# The Role of Precursor Transformation on PFAS Fate and Transport in the Saturated Zone

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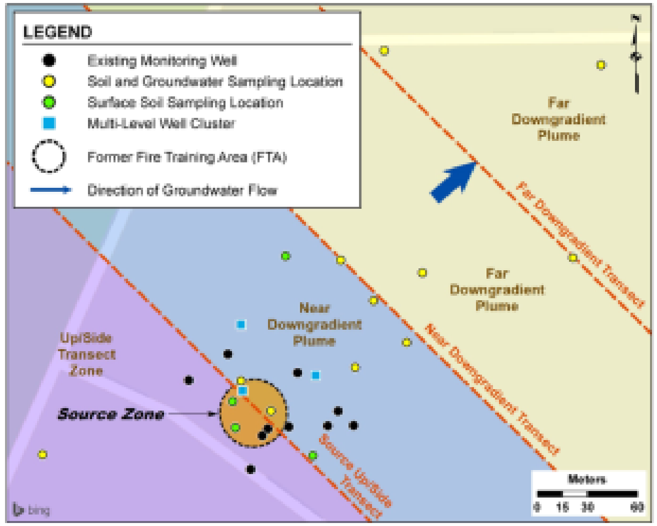
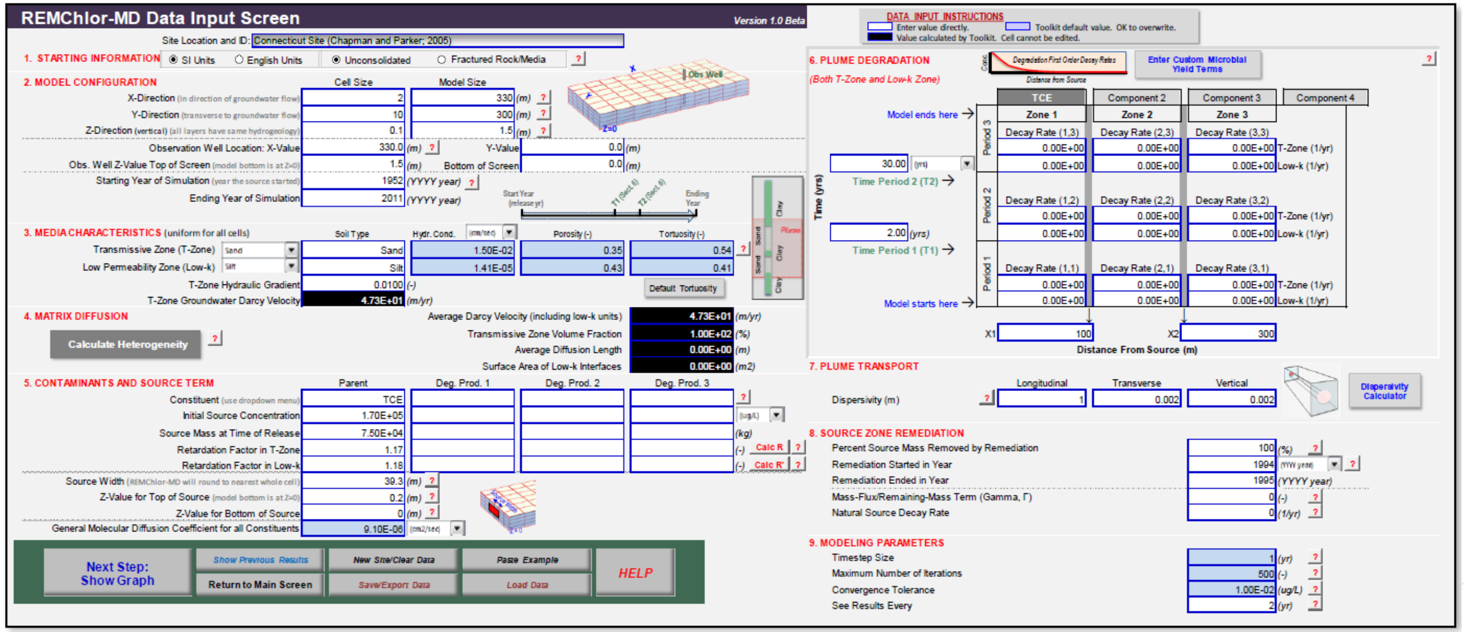
# Objectives

- Combine high-resolution field characterization data with semi-analytical modeling
- Determine relative transformation rates of different PFAS classes
- Document key fate and transport parameters at an AFFF release site
- Establish how precursor transformation influences PFAS plume development




# REMChlor-MD Overview

- Semi-analytical model
- Free, available via ESTCP website
- Easy to use for non-modelers
- Simulates:
  - Matrix diffusion
  - Retardation
  - Molecular diffusion
  - Plume degradation
  - Dispersion
  - Source zone remediation

# Field Site Overview

- High-resolution sampling at 11 locations
  - Groundwater at ~5 depths
  - Soil at ~ 10 depths
- Analysis for <u>79</u> PFAS in Groundwater (Dr. Field, Oregon State University)
  - 57 Precursors
  - 22 PFAAs
- Analysis for <u>136</u> PFAS in Soil (Dr. Higgins, Colorado School of Mines)
  - 115 Precursors
  - 21 PFAAs

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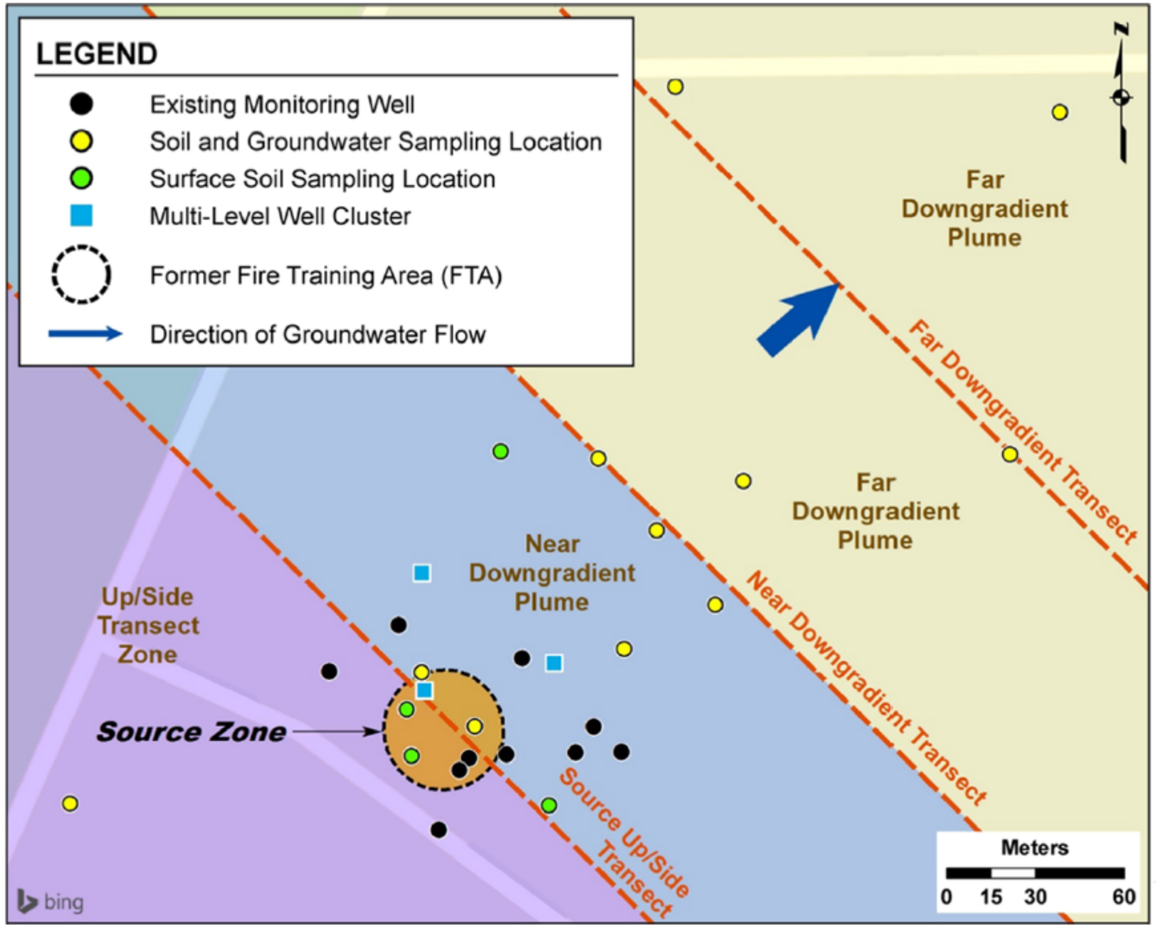
Article

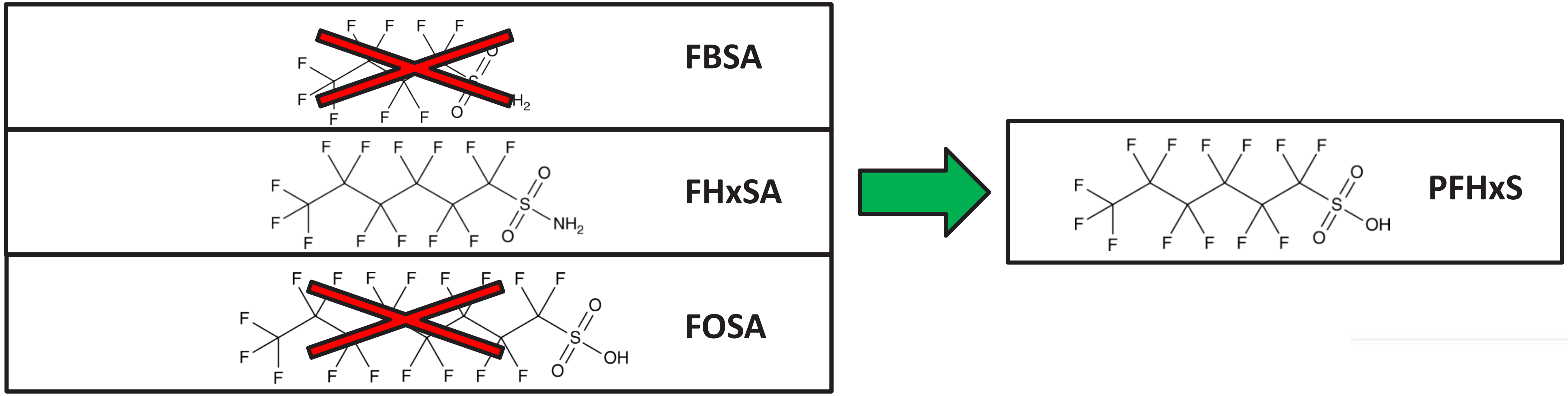
**Mass-Based, Field-Scale Demonstration of PFAS Retention within AFFF-Associated Source Areas**

David T. Adamson,* Anastasia Nickerson, Poonam R. Kulkarni, Christopher P. Higgins, Jovan Popovic, Jennifer Field, Alix Rodowa, Charles Newell, Phil DeBlanc, and John J. Kornuc

