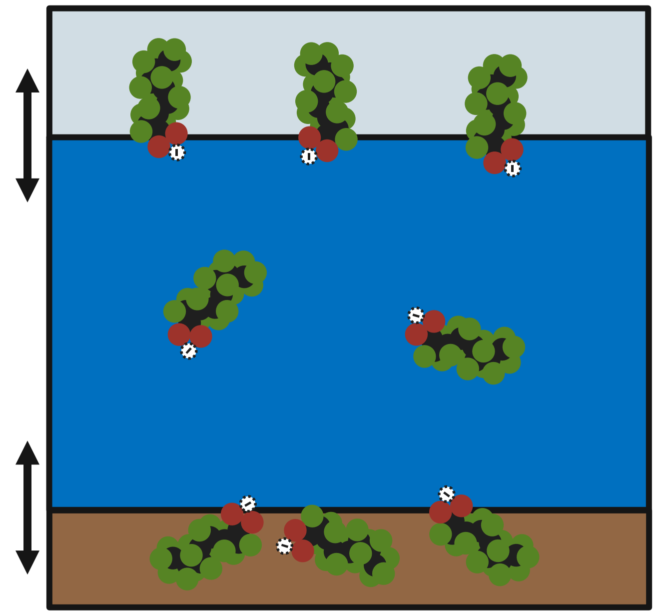
PFOA/PFOS Phase Partitioning

Key Factors:

- Soil and water chem, e.g.
  - Organic carbon
  - Co-contaminants
  - pH & surface charge
  - Major ions
- PFOA/PFOS concentration — *nonlinear*
- Previous conditions — *hysteresis*



Not to scale

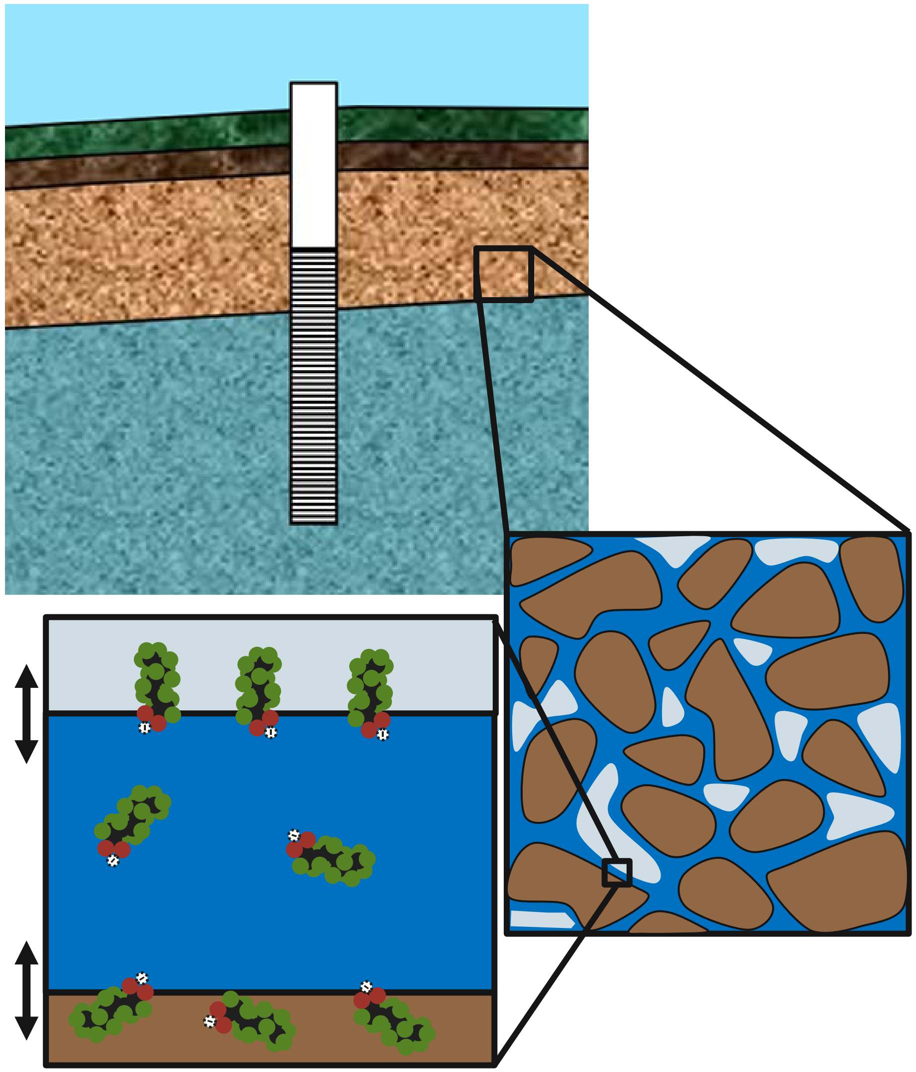
For more information, see ITRC PFAS Technical and Regulatory Guidance Document: https://pfas-1.itrcweb.org/5-environmental-fate-and-transport-processes/#5_2

Field Conditions Phase Partitioning

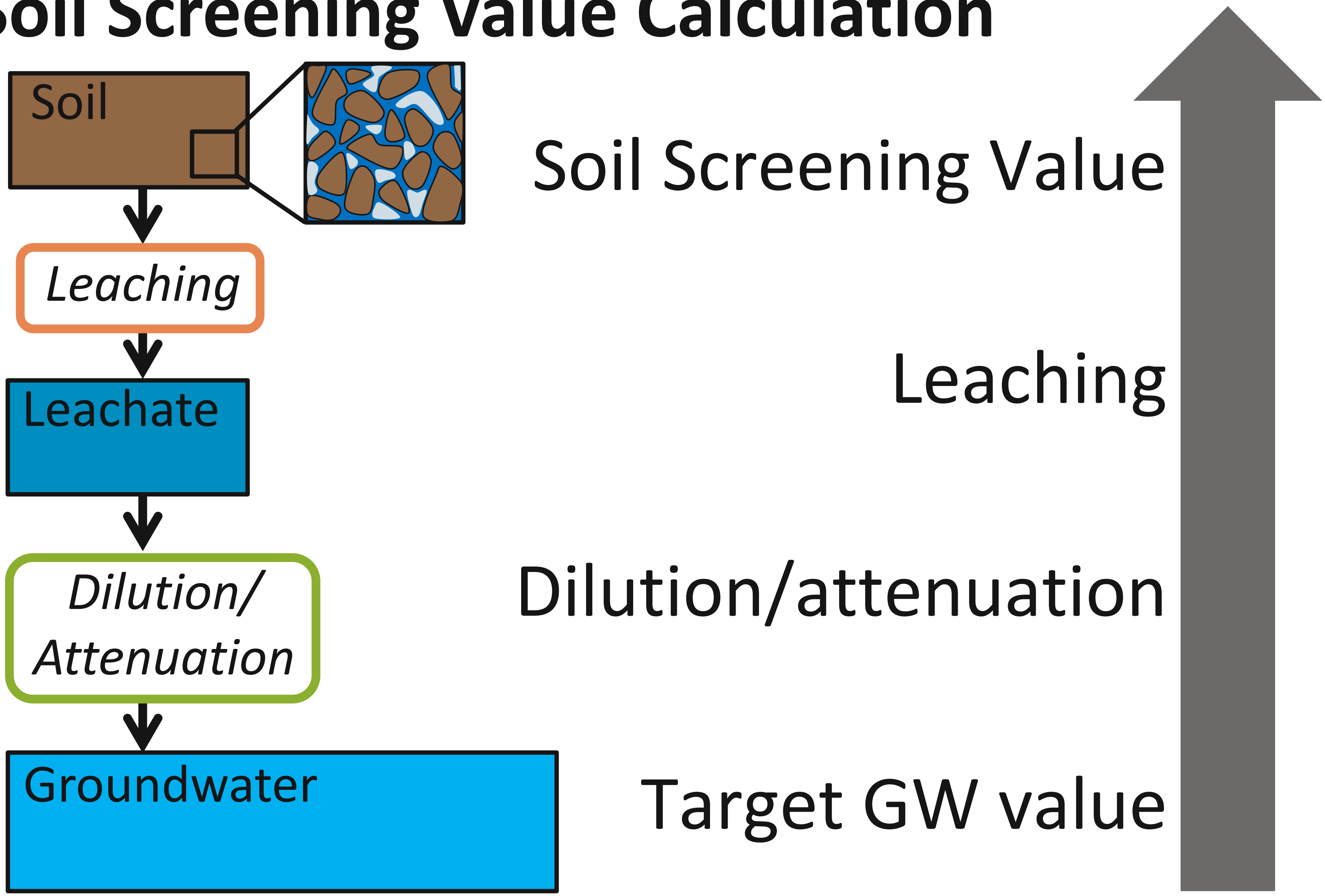
- Hydraulics
  - Microscale
  - Macroscale
- Kinetics/mass transfer

Field conditions:

- *Approach* equilibrium
- Complex/variable
  - Heterogeneous
  - Cannot replicate in a lab
- Delicate
  - Disturbed by sampling



Soil Screening Value Calculation



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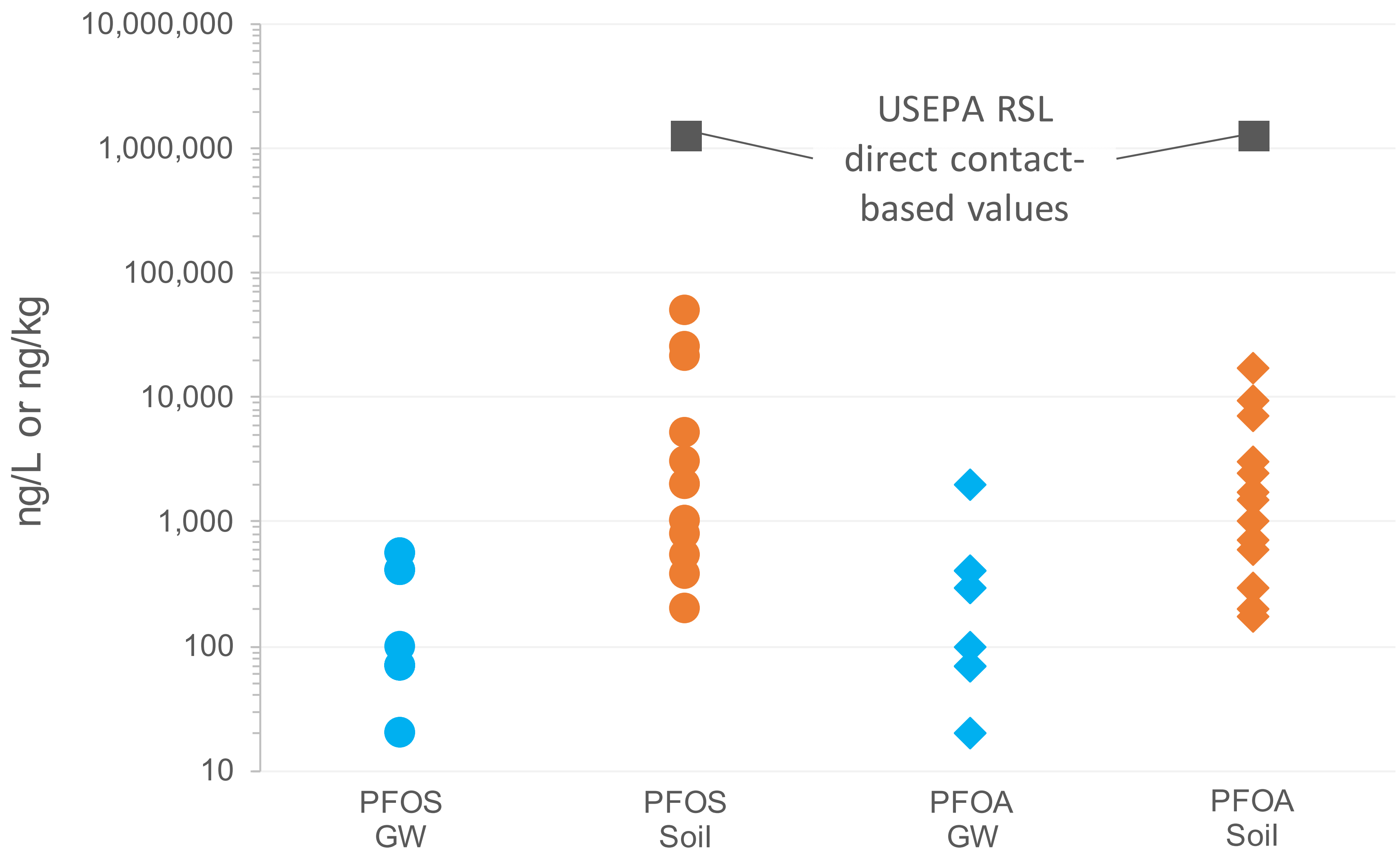
GW and Soil Leaching Values



