Exploring PFAS Fate and Transport in Subsurface and Groundwater:

The Role of Precursors, Subsurface Heterogeneity, and Environmental Dynamics

Presented by

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Collaborators

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Objectives

- Why PFAS are important for subsurface and groundwater
- Focus on PFAS transport and transformation
- Role of PFAS precursors
- Influence of soil and sediment variability
- Application of numerical modeling
- Implications for risk assessment and remediation

PFAS

- PFAS as emerging contaminants
  - Synthetic chemicals widely used in industrial and consumer products
  - Highly persistent in the environment ("forever chemicals")
  - Pose potential risks to human health and ecosystems

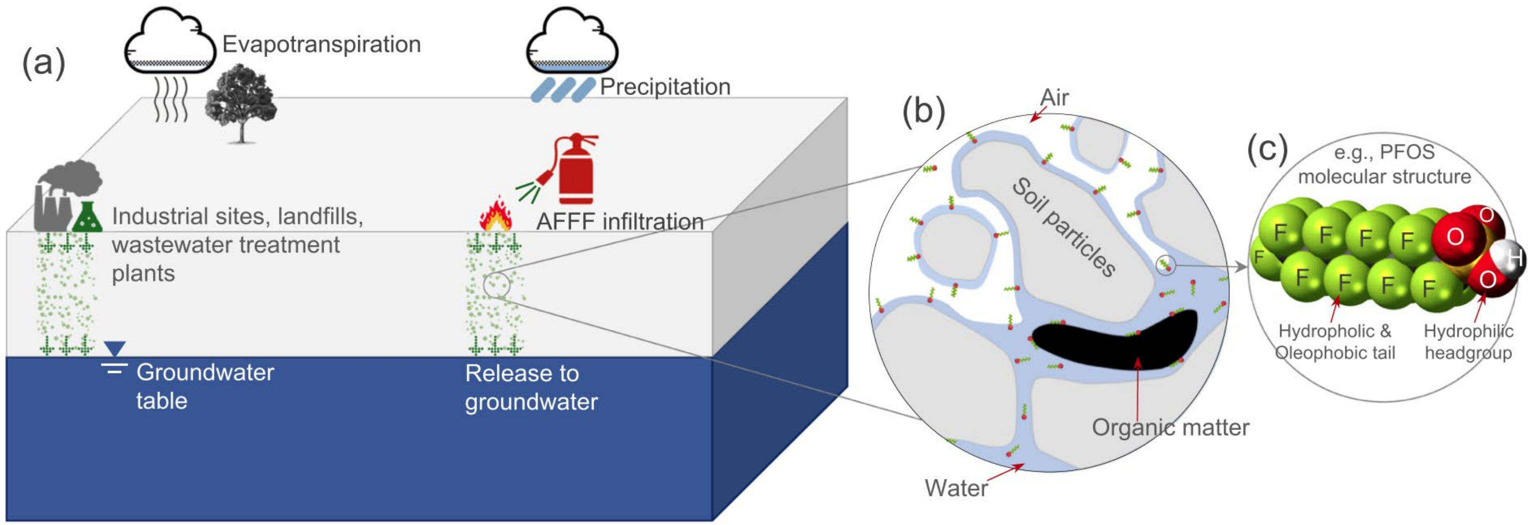


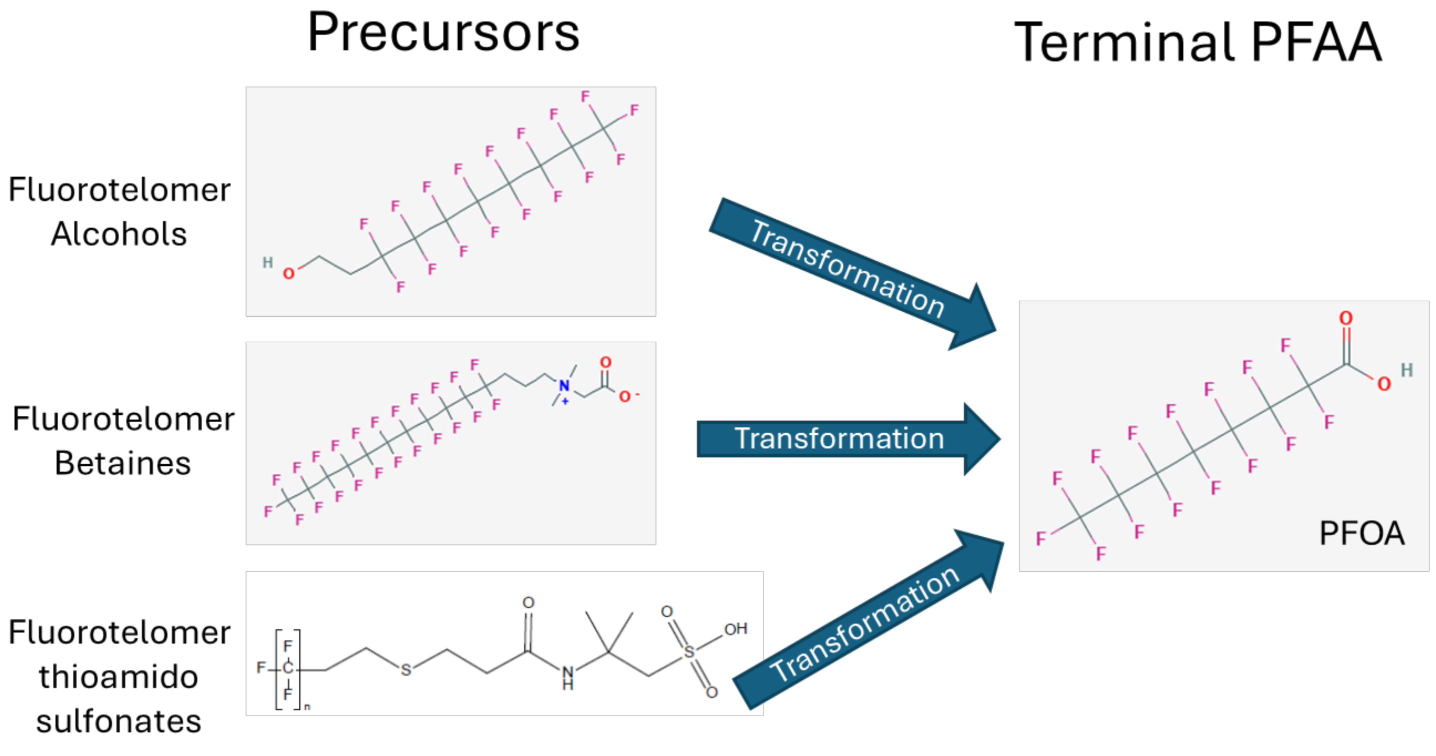
Image from Guo et al. 2019

- Subsurface transport and groundwater contamination
- Complex behavior in the subsurface
- Remediation challenges