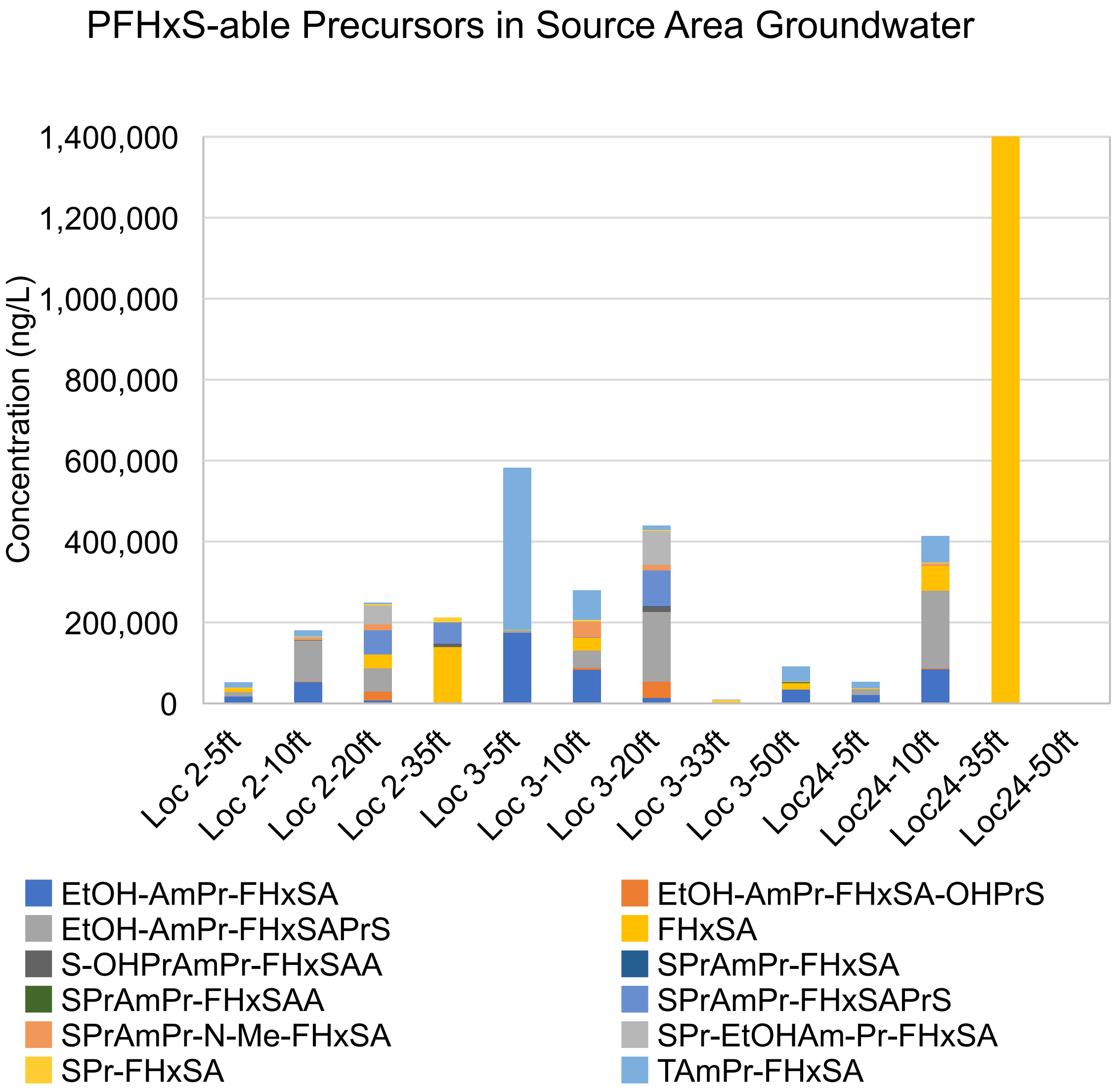


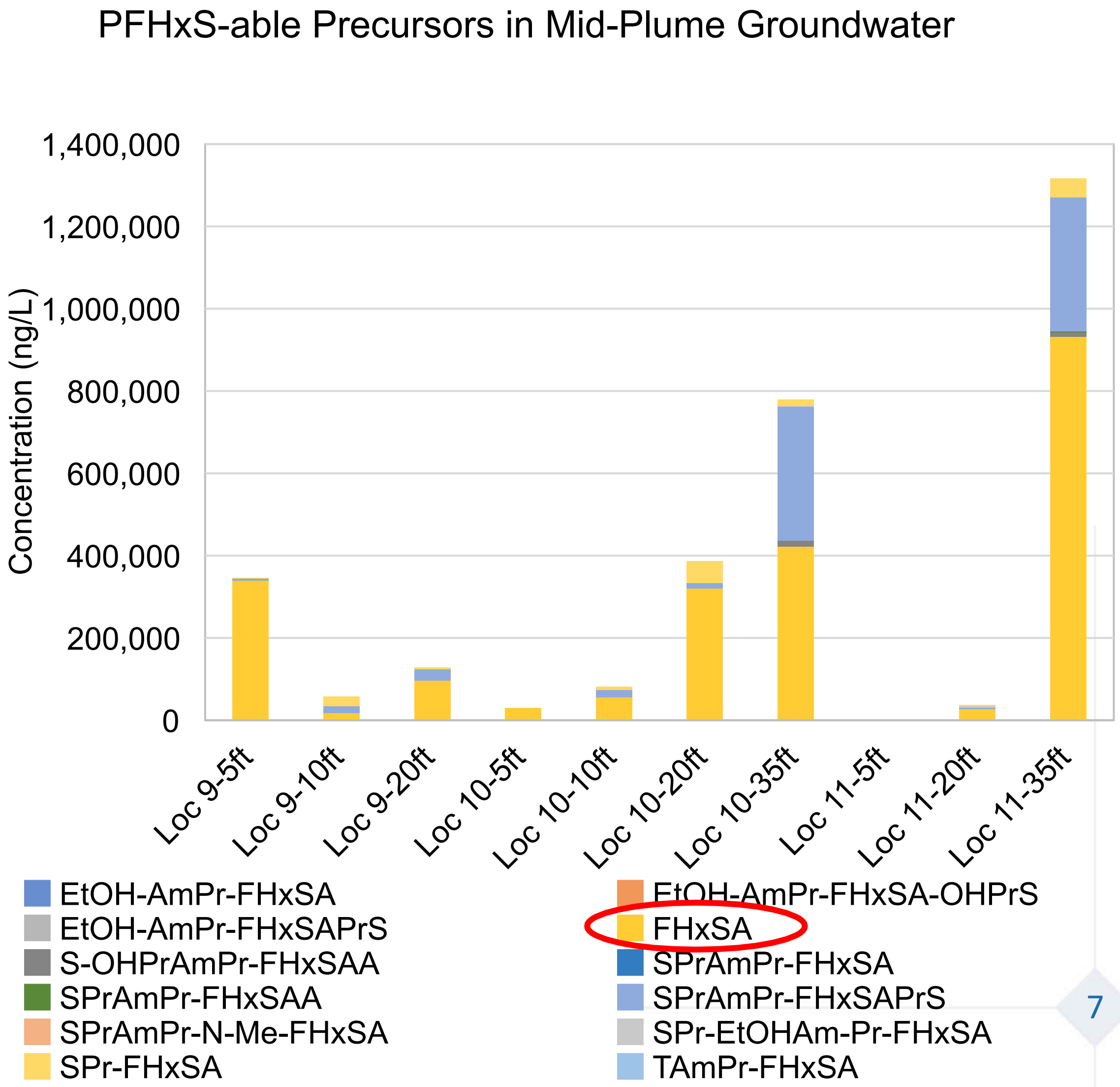
# Key Assumptions For Incorporating Precursor Transformation into REMChlor-MD

- The PFAS identified in the data set represent all PFAS at the site
  - In groundwater, the 57 identified precursors represent all precursors
  - In soil, the 115 identified precursors represent all precursors
- "**PFOS-able precursors**" are PFSA precursors with 8 fully fluorinated carbons
- "**PFOA-able precursors**" are PFCA precursors with 7 or 8 fully fluorinated carbons
- "**PFHxS-able precursors**" are PFSA precursors with 6 fully fluorinated carbons
- "**PFBS-able precursors**" are PFSA precursors with 4 fully fluorinated carbons



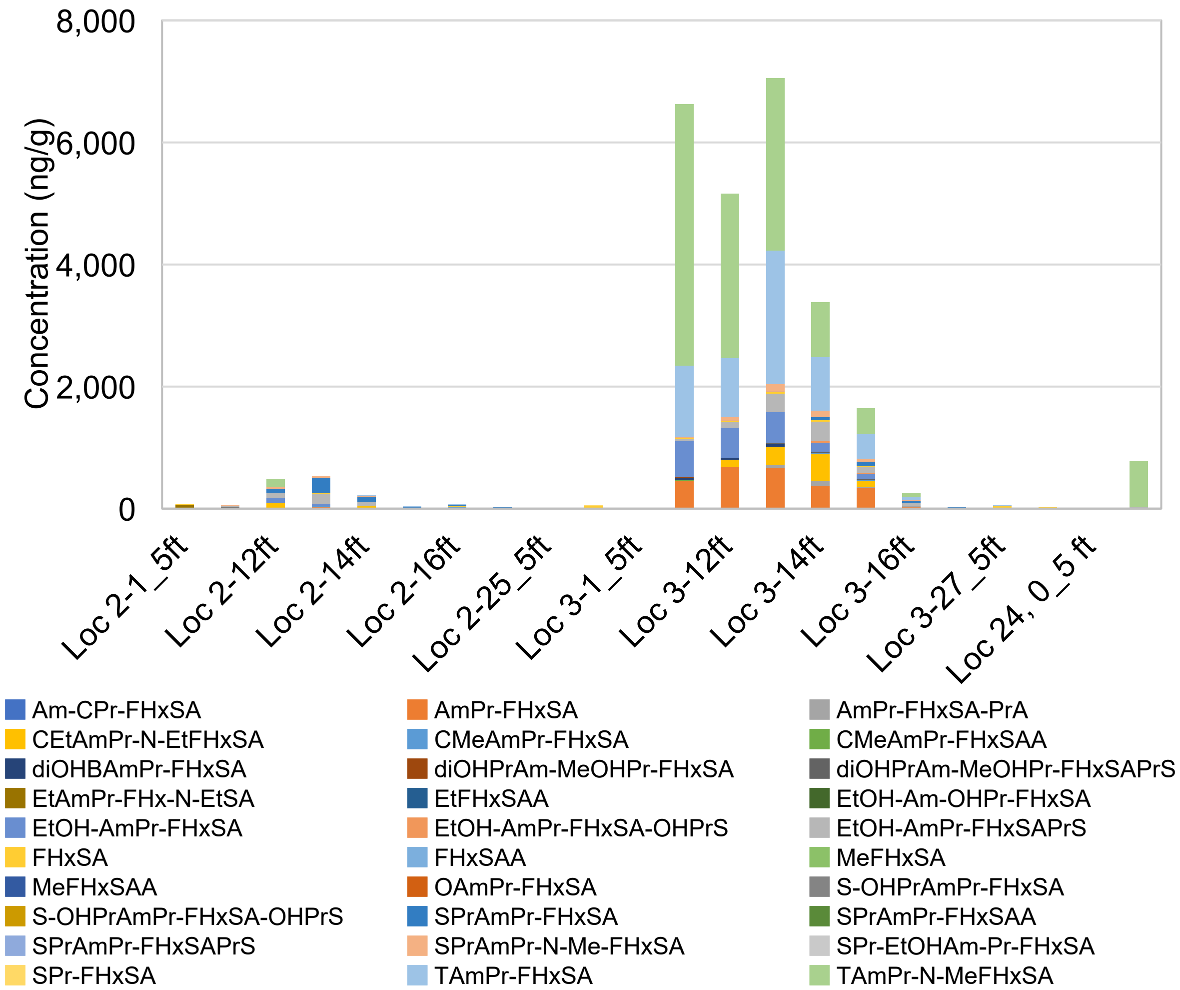
# Field Site PFHxS-able Precursors in Groundwater