1. "GW Values" and "Soil to GW Protection Values" were largely obtained from the ITRC fact sheet spreadsheet updated June 2020 (https://pfas-1.itrcweb.org/fact-sheets/). Some proposed or draft values, which may be on-hold or now replaced with updated values, are also included.
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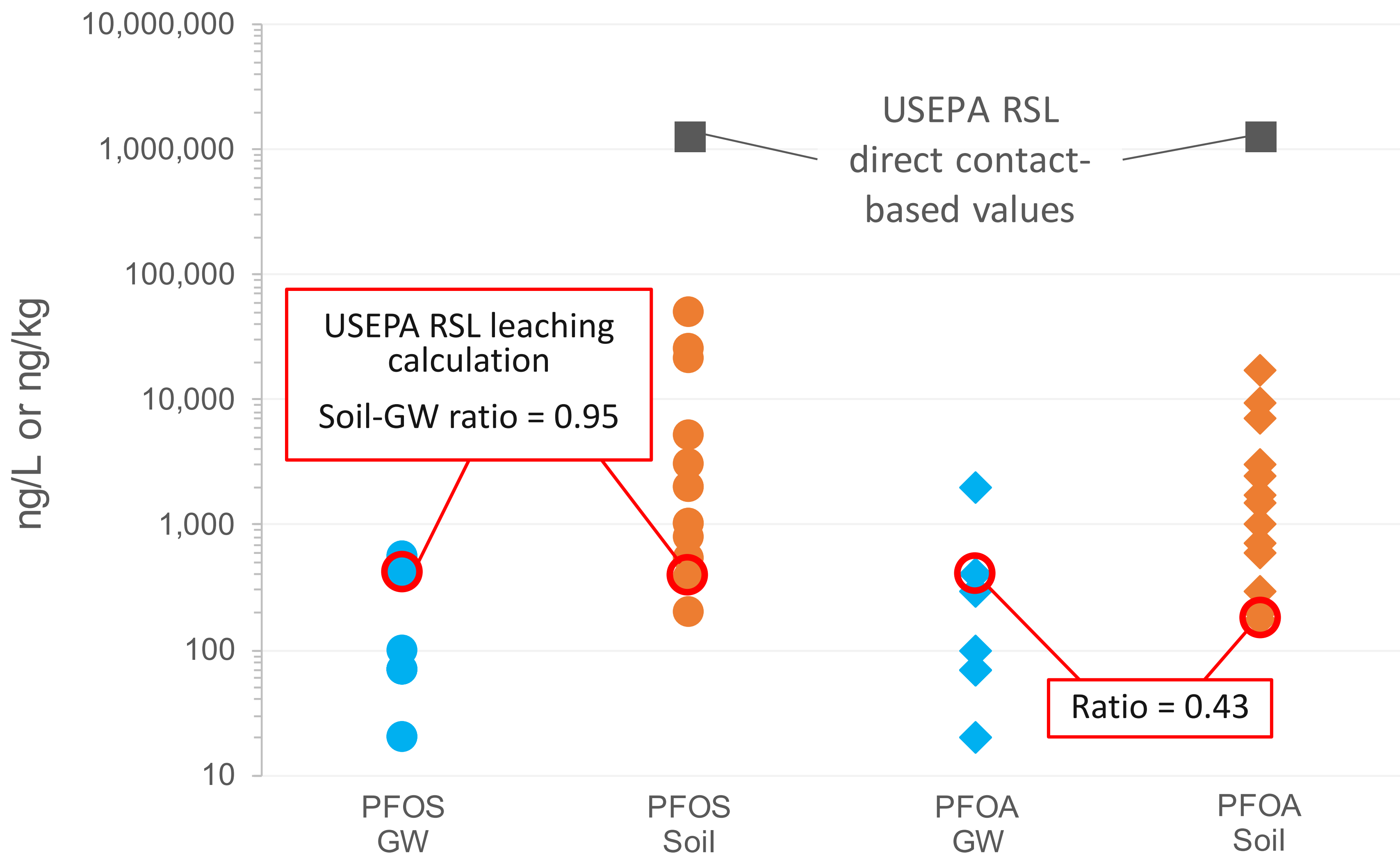
GW and Soil Leaching Values



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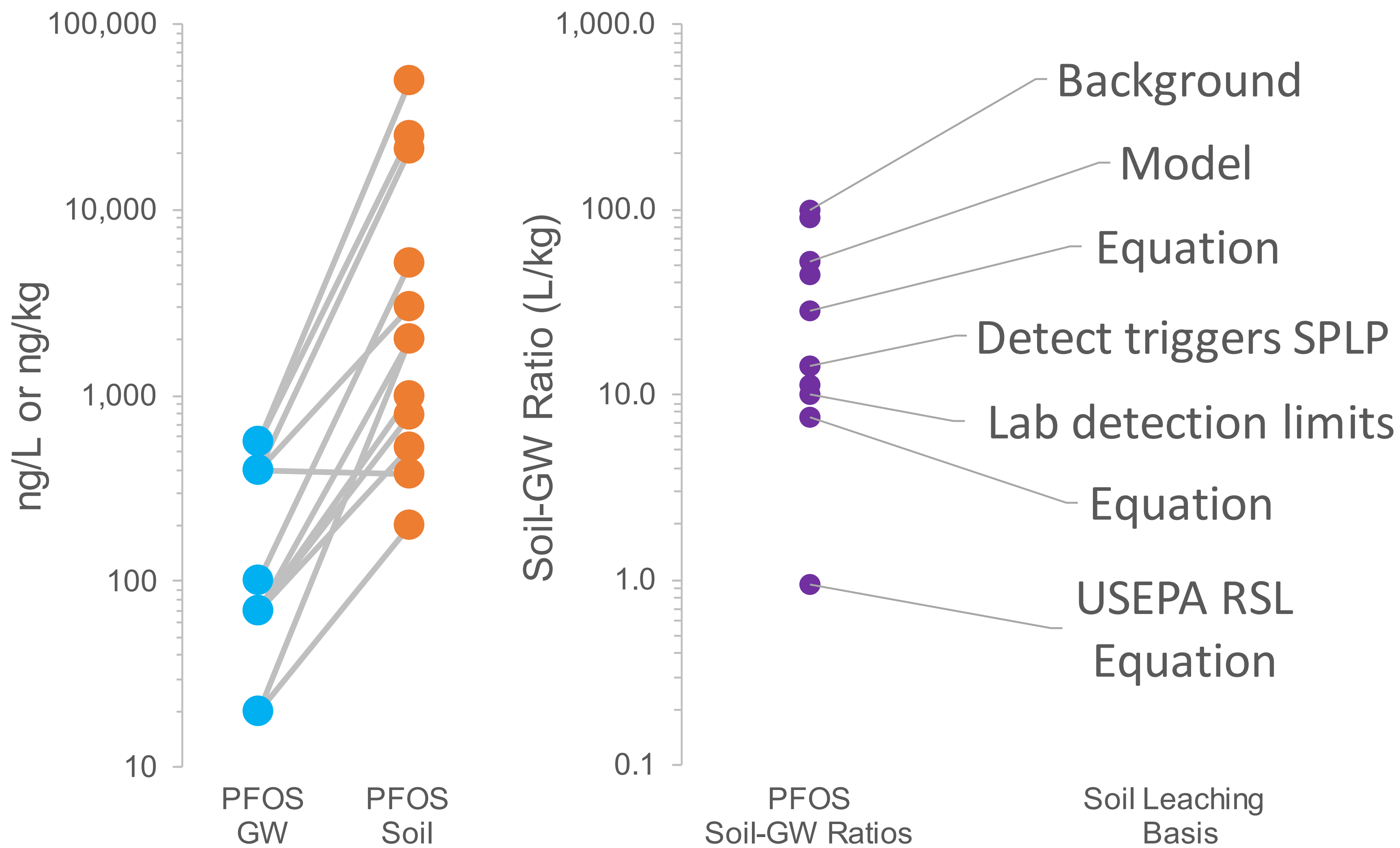
PFOS Soil Leaching Soil-GW Ratios



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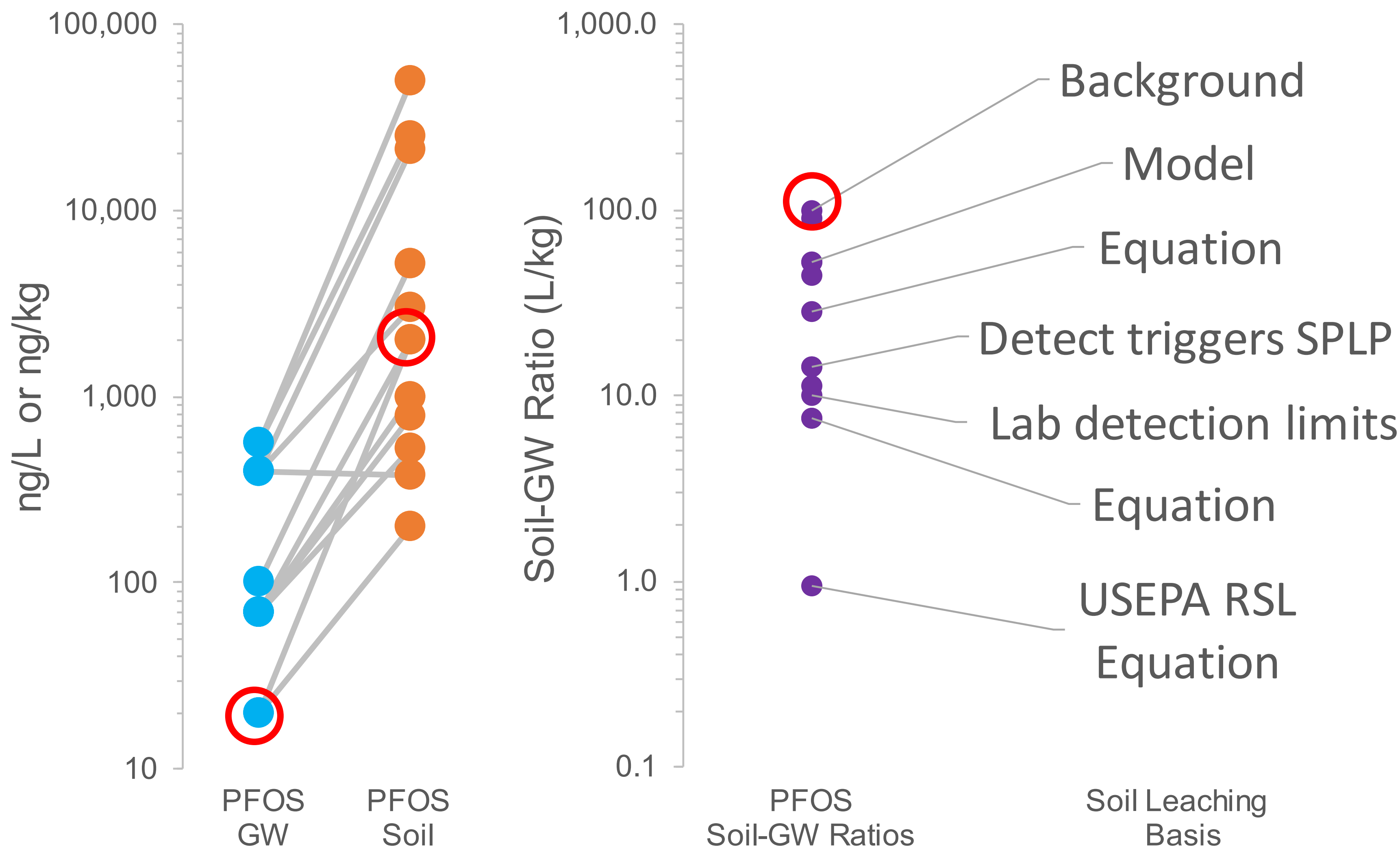