PFOA Plume Development and Remediation

Perfluoroalkyl Acid (PFAA) Precursors

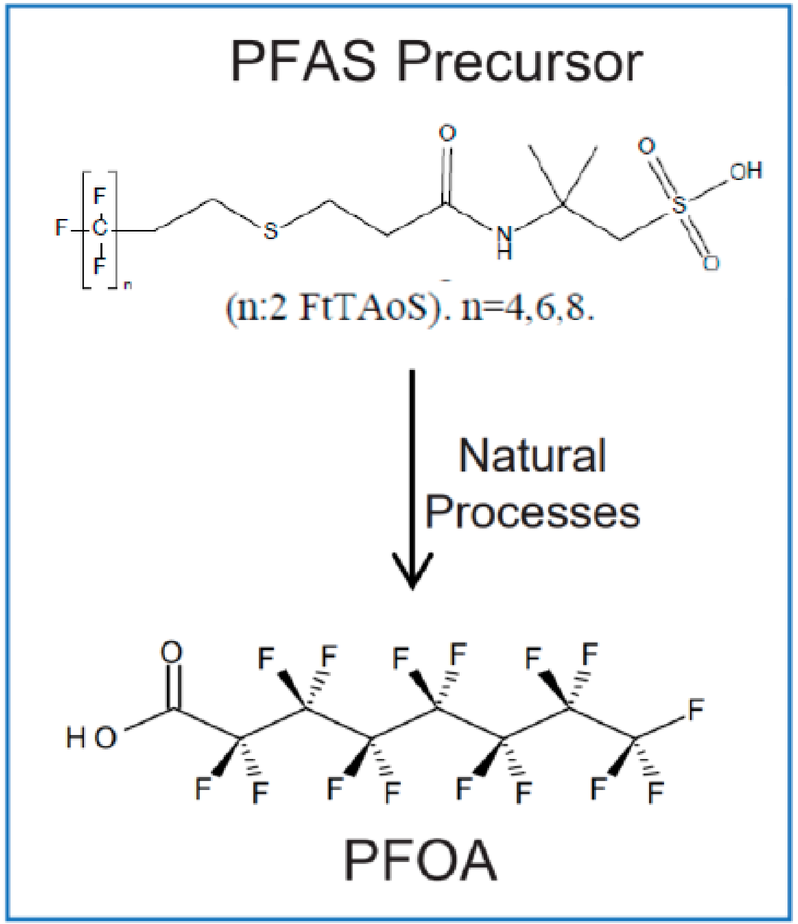
- Chemical compounds that have potential to transform and degrade into persistent and mobile PFAS compounds
- The degradation pathways are through environmental or biological processes
- Can prolong contamination and alter concentrations in groundwater and soil



Images from Chemspider 2021 and Houtz et al. 2013

Fate and Transport Modeling

- Simulate perfluorooctanoic acid (PFOA) fate and transport in heterogeneous aquifer
- Hypothetical source: precursor or PFOA
- Include precursor transformation to PFOA
- Evaluate remediation
  - Source removal
  - Pump and treat (P&T)
  - Permeable reactive barriers (PRBs)



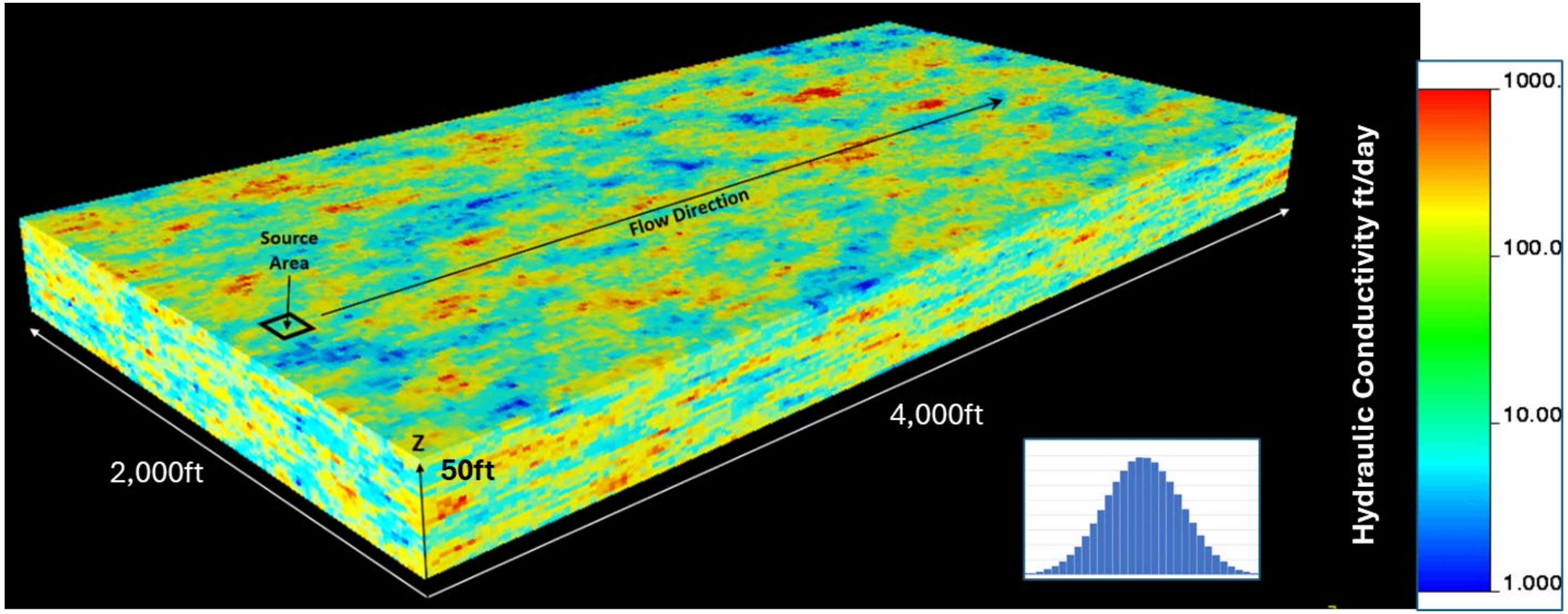
Images from Houtz et al. 2013 and Zhang et al. 2013