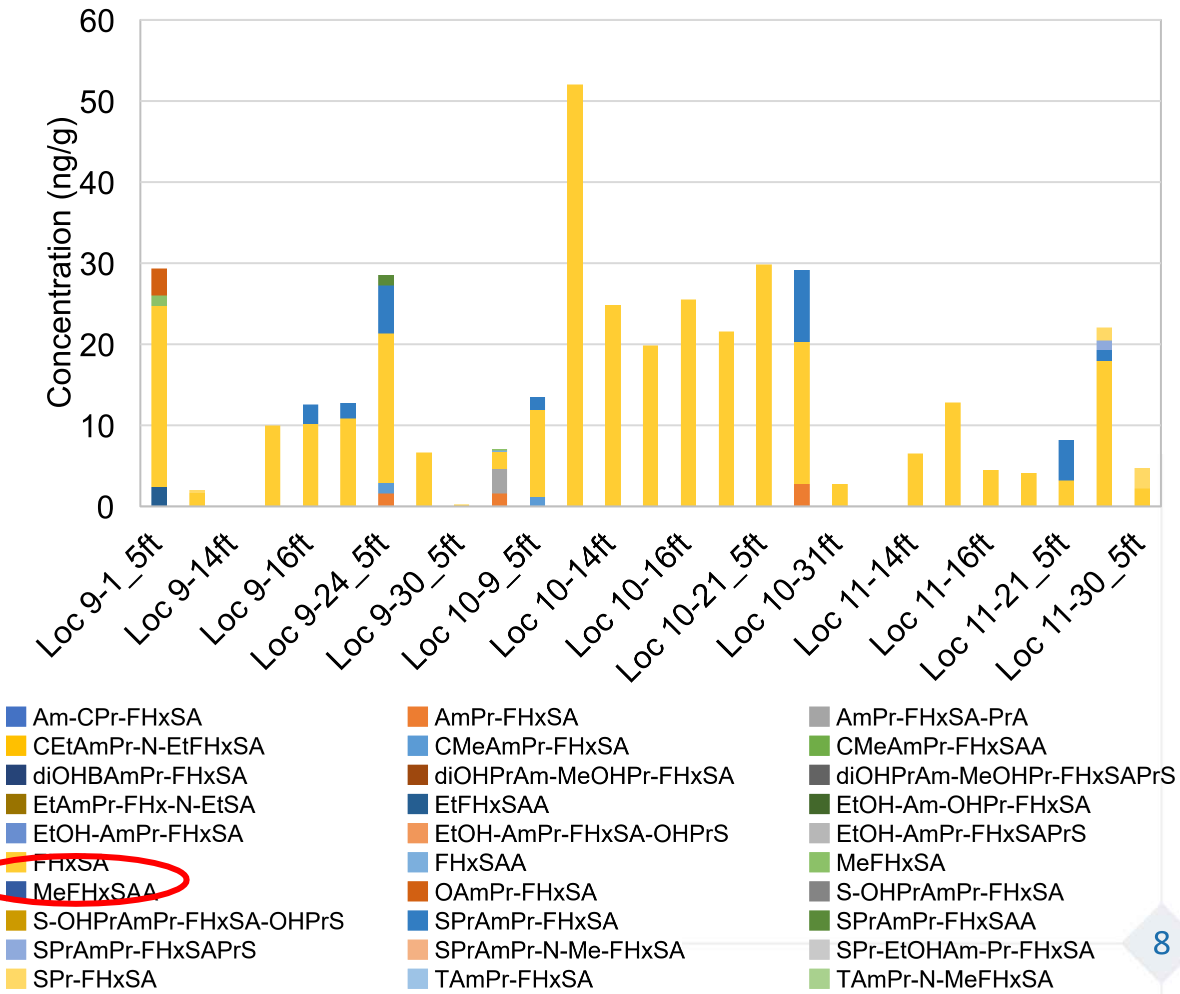



# Field Site PFHxS-able Precursors in Soil

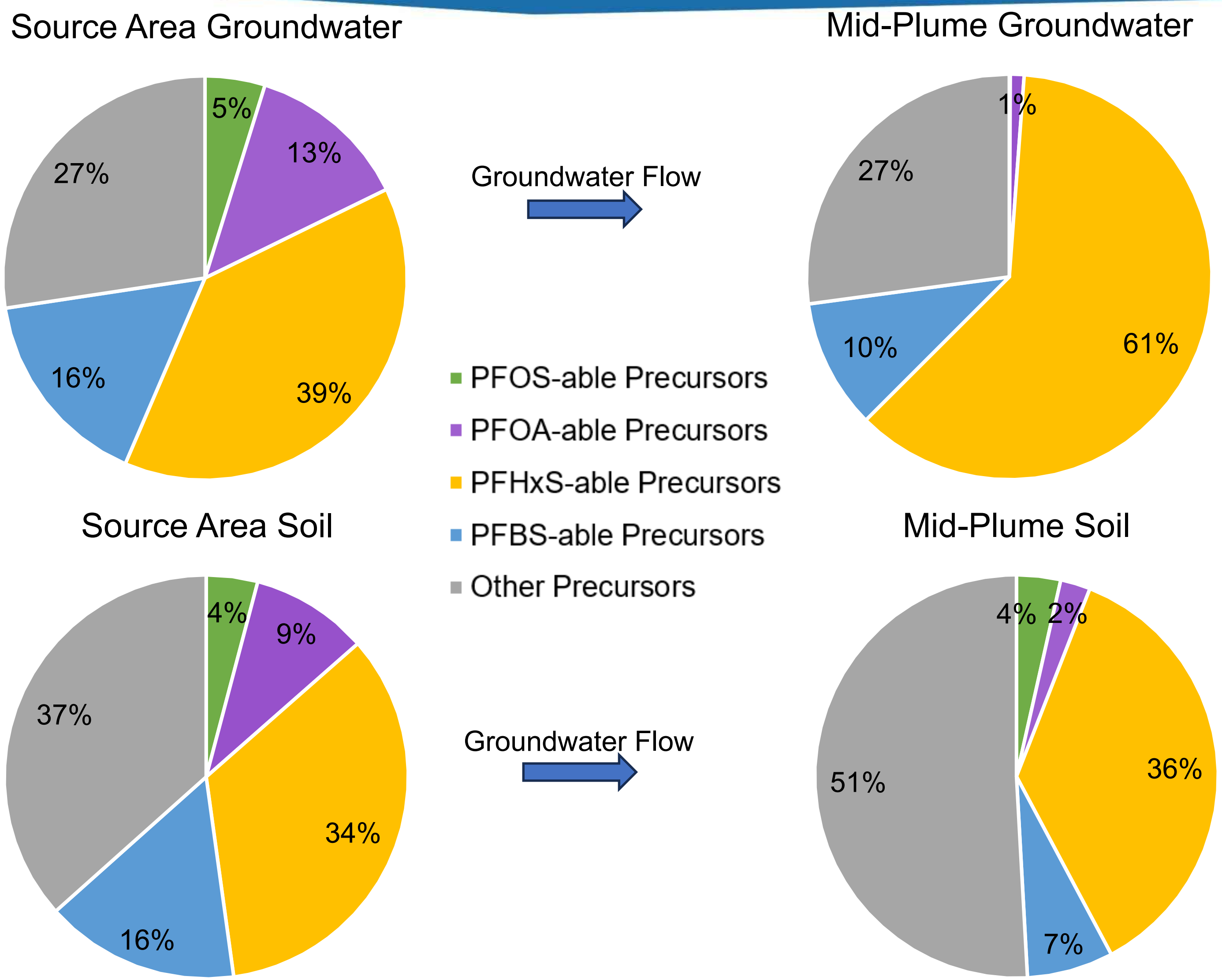
PFHxS-able Precursors in Source Area Soil




PFHxS-able Precursors in Mid-Plume Soil



# Field Site Precursor Characterization




Precursor mass by proportion:

- PFHxS-able
- PFBS-able
- PFOA-able
- PFOS-able

# Field Site Model Inputs

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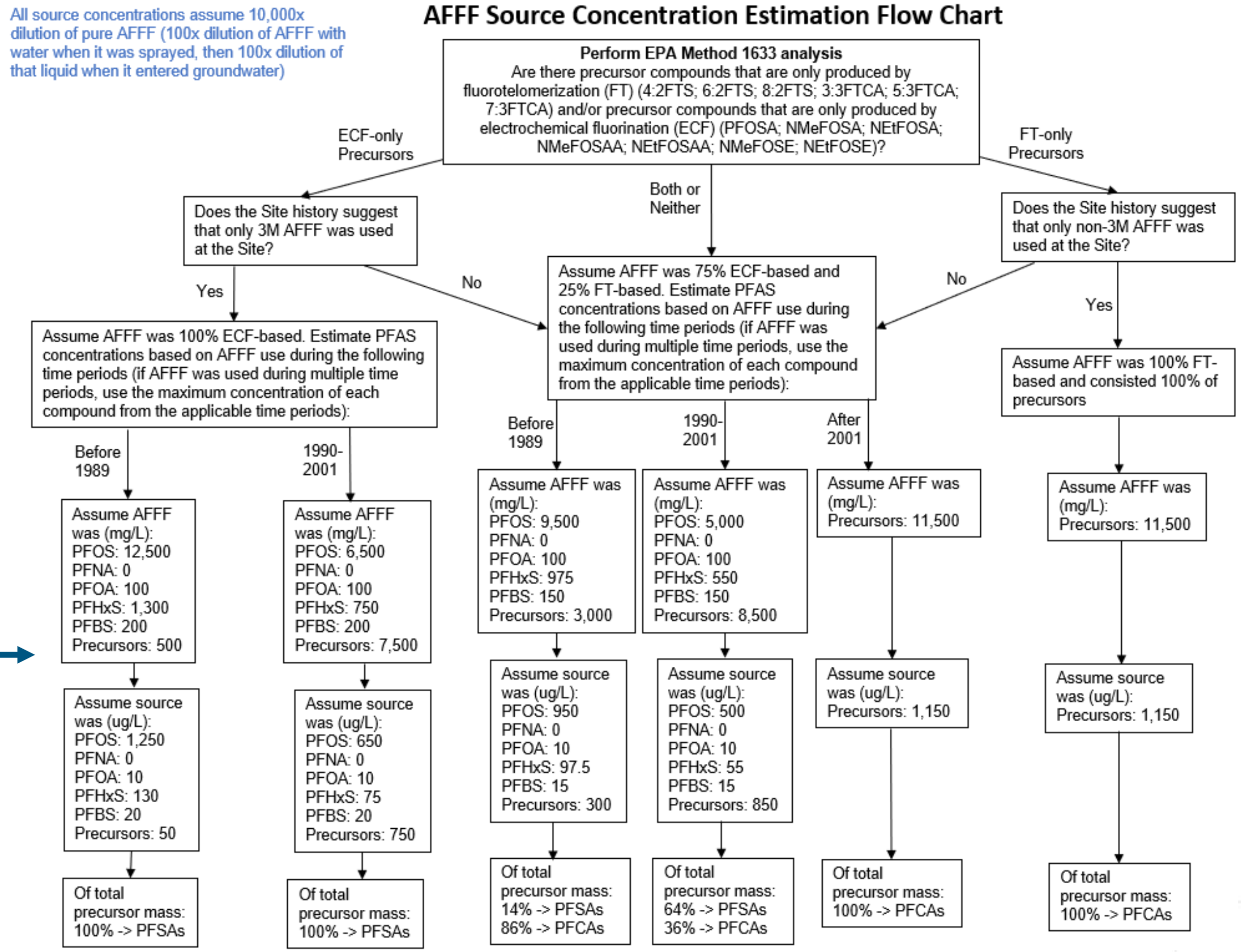
- Soil and Groundwater Properties
- Molecular Diffusion Coefficients
- Precursor Yields
- Source Mass at Time of Release
- Retardation Factors*
- Precursor Transformation Rates*
- Initial Source Concentrations*