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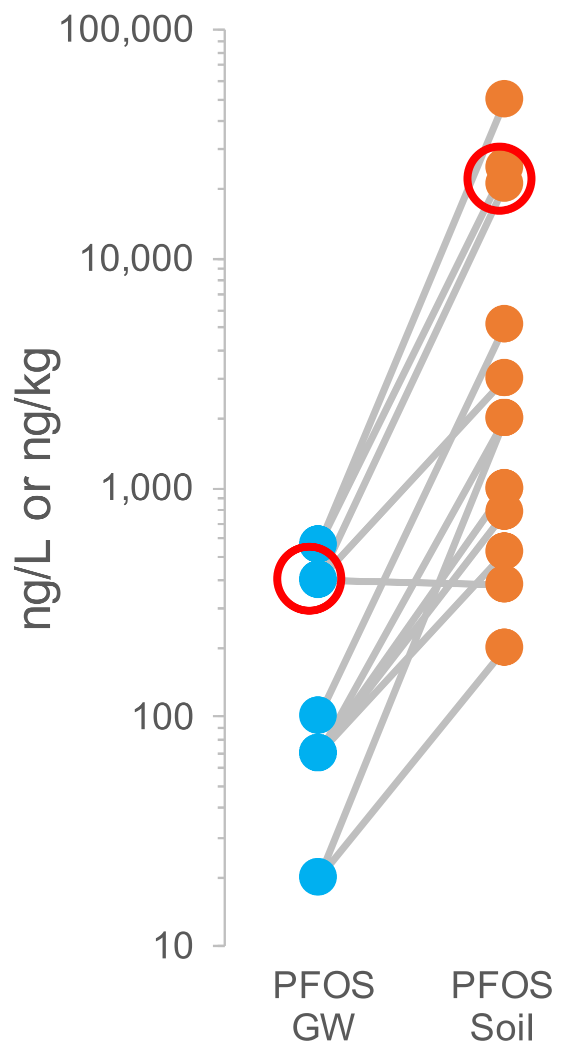

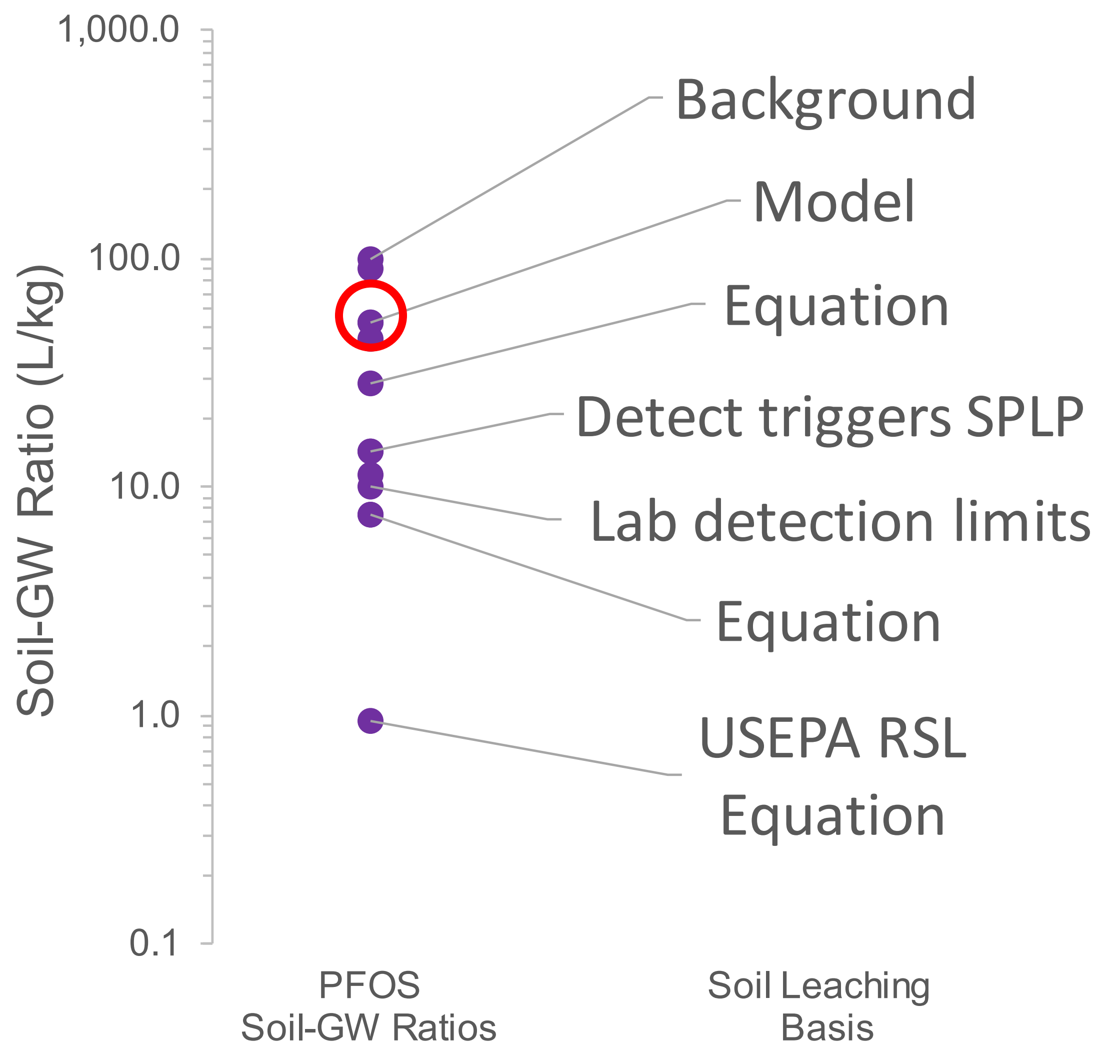

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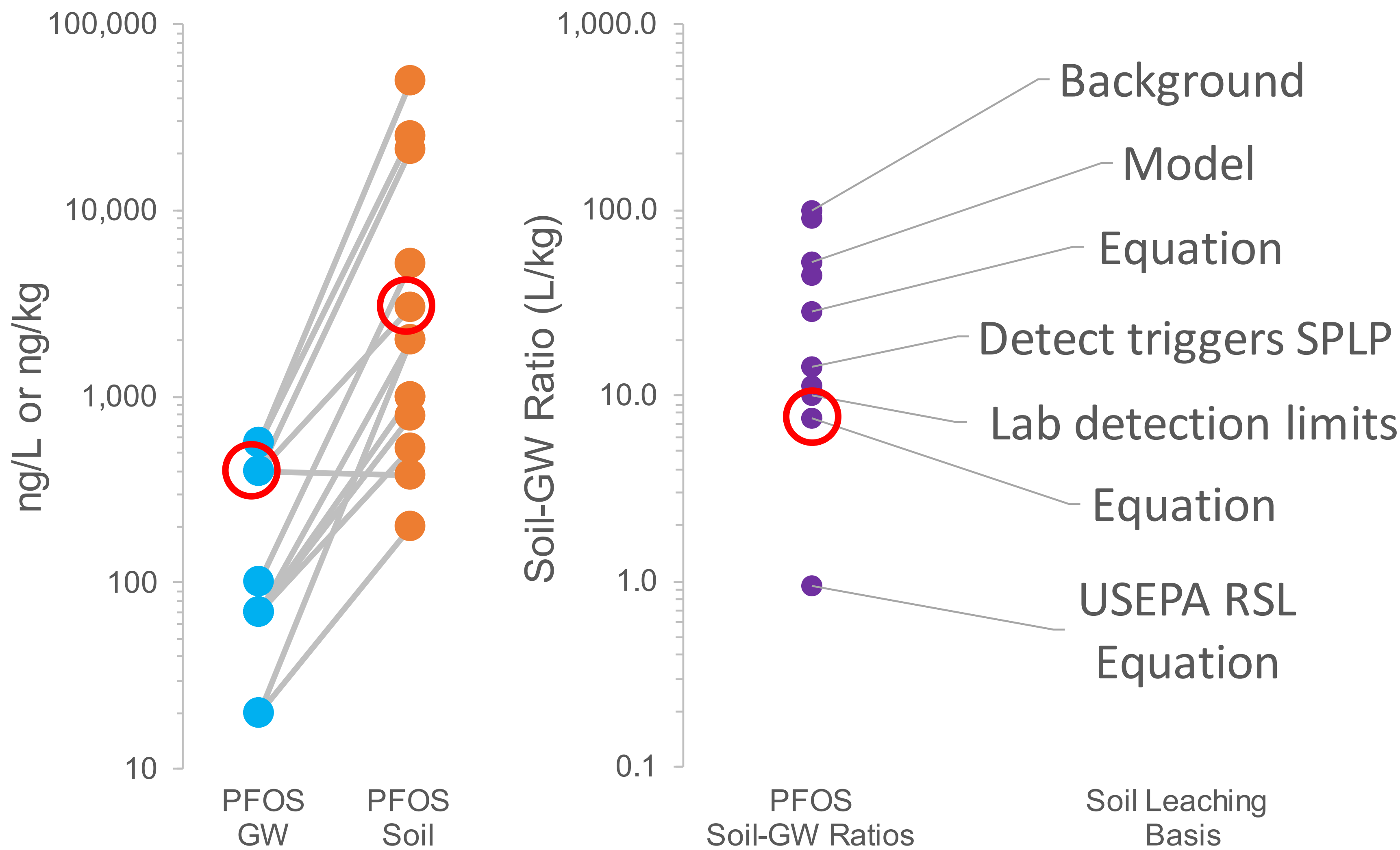

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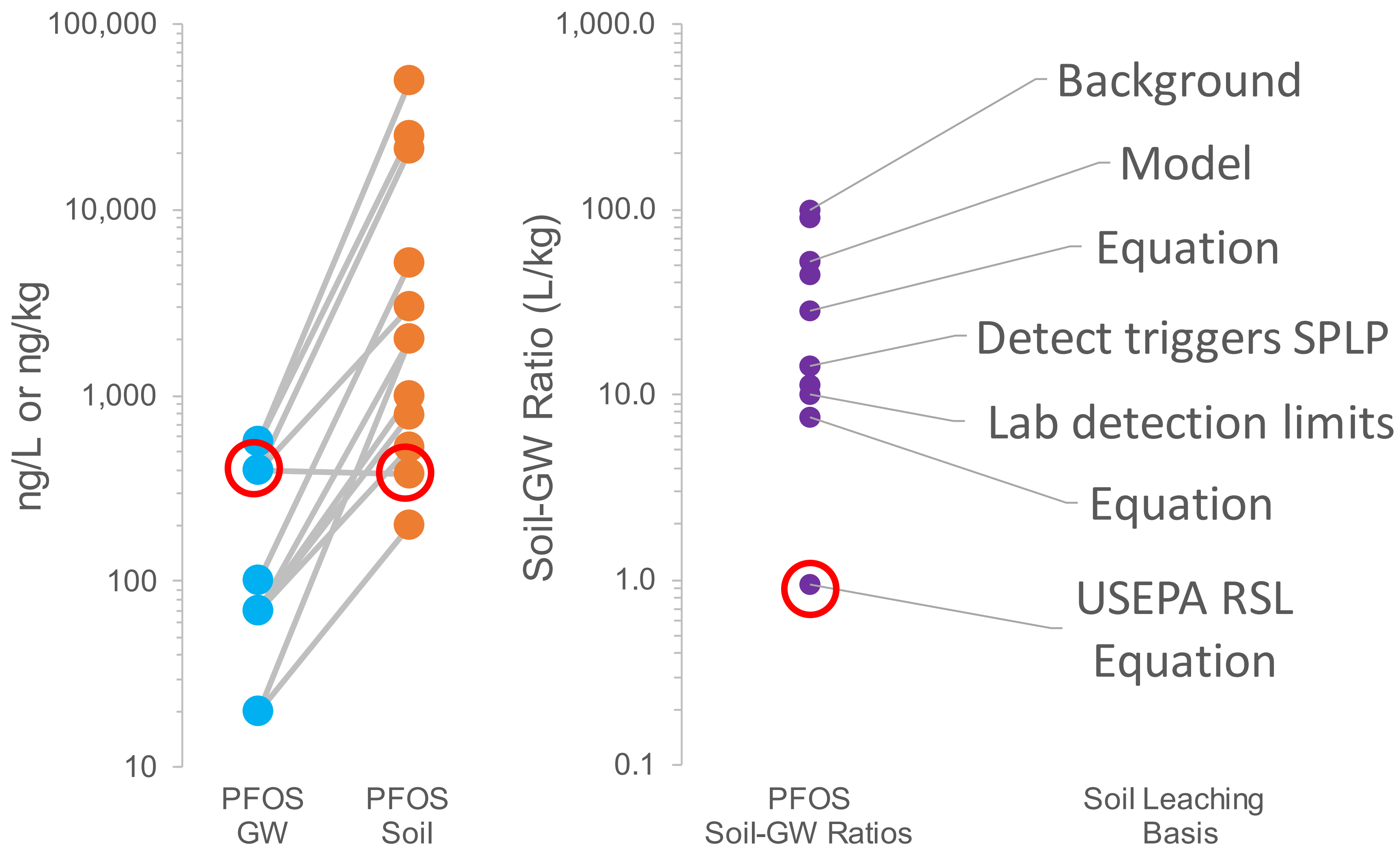