Methods

- 3D MODFLOW/MT3D model
  - Hypothetical alluvial aquifer with silty, fine sand to clean sand and gravel
  - Heterogeneous hydraulic conductivity and organic carbon distribution
  - Two source-area conditions (precursor or PFOA loading)
- Fate and transport simulated using literature values for PFOA and PFOA precursors, including transformation rate and yield from a generic precursor to PFOA
- Hypothetical, realistic assumptions used to illustrate a modeling approach and compare results

Model Overview (Flow)

- Grid 6 meters (m; 20 feet) horizontal and 0.6 m (2 feet) vertical
- Log-normal, spatially correlated hydraulic conductivity
- Gradient 0.0025; recharge 0.15 m/year (0.5 feet/year)



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Model Overview (Transport)

Parameter	Precursor	PFOA
K_{oc} (mL/g)	13,490	108
K_d (mL/g) range	1.35–13.5	0.0108–0.108
Half-life in aqueous phase (days)	27	Not applicable
Yield ratio (relative mass)	10	1
Effective molecular diffusion coefficient (cm^2/day)	0.19	0.23
Dispersivity (m) (longitudinal, transverse horizontal, transverse vertical)	0.6, 0.06, 0.02	
Fraction of organic carbon	0.0001 to 0.001	
Porosity	0.35	

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Fate and Transport Modeling Scenarios

Simulated Time Since Beginning of Release

Time 0 | 25 years | 50 years | 75 years

Loading → Flushing

<u>Scenarios 1</u>
Precursor loading
10,000 ng/L

<u>Scenario 2</u>
PFOA loading
840 ng/L

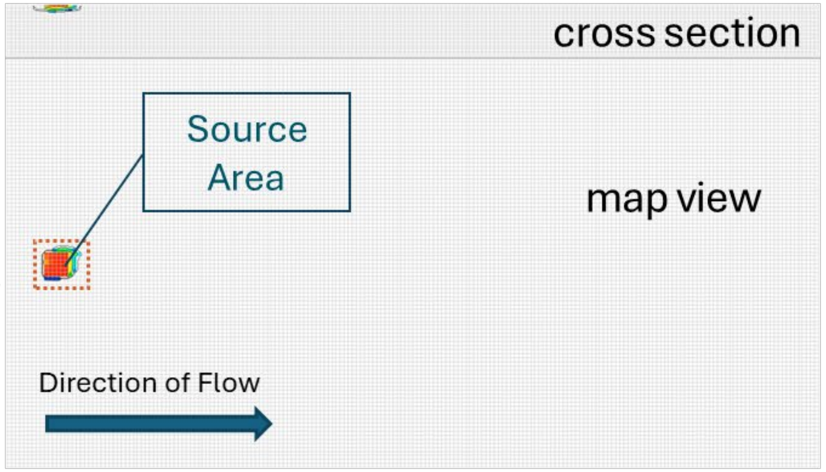
Stop loading, source removed (all simulations)