* Calibration parameter

## Source Concentration Estimation Method



# Field Site Model Calibration

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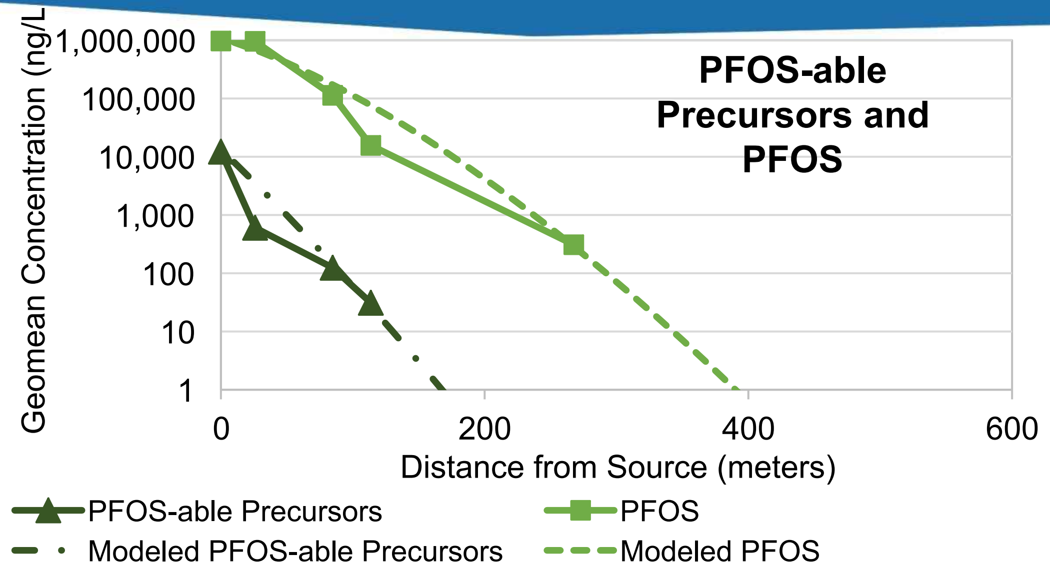
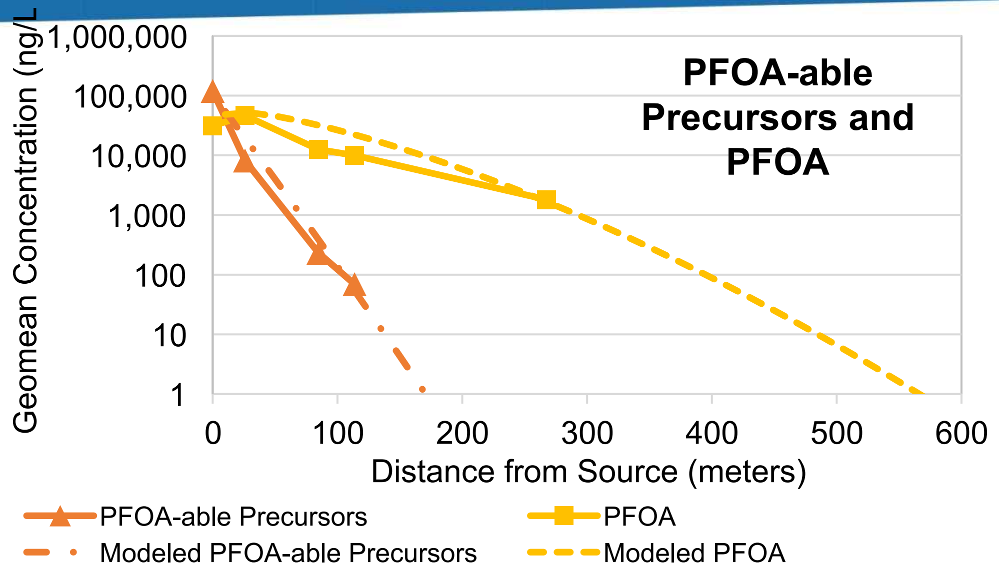
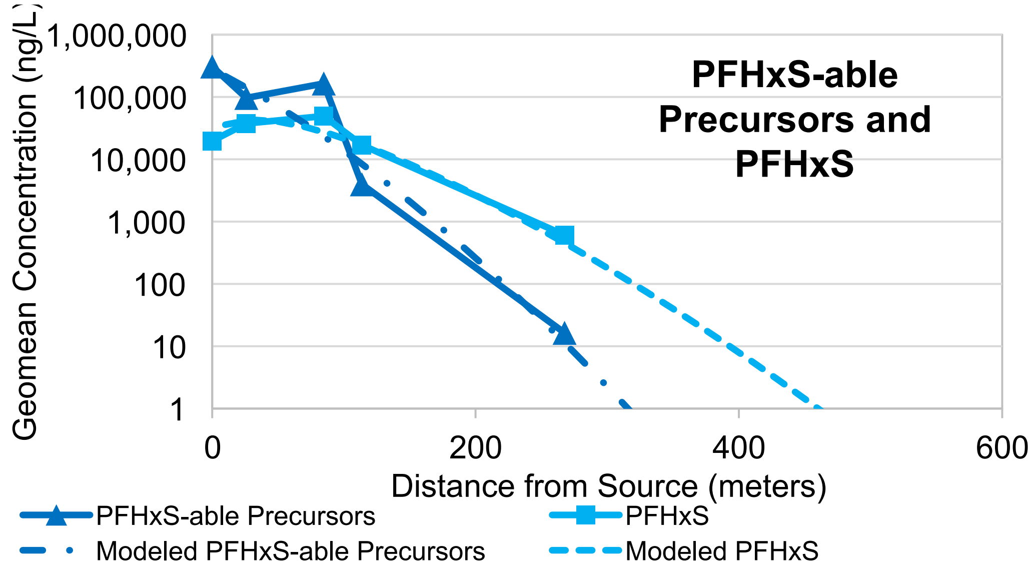
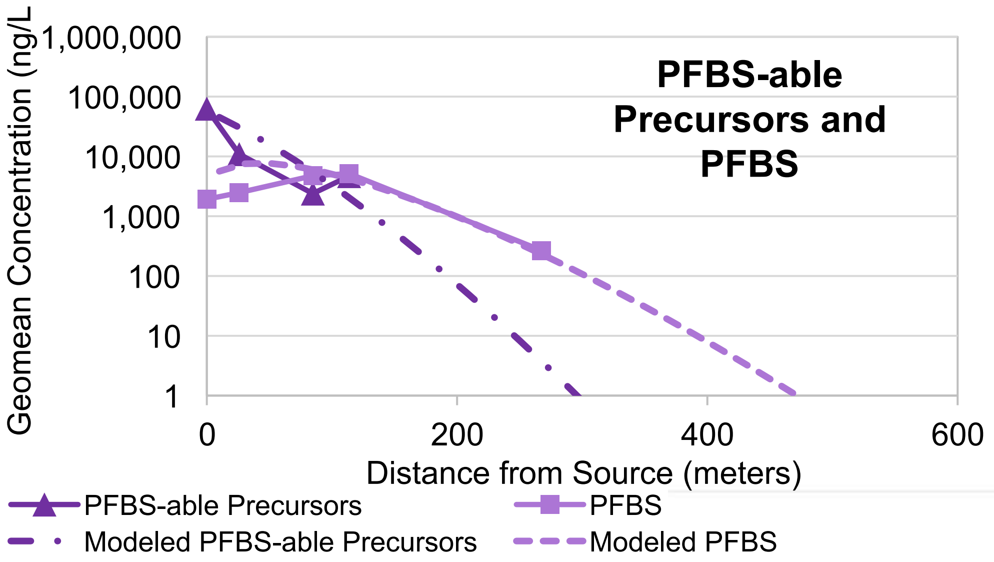
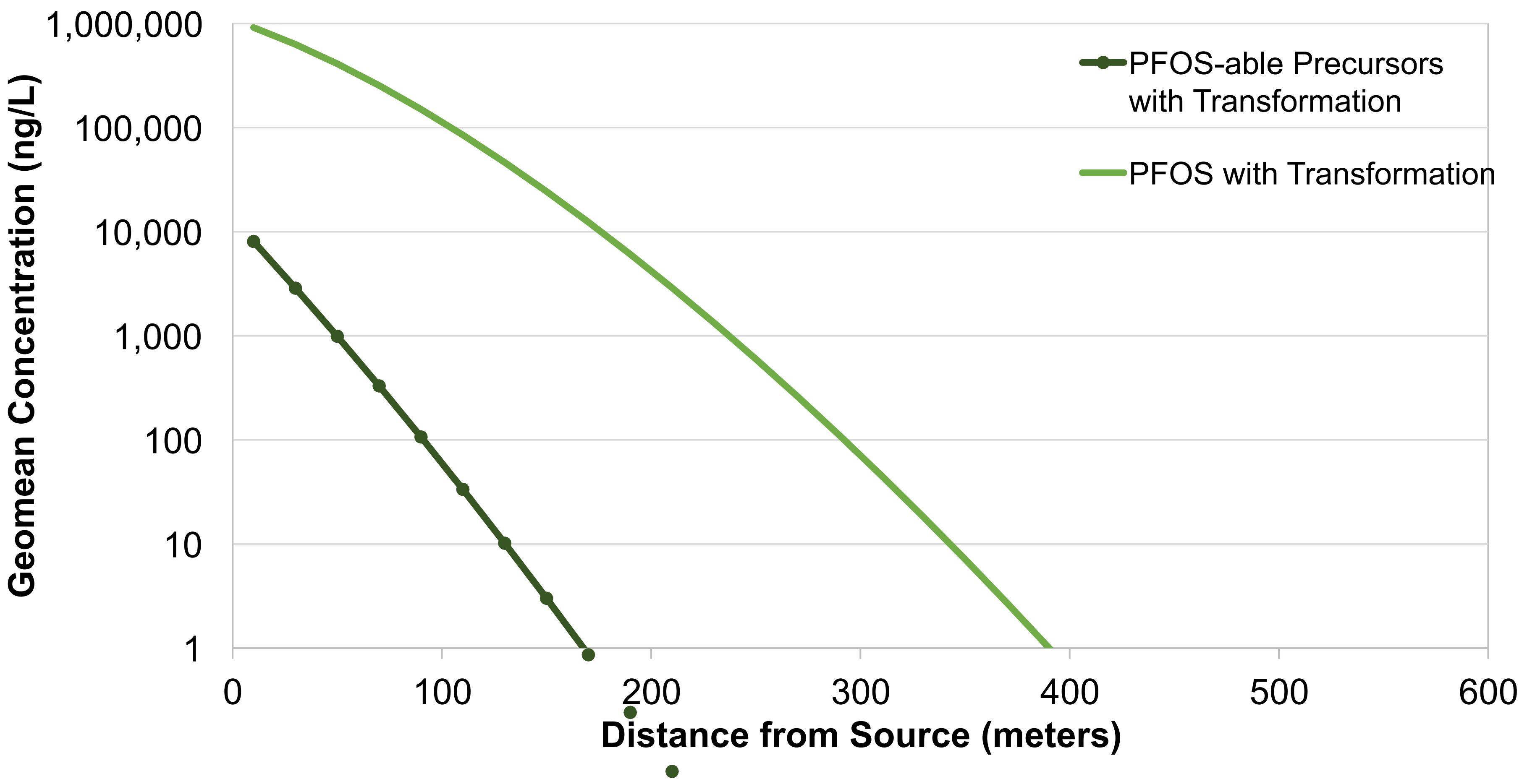