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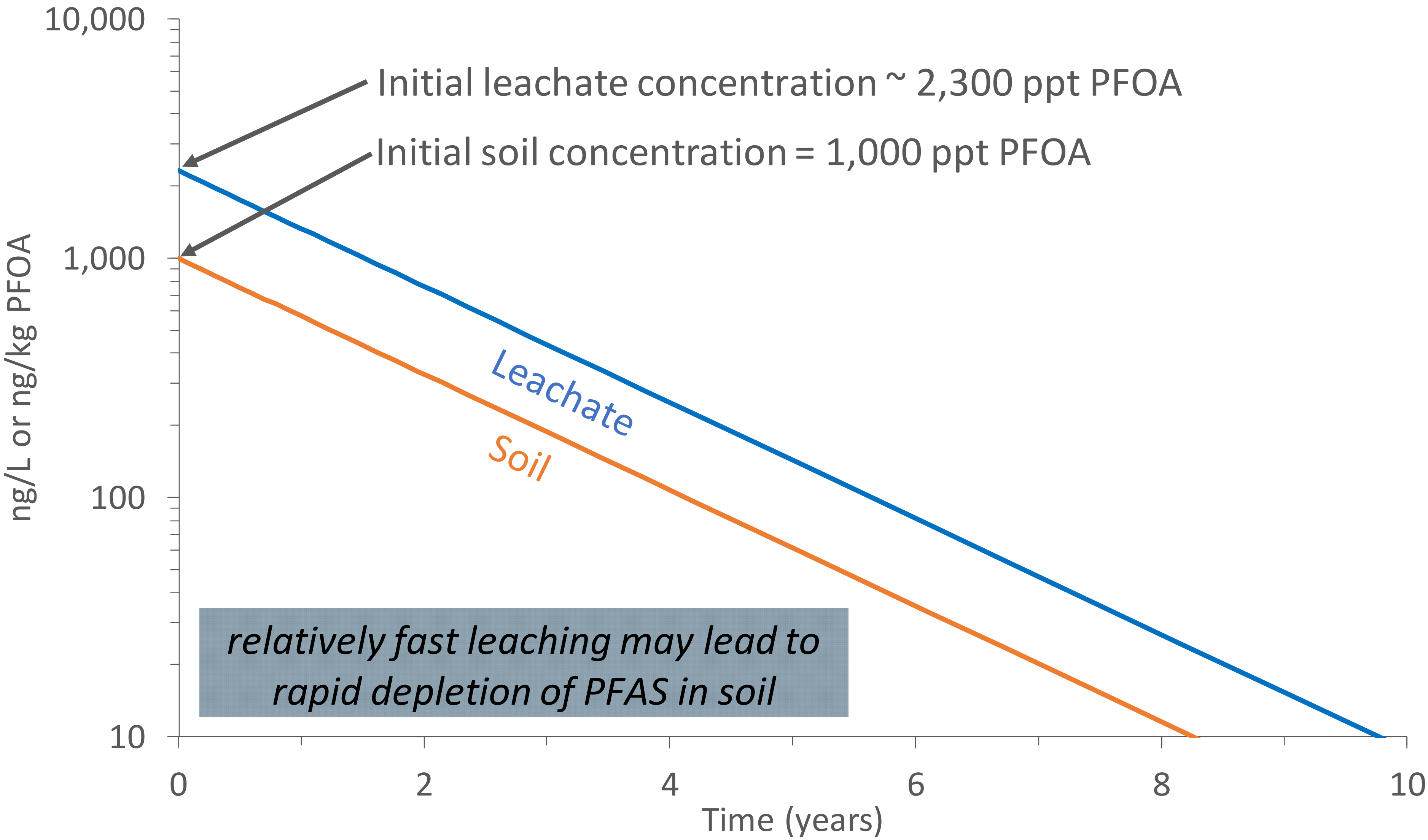
Depletion Model Check



Basic model assumptions include: *1st-order, USEPA RSL leaching; complete mixing, steady-state hydraulics; 0.5 meters of soil, 0.18 meters per year infiltration*

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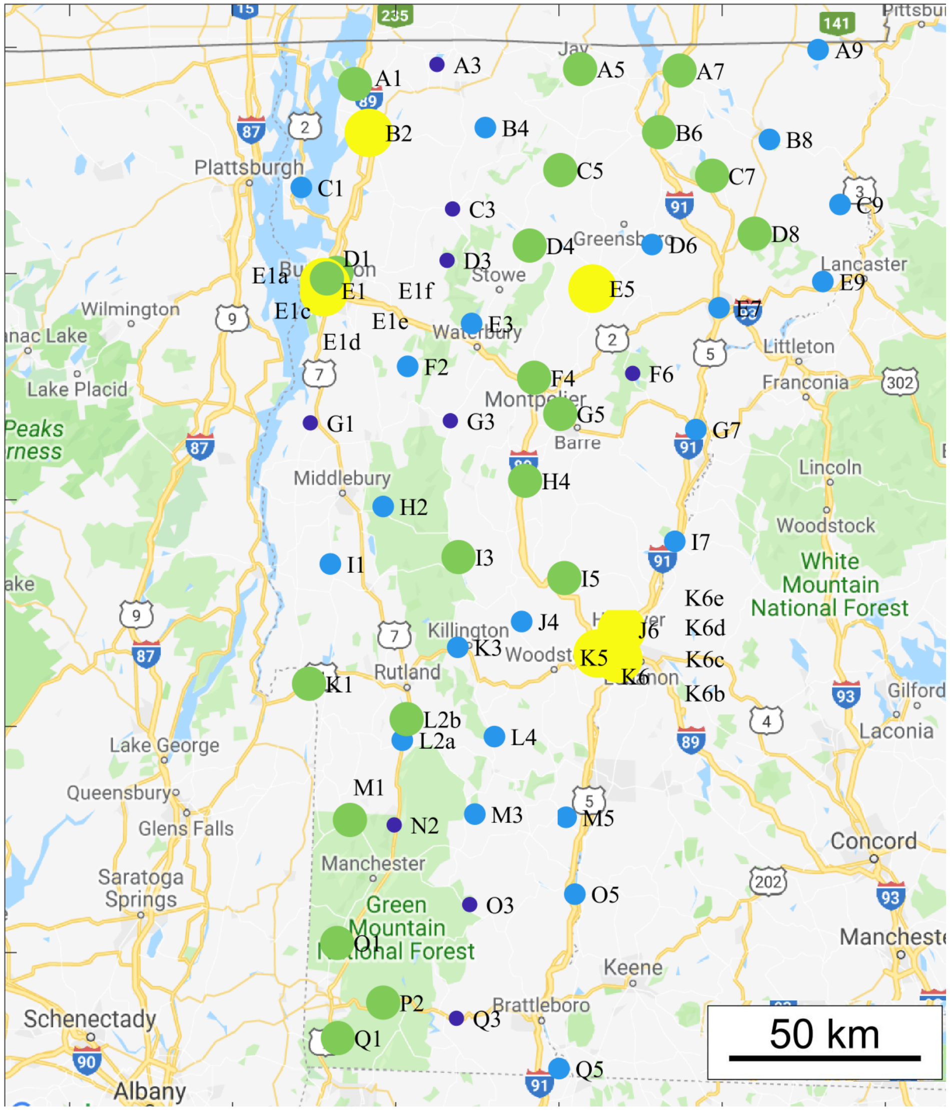
PFAS in Background Vermont Shallow Soils



- 66 locations, 0-6" depth
- Parks, grass areas, forests
- 13 PFCAs & 4 PFSAs

ΣPFAS (ng/kg)

- >5,000 [n = 8]
- 2,000-5,000 [n = 23]
- 1,000-2,000 [n = 25
- <1,000 [n = 10]

Source, University of Vermont and Sanborn Head:
https://anrweb.vt.gov/PubDocs/DEC/PFOA/Soil-Background/PFAS-Background-Vermont-Shallow-Soils-03-24-19.pdf

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Soil Leaching Values & VT Background

1. ***The intent of this aggregate comparison is to contextualize the regulatory and guidance values. The individual data in this study were not collected for comparison to regulatory or guidance values and should not be used for that purpose.***
2. *"Soil to GW Protection Values" were largely obtained from the ITRC fact sheet spreadsheet updated June 2020 (https://pfas-1.itrcweb.org/fact-sheets/). Some proposed or draft values, which may be on-hold or now replaced with updated values, are also included.*