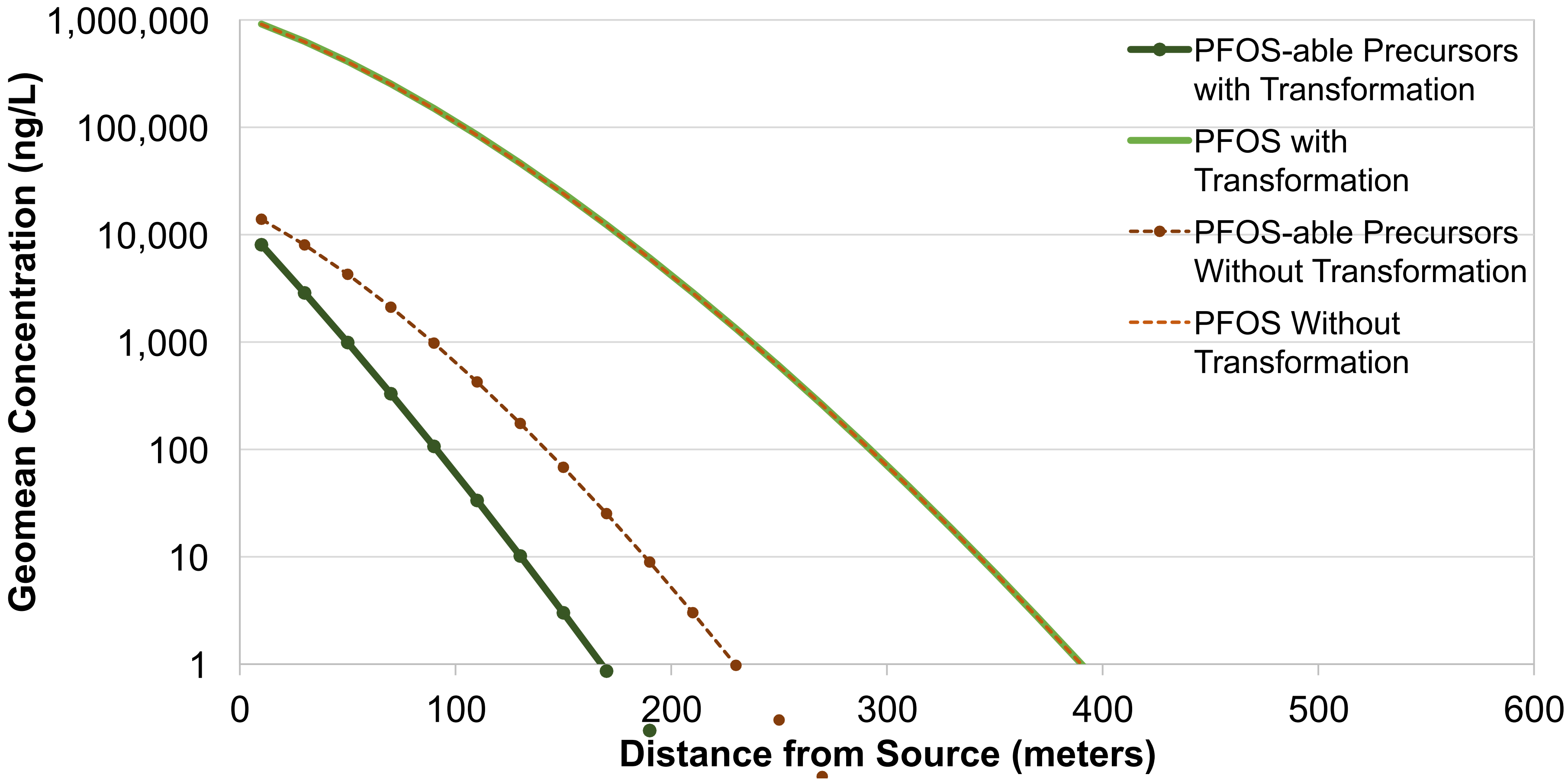



# Field Site PFOS Model – Year 40



# Field Site PFOS Model – Year 40




**Even though PFOS-able precursor transformation occurs, the concentrations of PFOS are so much higher that precursor transformation has no impact on PFOS plume length or concentration**

# Field Site PFOS Model – Year 40

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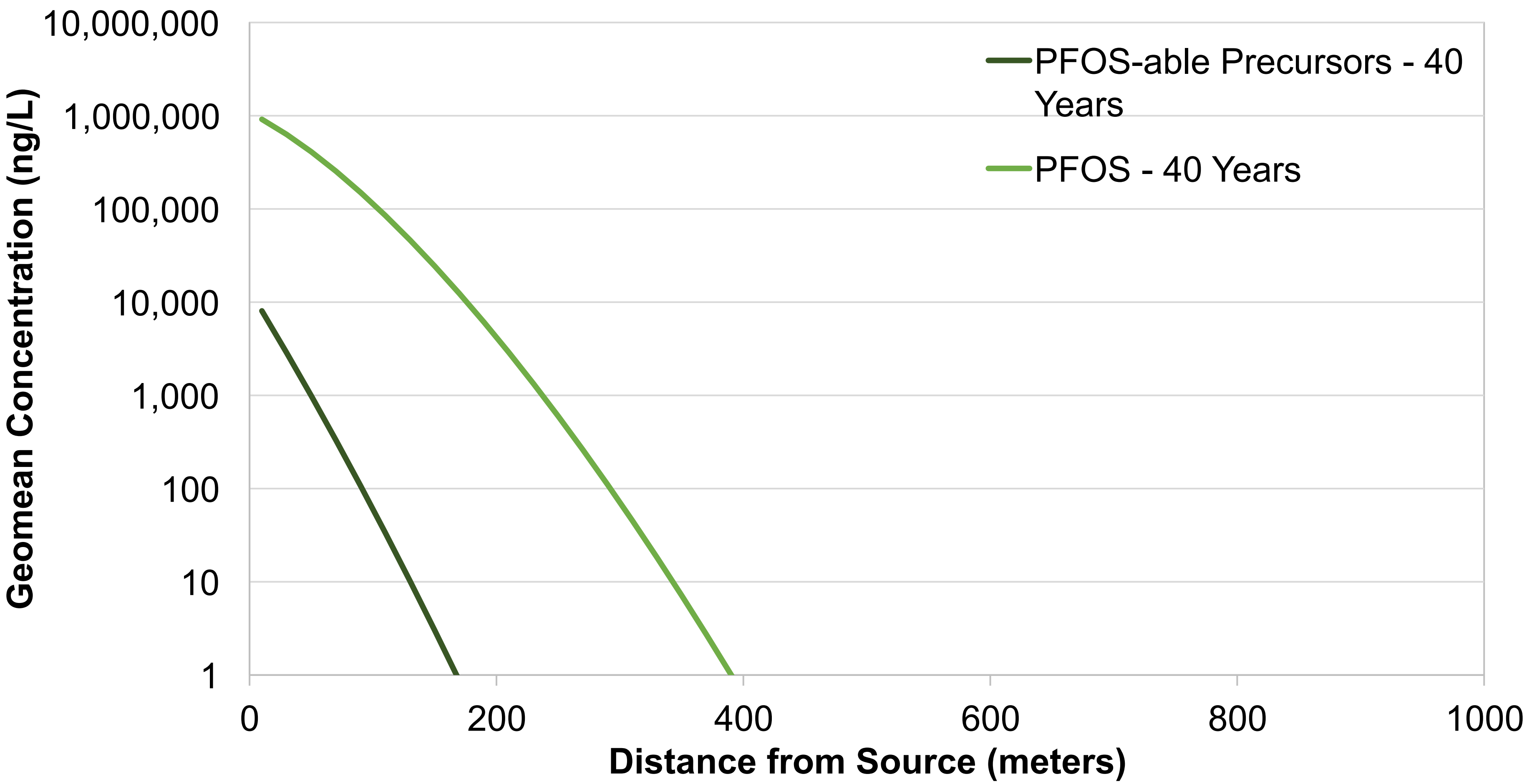
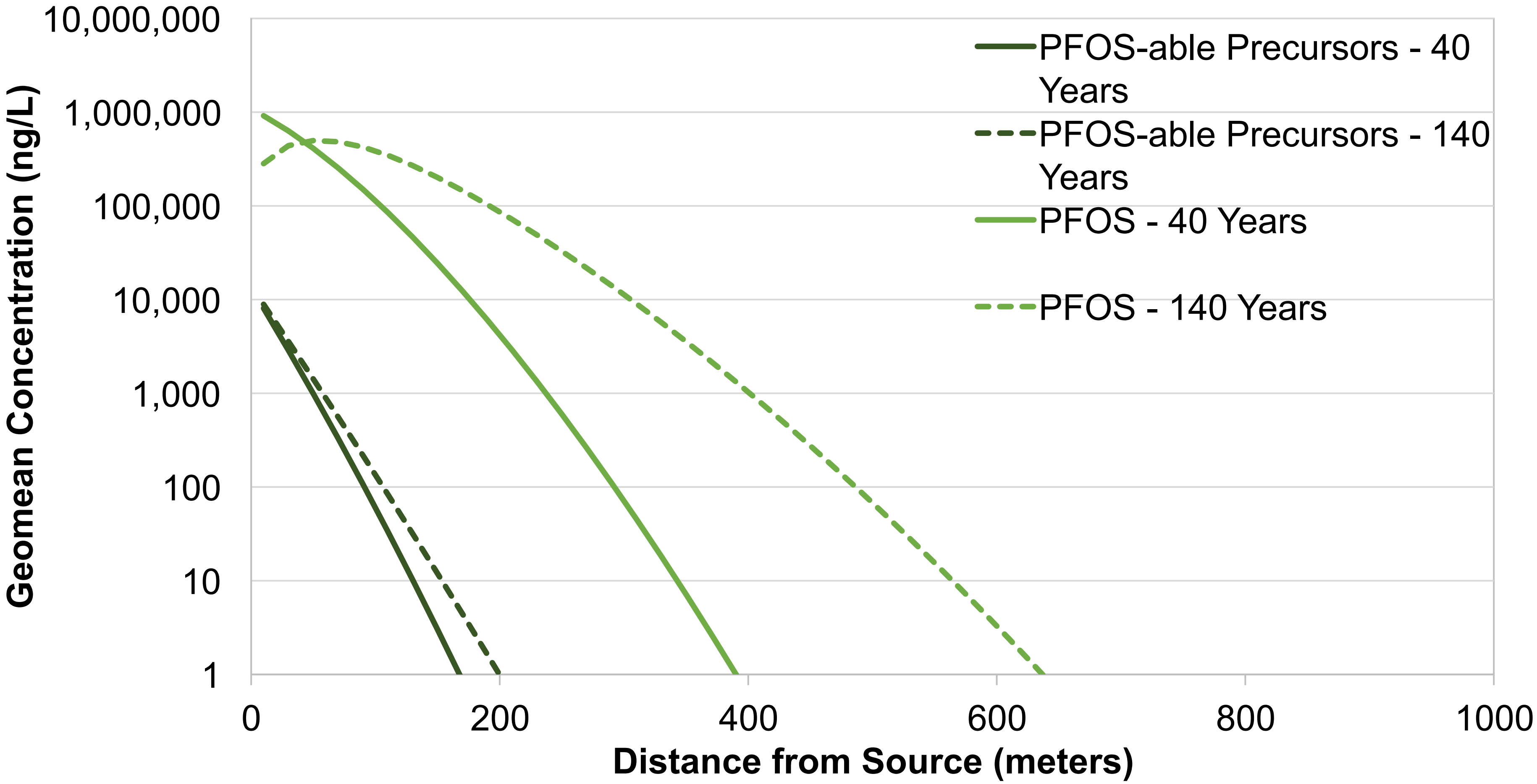
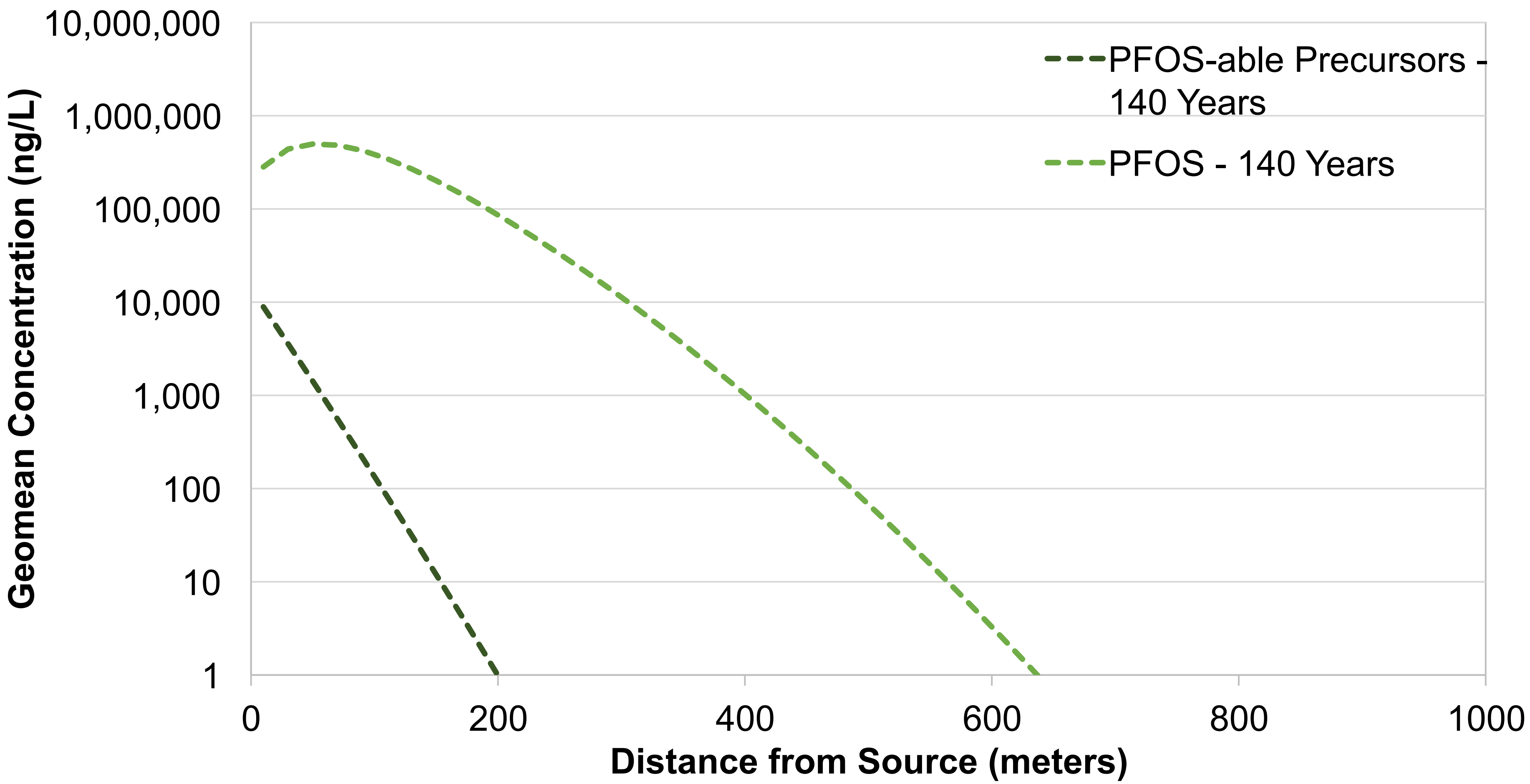