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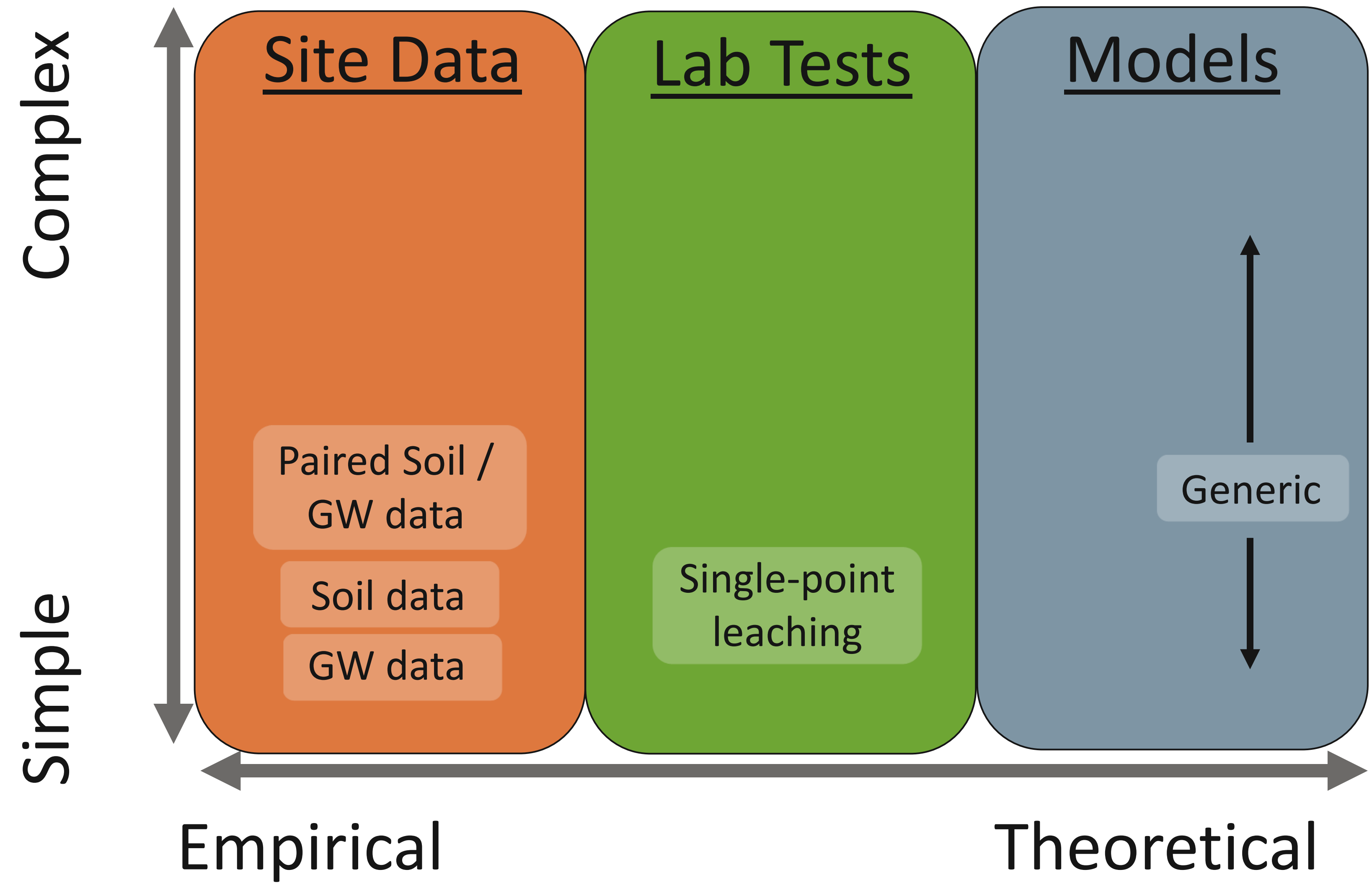
Common Tools Rely on Key Assumptions and Interpretation



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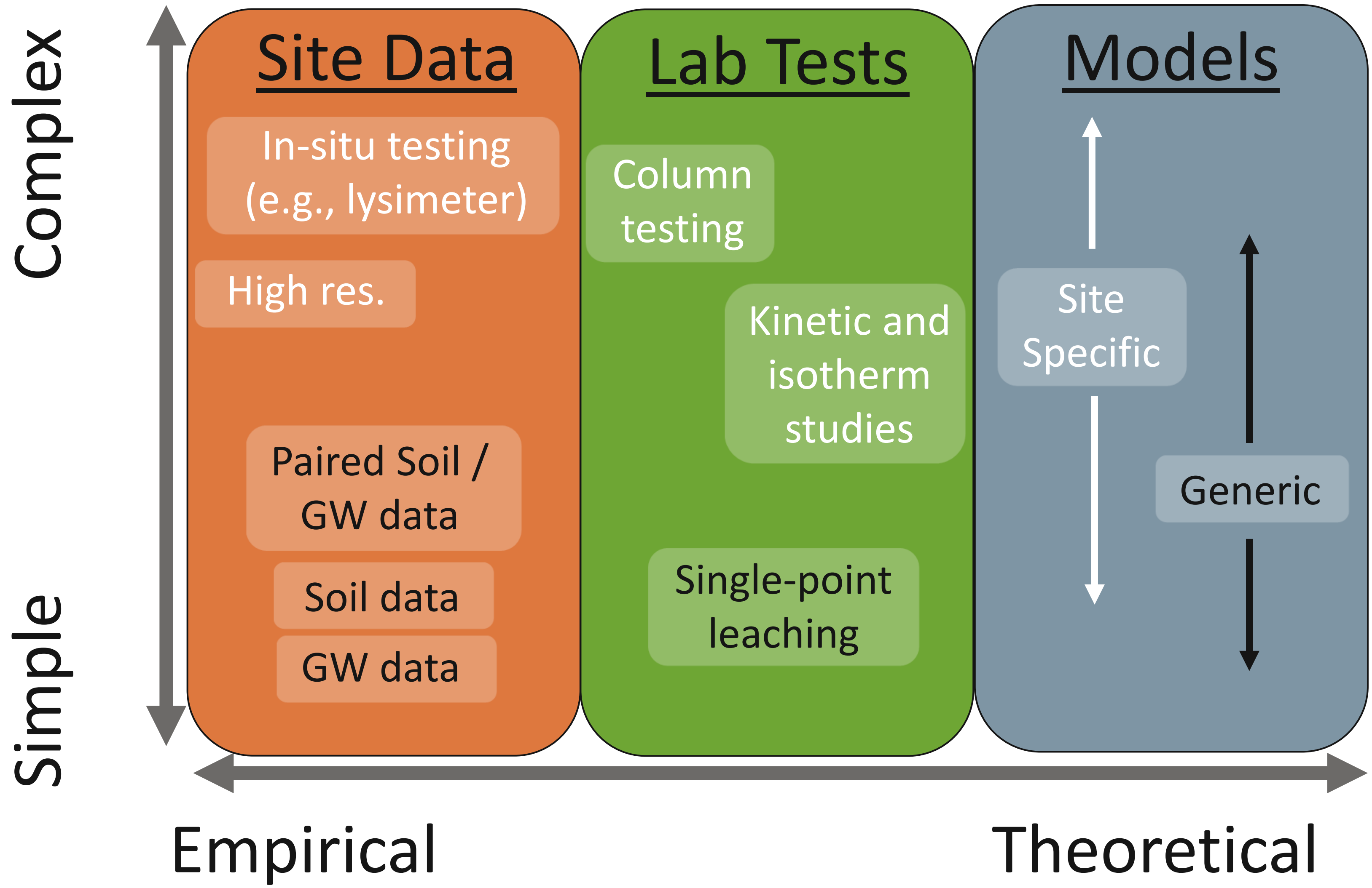
Consider Empirical and Complex Tools



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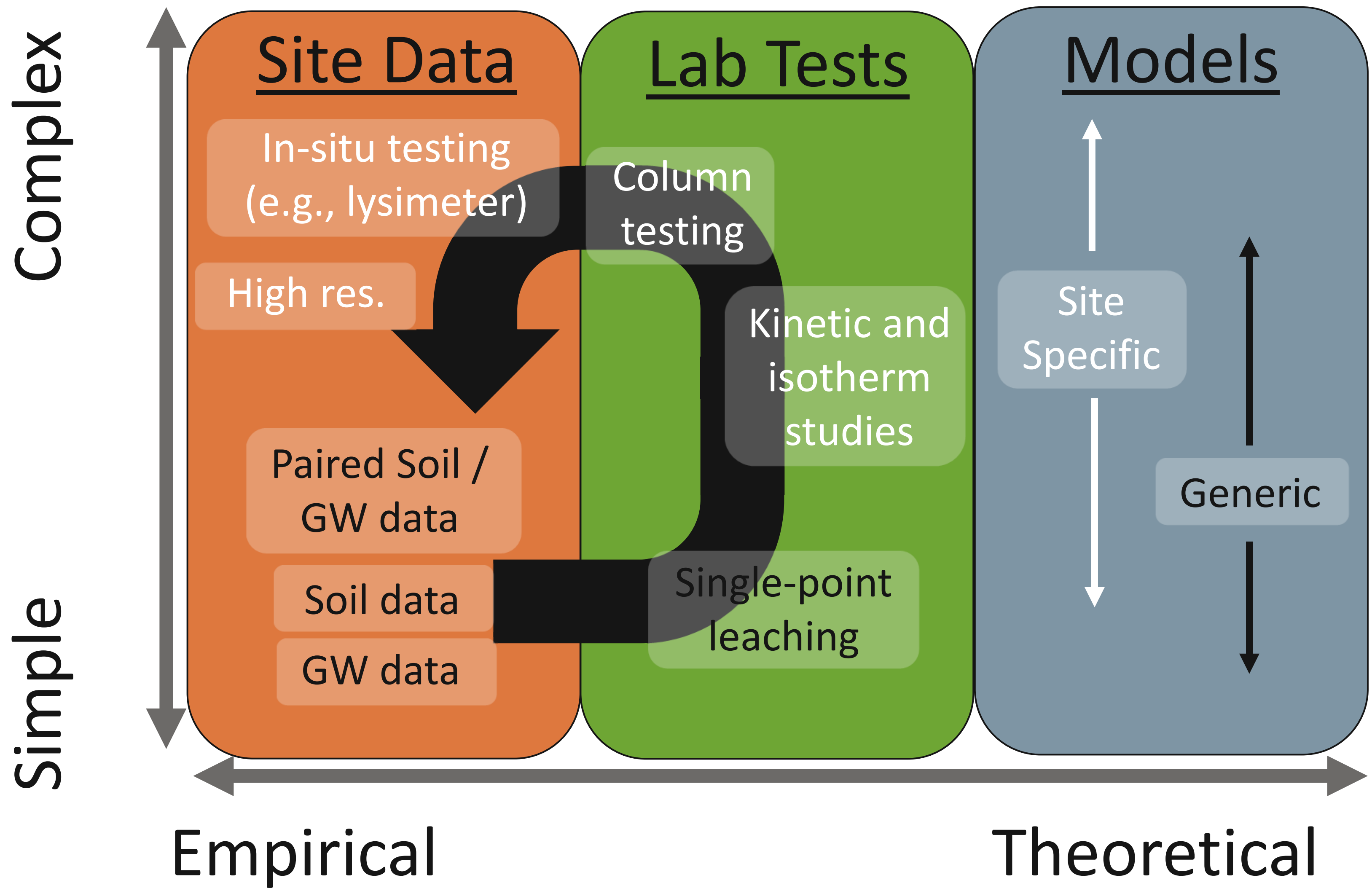
Build Multiple Lines of Evidence



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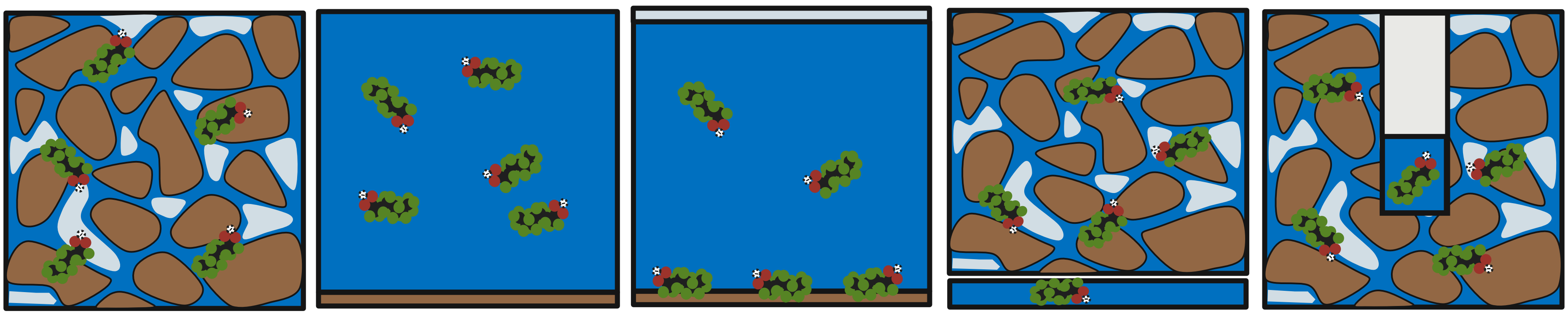
Soil Analysis Methods