# Field Site PFOS Model – Year 140

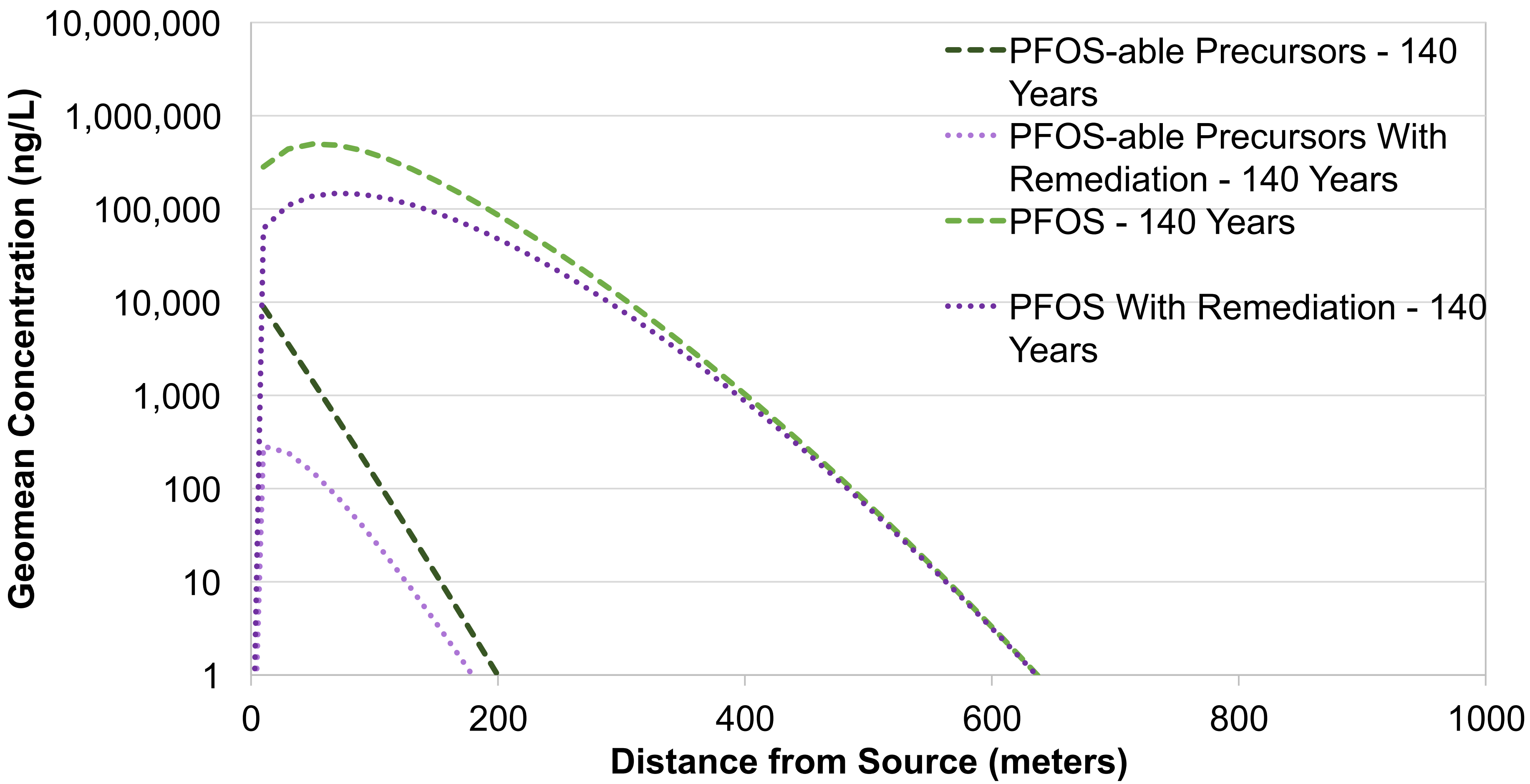



**PFOS-able precursor and PFOS plumes are still expanding due to continued release from source zone and migration of downgradient plume**