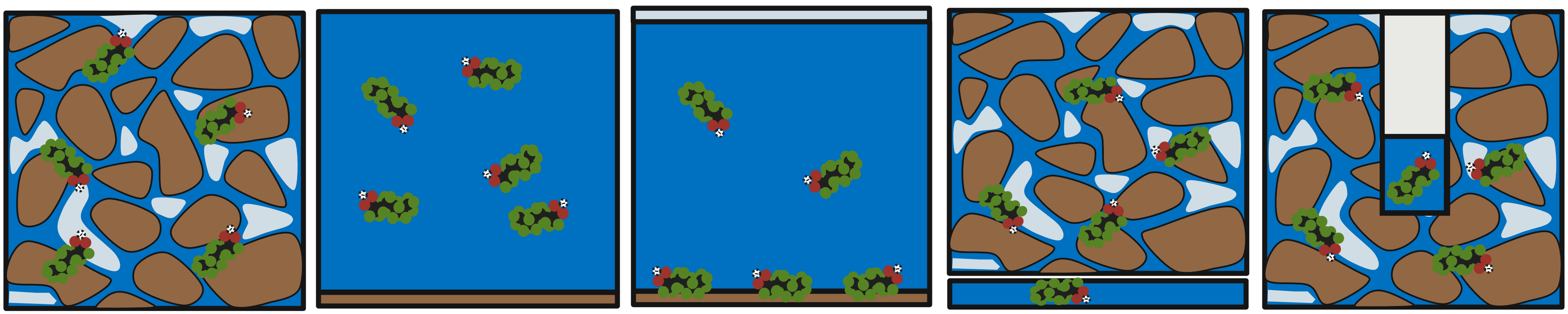
Soil sample | Solids analysis | SPLP | Column testing | Lysimeter



- Three phases: Air, Water, Solids

Soil Analysis Methods

Soil sample	Solids analysis	SPLP	Column testing	Lysimeter



Soil sample

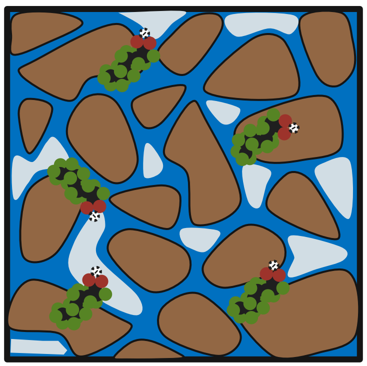
- Three phases: Air, Water, Solids

Solids analysis

- Solvent extraction
- High lab RLs

Soil Analysis Methods

Soil sample



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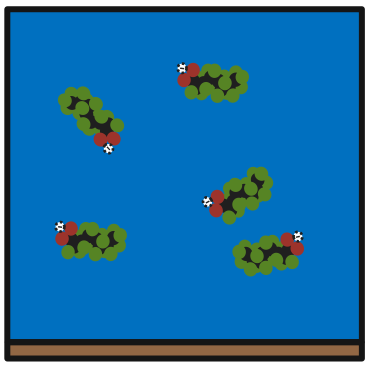

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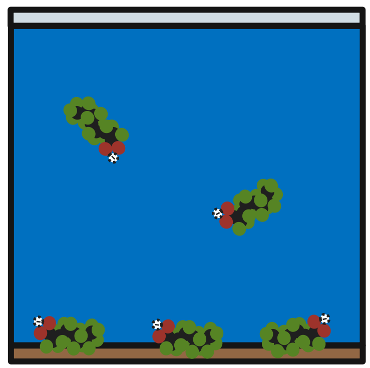
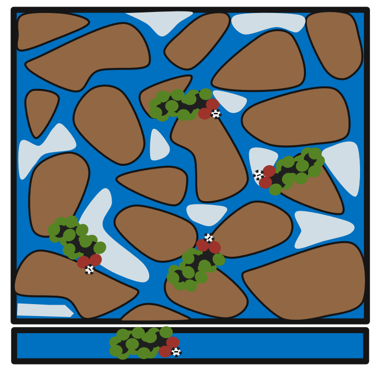
SPLP

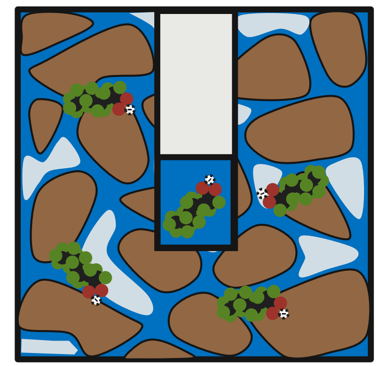


- Water extraction
- High liquid-solid ratio

Column testing



Lysimeter



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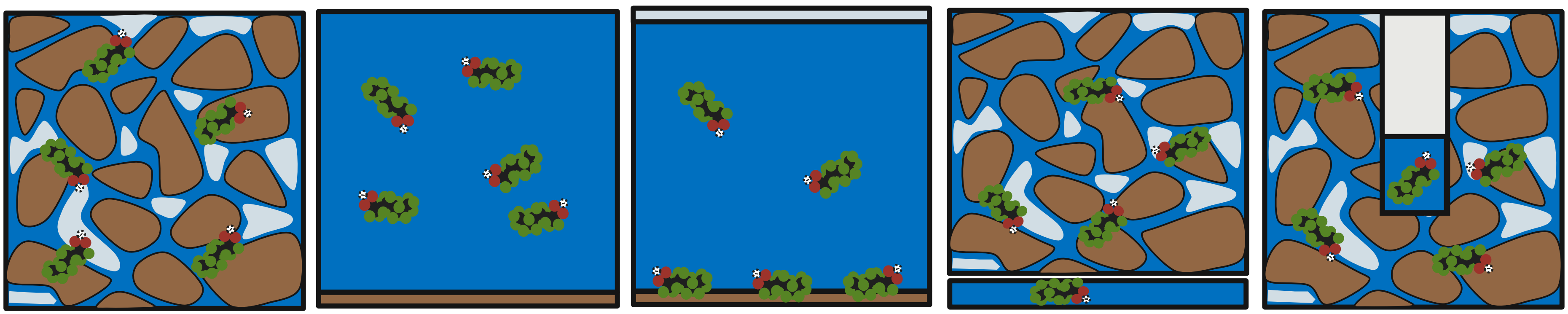

Soil sample

- Three phases: Air, Water, Solids

Solids analysis

- Solvent extraction
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SPLP

- Water extraction
- High liquid-solid ratio

Column testing

- May customize conditions
- Lower liquid-solid ratio

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Soil Analysis Methods

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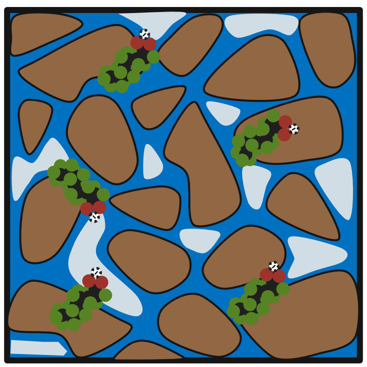

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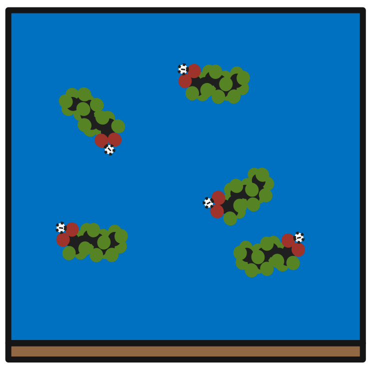

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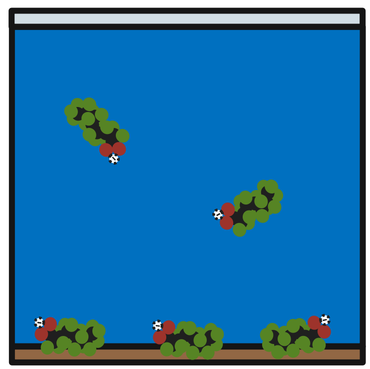

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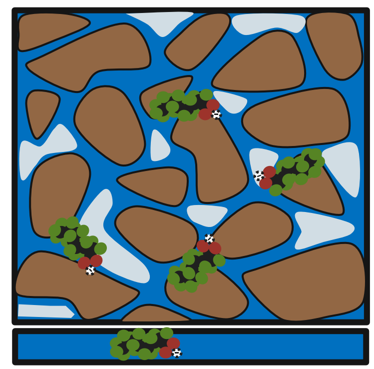

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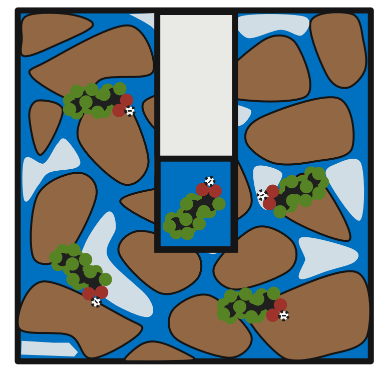
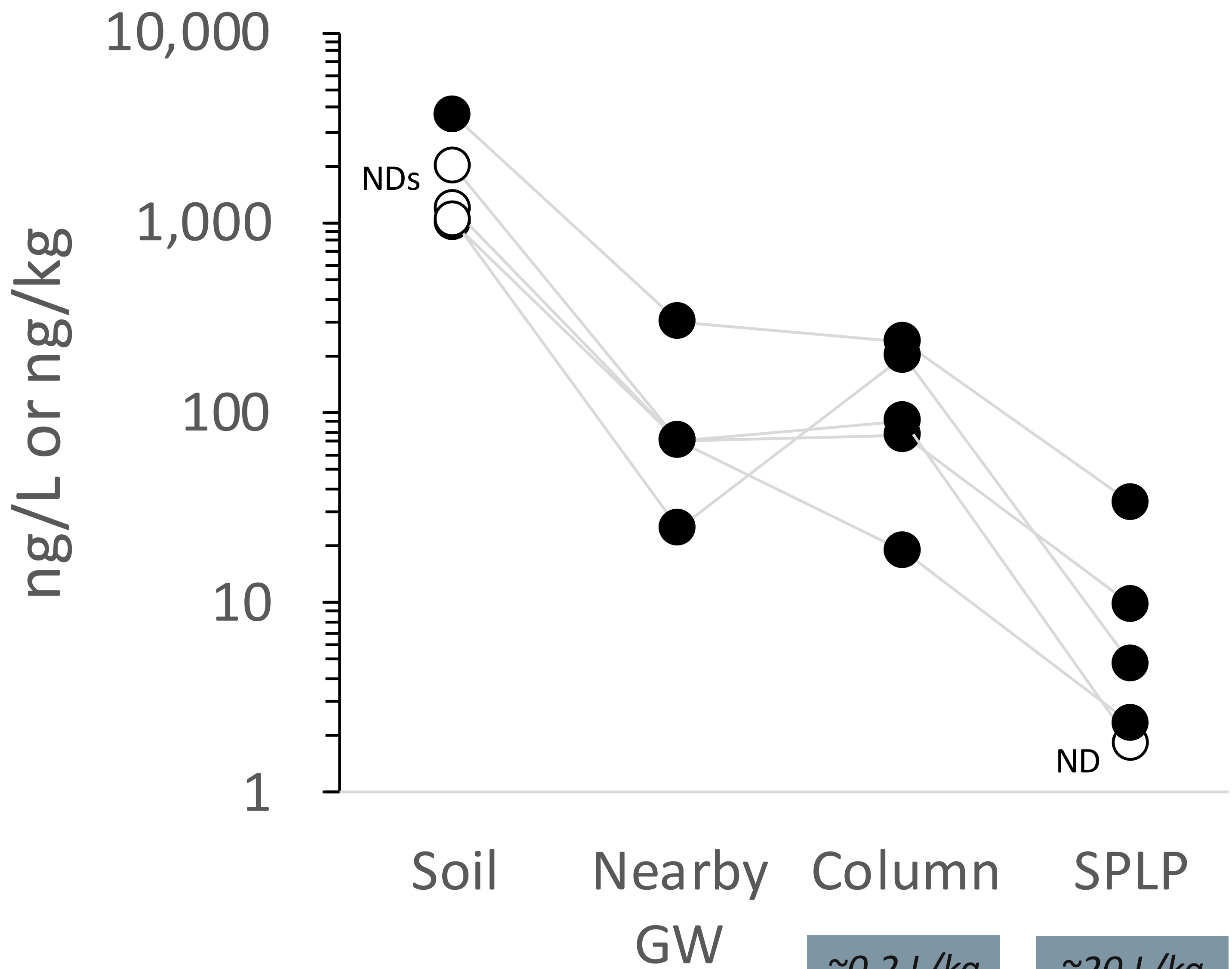
Lysimeter



- Vadose zone liquids
- Near field conditions

PFOA Atmospheric Deposition Case Study



Column testing and photographs by XDD Environmental, LLC.

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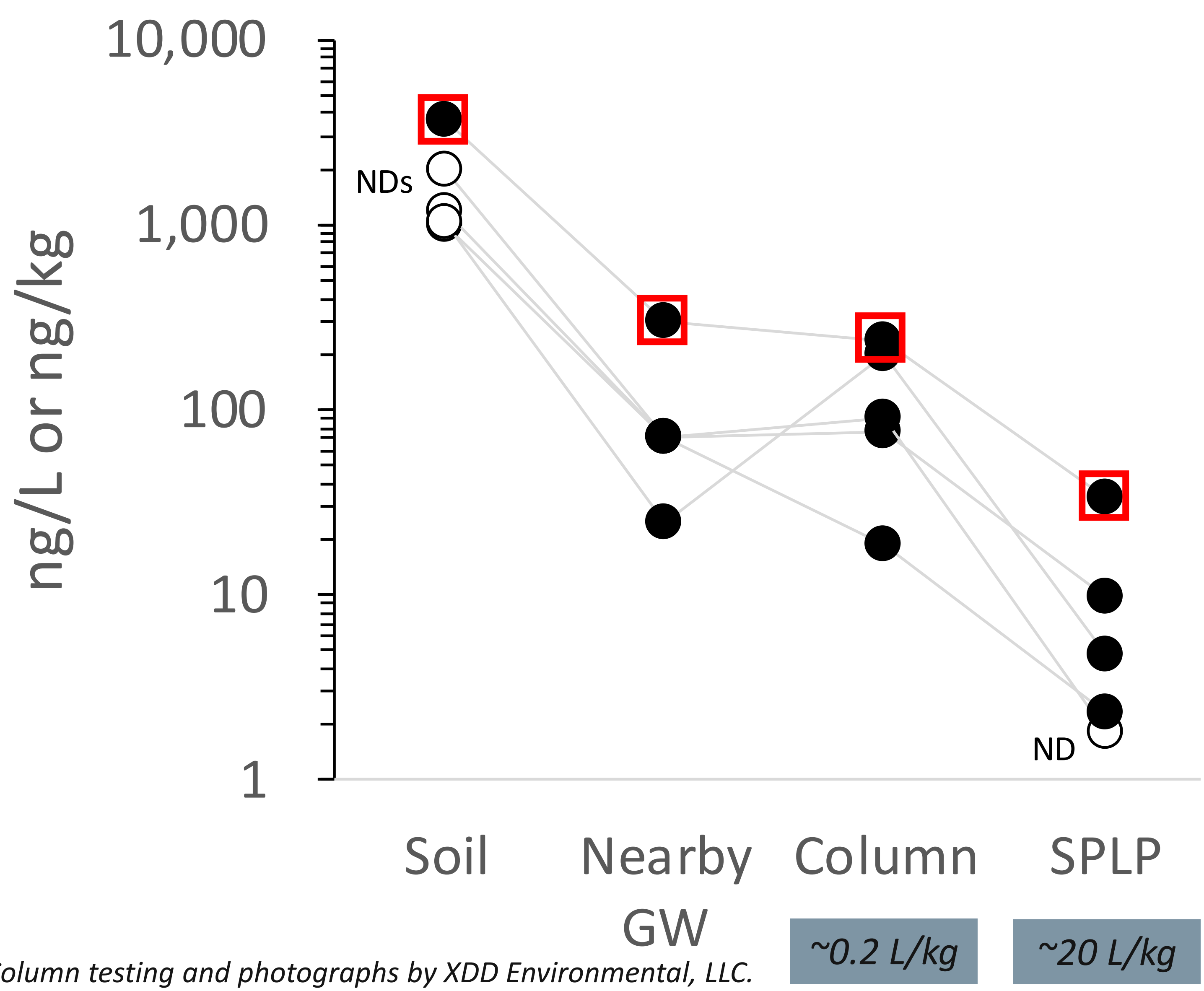

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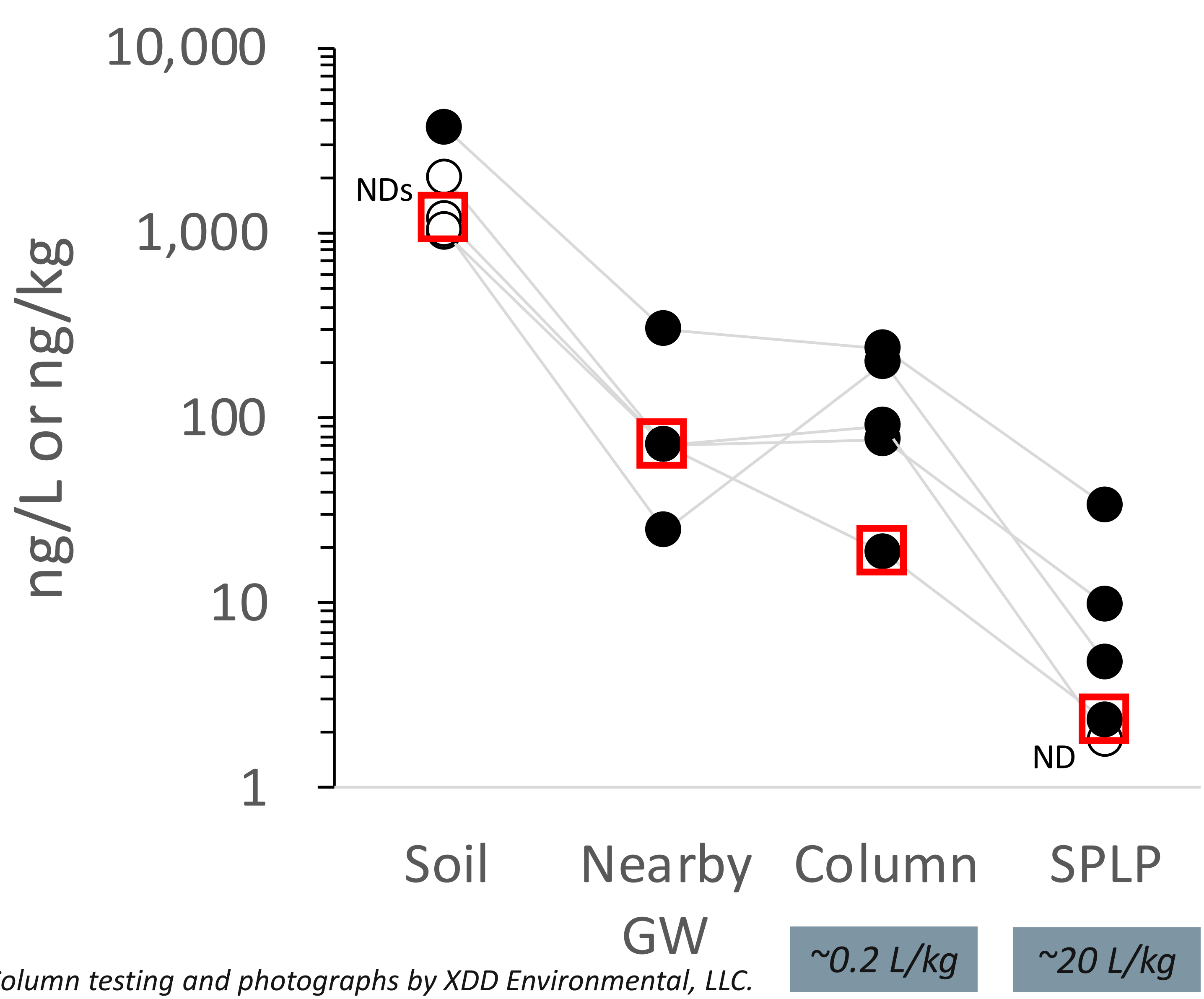

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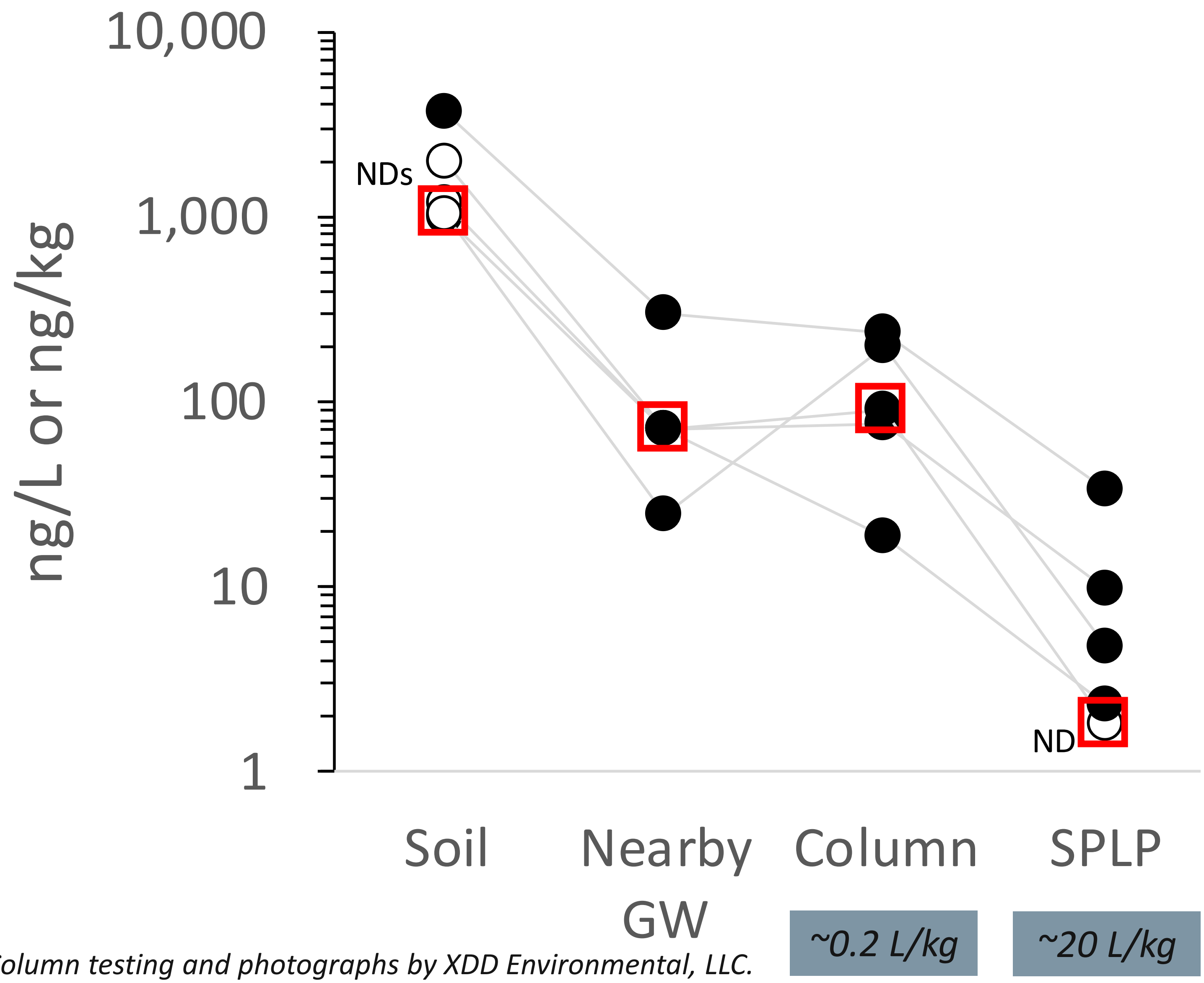