# Field Site PFOS Model – Year 140

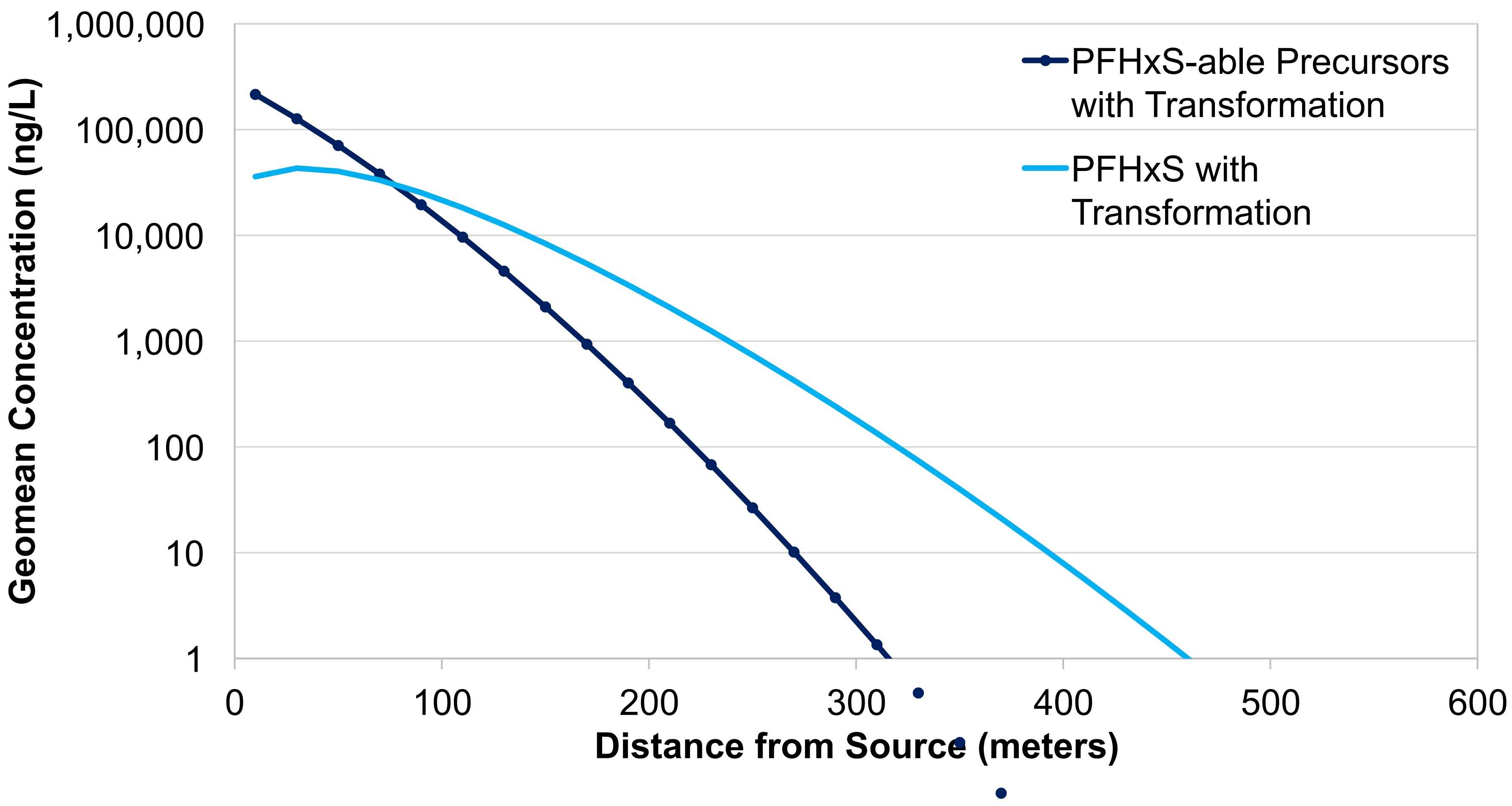


# Field Site PFOS Model – Year 140, With Source Remediation at Year 40

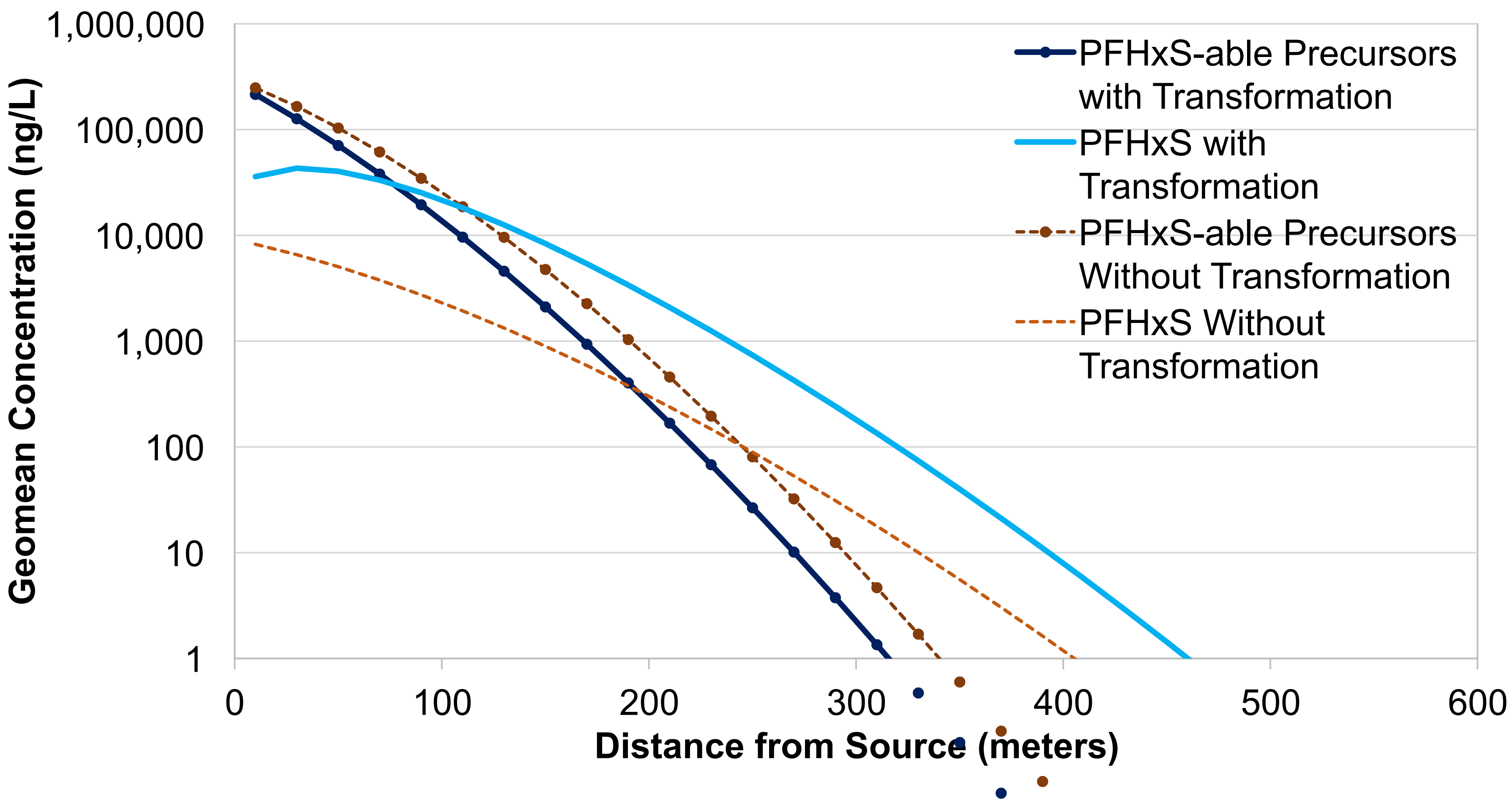



**Source concentrations decrease, but plumes persist and continue to expand downgradient due to continued migration of downgradient plume**