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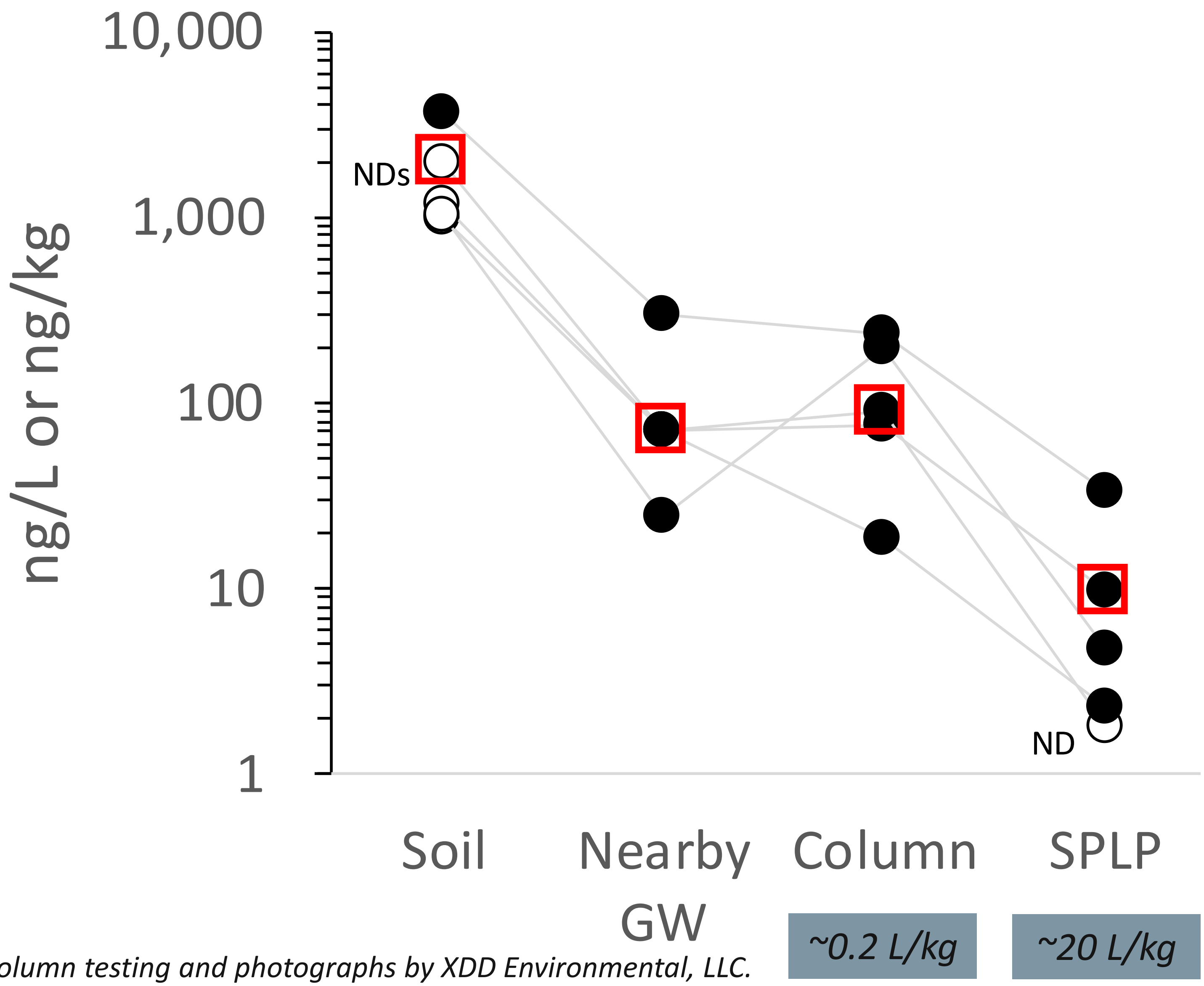

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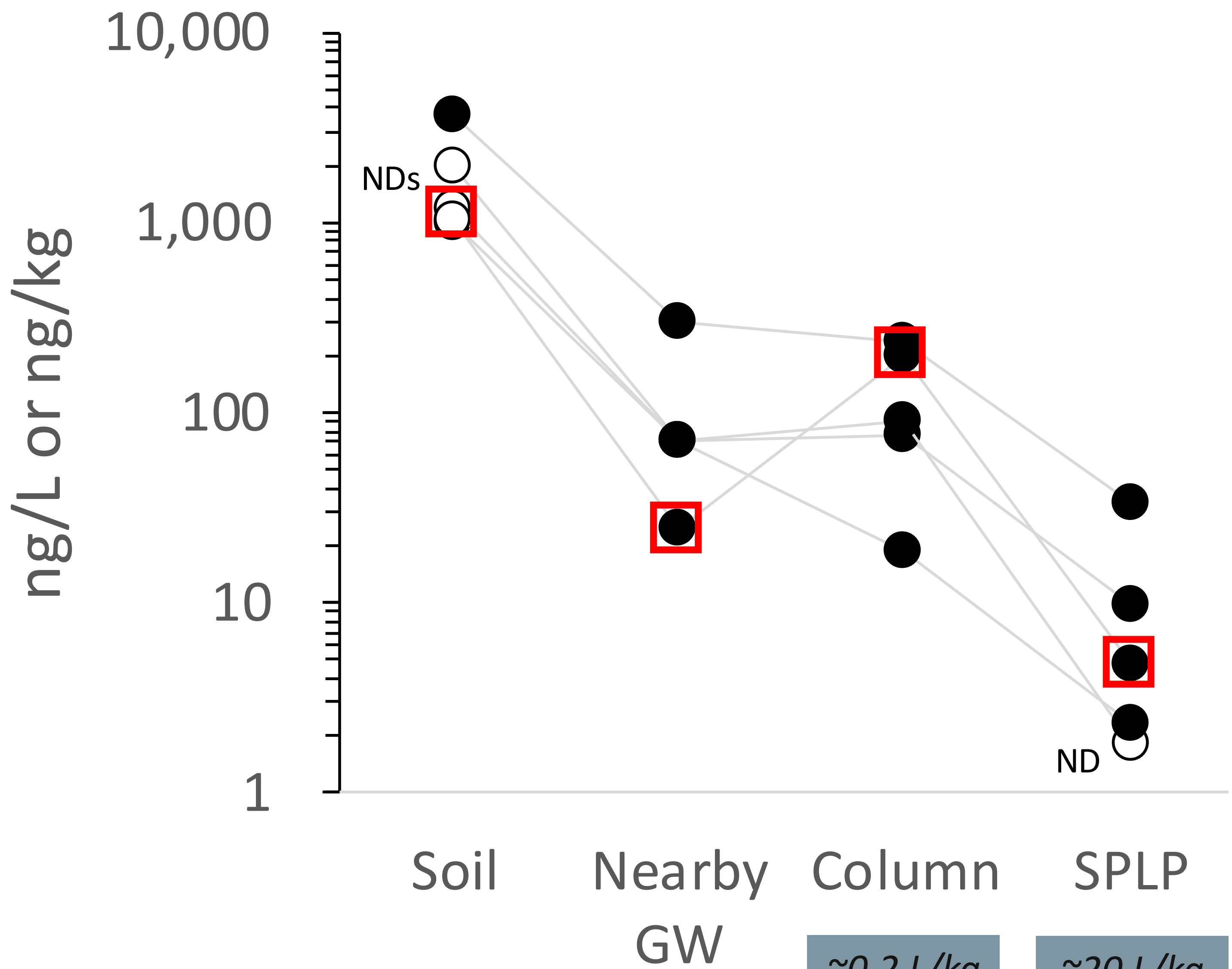

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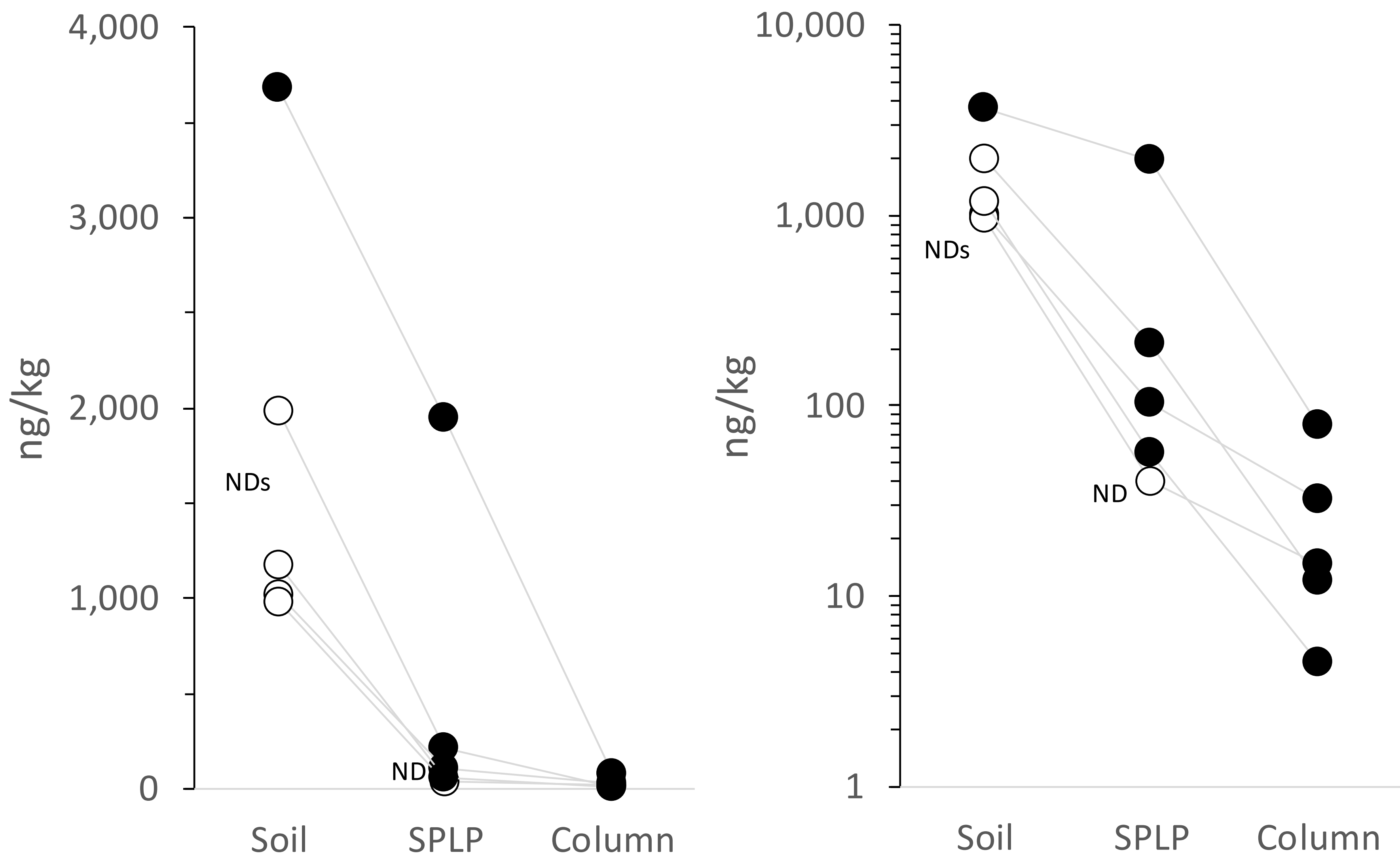
Normalized to Soil Dry Weight



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Summary

Leaching
- Wide-ranging field data
- Default models not built for PFOA/PFOS

Leaching-Based Screening Values
- Typically lower than direct contact-based values
- Variety of methods and large range of values

Anthropogenic Background
- PFOA and PFOS present in many background soils
- Lower leaching-based screening values at or below VT background
- Background leaching values not known

Screening Approaches
- Underlying assumptions for interpretation are important
- Consider more empirical and complex tools
- Multiple lines of evidence

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Questions and Comments Appreciated!

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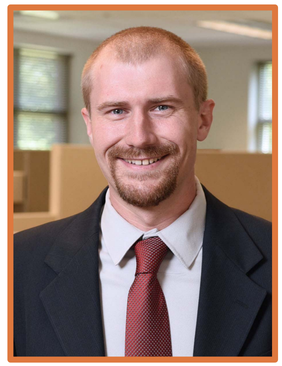

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