# Field Site PFHxS Model – Year 40

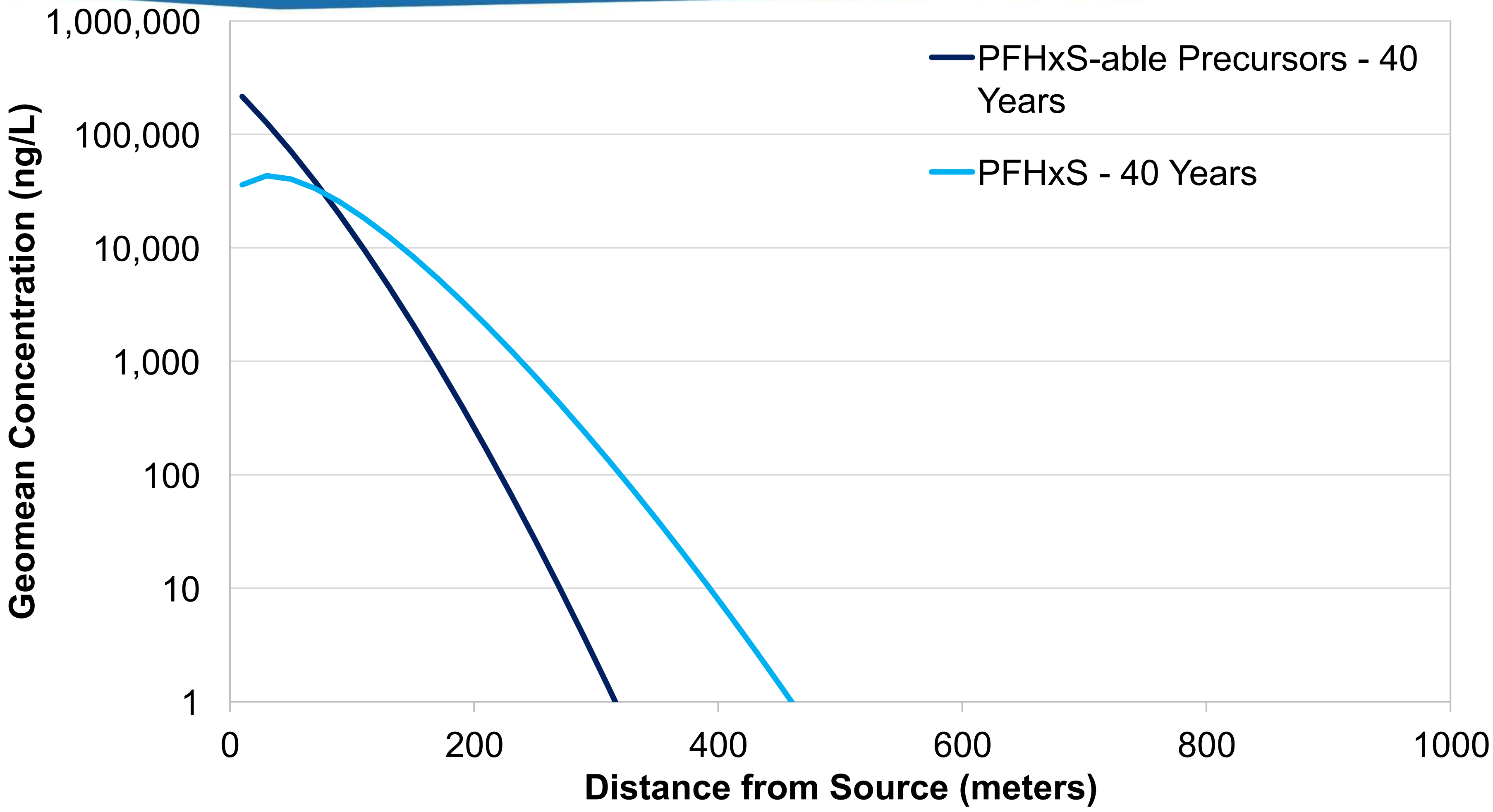


# Field Site PFHxS Model – Year 40

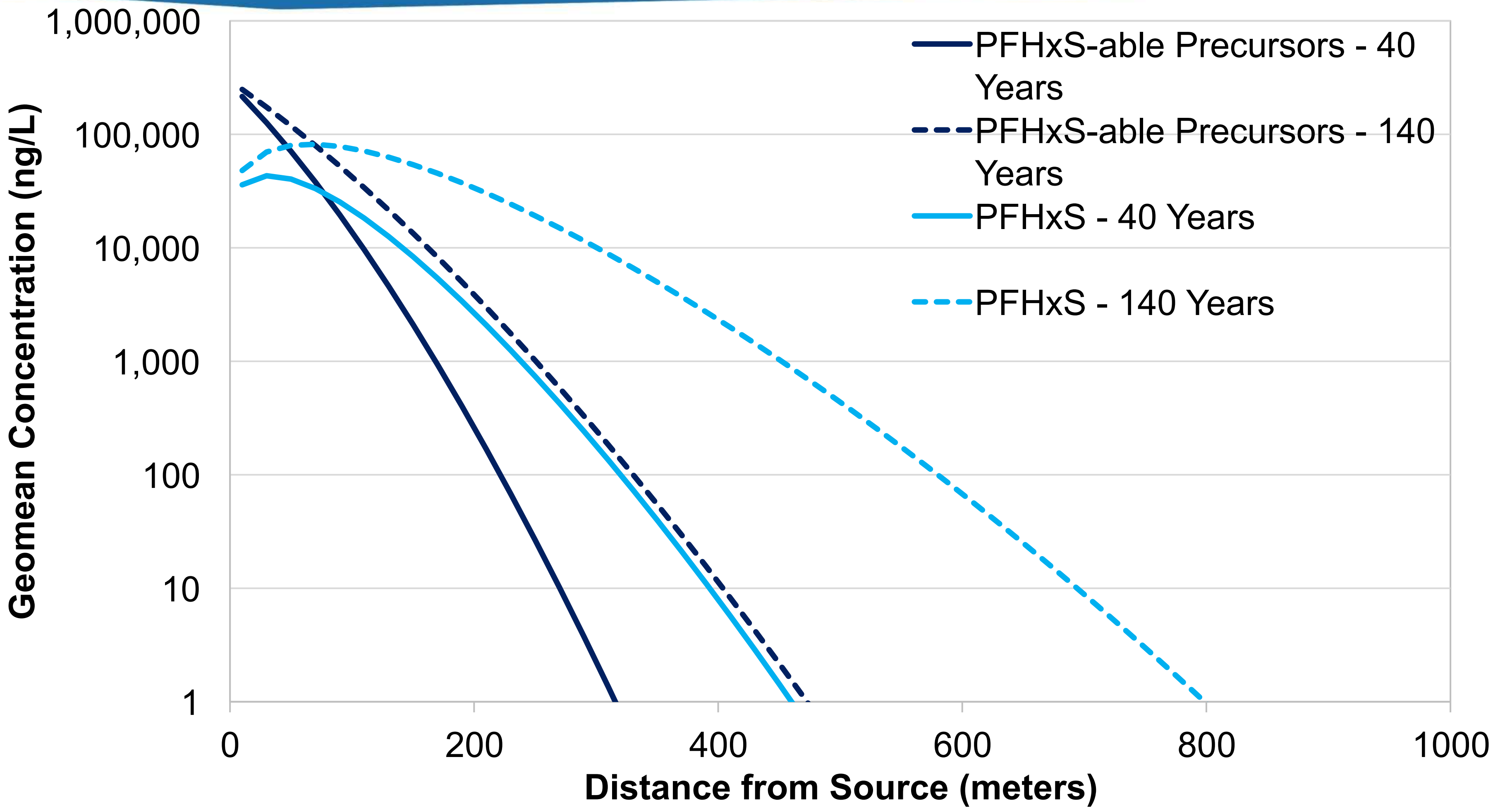



**PFHxS precursor transformation results in higher PFHxS concentrations and longer PFHxS plume**

# Field Site PFHxS Model – Year 40

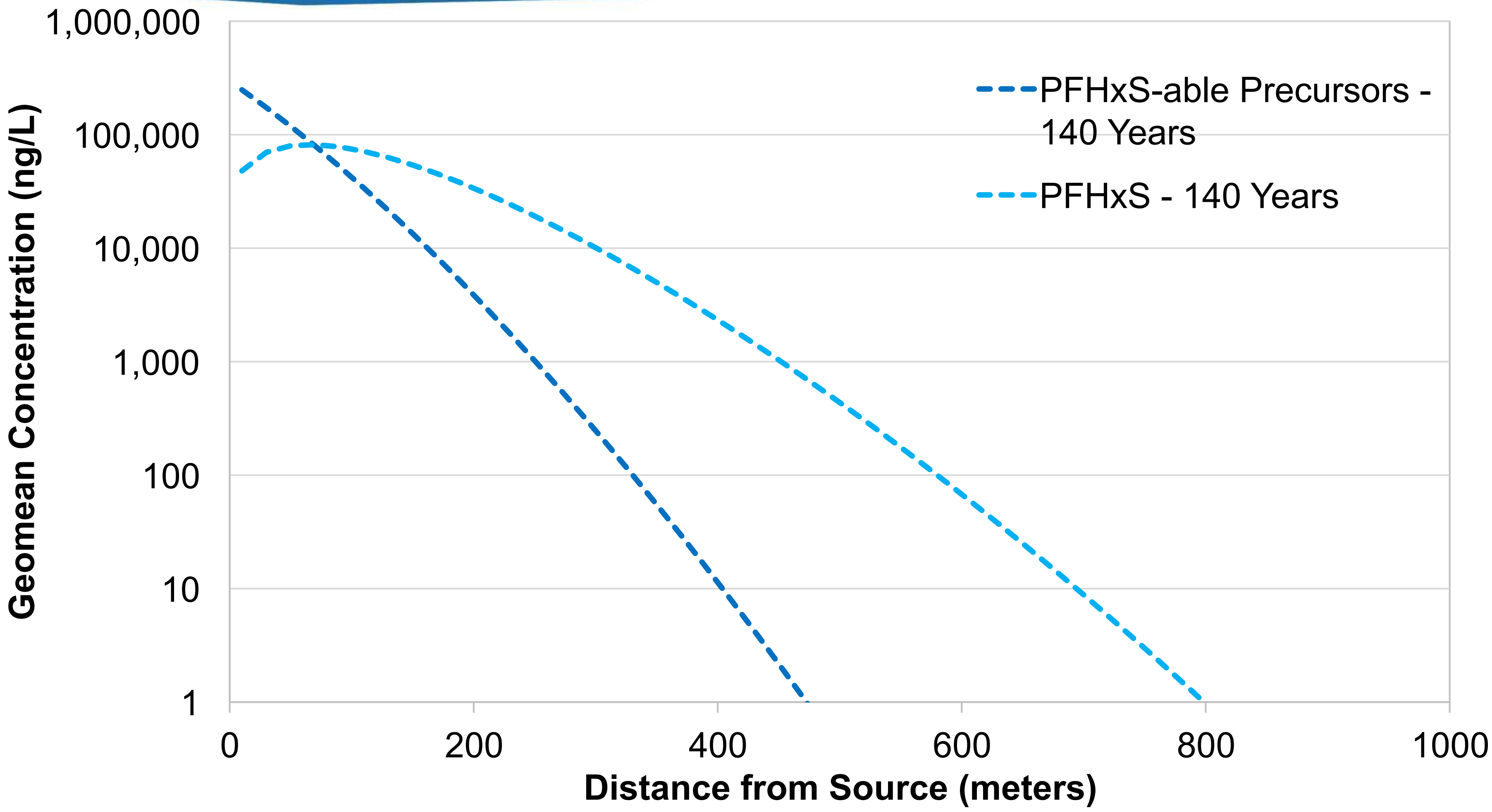


# Field Site PFHxS Model – Year 140

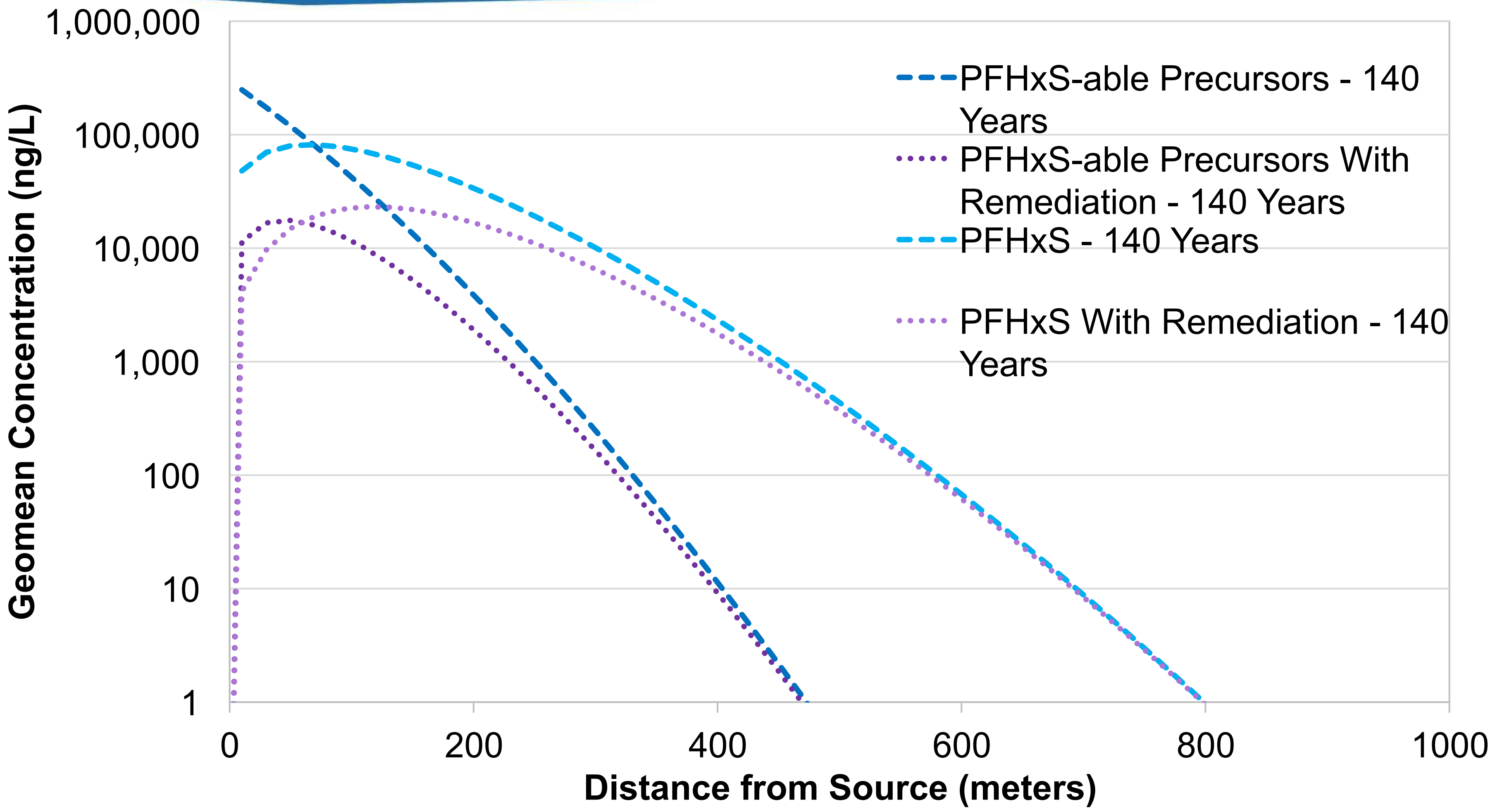



**PFHxS-able precursor and PFHxS plumes still expanding due to continued release from source zone and migration of downgradient plume; PFHxS plume also expanding due to precursor transformation**

# Field Site PFHxS Model – Year 140



# Field Site PFHxS Model – Year 140, With Source Remediation at Year 40




**Source concentrations decrease, but plumes persist and continue to expand downgradient due to continued migration of downgradient plume**

# Sensitivity Analysis Results

- Key Fate and Transport Parameters:
  - Retardation in low-k zones
  - Precursor transformation rates
  - Source mass at the time of release

| PFAS | Parameter | Precursor Plume Length % Difference from Base Case | PFAA Plume Length % Difference from Base Case |
|---|---|---|---|
| PFOS | PFOS Retardation in T-Zone | ±0% | ±8-13% |
| | PFOS Retardation in Low-k | ±0% | ±15-18% |
| | Precursor Retardation in T-Zone | ±3-6% | ±0% |
| | Precursor Retardation in Low-k | ±6% | ±0% |
| | Precursor Yield in T-Zone | ±0% | ±0% |
| | Precursor Transformation Rate | ±18-24% | ±0% |
| PFHxS | PFHxS Retardation in T-Zone | ±0% | ±7-9% |
| | PFHxS Retardation in Low-k | ±0% | ±16-21% |
| | Precursor Retardation in T-Zone | ±8-11% | ±1-2% |
| | Precursor Retardation in Low-k | ±14% | ±2% |
| | Precursor Yield in T-Zone | ±0% | ±2% |
| | Precursor Transformation Rate | ±5-6% | ±2-3% |

# Summary and Conclusions

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- Categorized potential precursors based on fluorinated carbon chain length
- High-resolution field site precursor characterization
  - Predominant precursor type = PFHxS-able precursors
  - Wide range of precursors in source area soil and groundwater; shorter-chained, anionic precursors dominate mid-plume soil and groundwater
- Modeled individual PFAAs and their grouped potential precursors using REMChlor-MD
  - Retardation and precursor transformation rates are key parameters
  - <u>Impact of precursor transformation strongly influenced by concentration difference between precursors and terminal PFAAs; greatest for PFBS, PFHxS, and PFOA; no impact on PFOS</u>
- Conclusions are specific to the modeled field site
- Manuscript of this work is currently in review
- Next up = REMFluor model