Scenario 1a: Begin P&T
Scenario 1b: Install PRBs

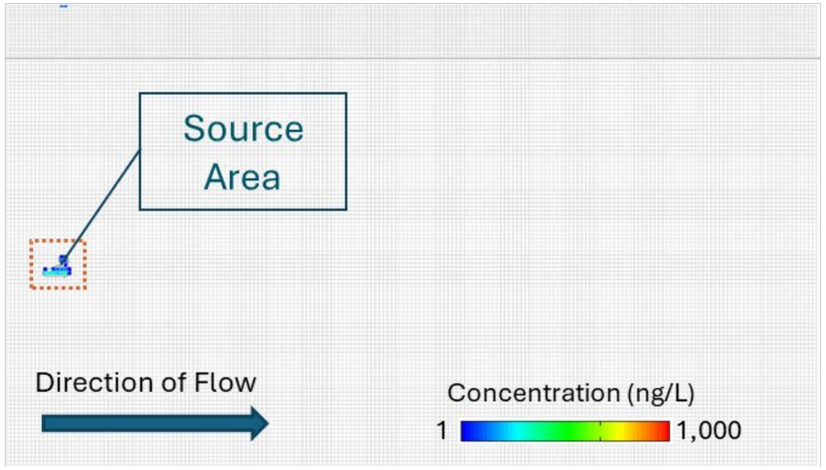
Results – Scenario 1: Precursor Loading

Precursor Plume

25 Years



50 Years

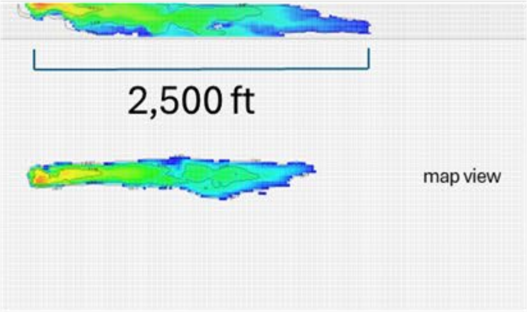


- Release occurs from t=0 to t=25 years
- Maximum 772 ng/L
- Precursor plume remains near source
- Precursor entirely transforms to PFOA before 75 years

PFOA Results – Scenarios

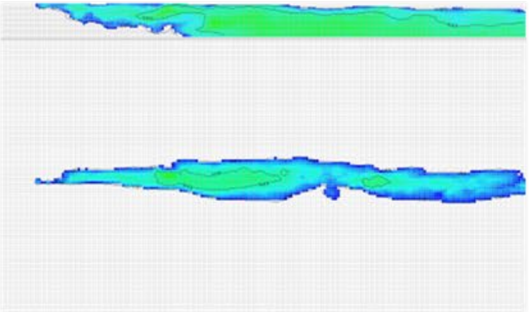
Scenario 1: Precursor Loading

25 Years



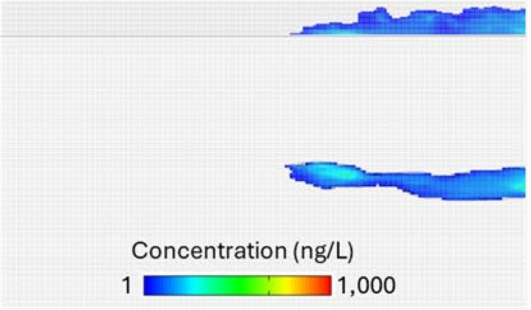
After 25 years' loading, PFOA >1 ng/L extends 2,500 feet (maximum 870 ng/L)

50 Years



Plume still attached to source area after 50 years (25 years flushing)

75 Years



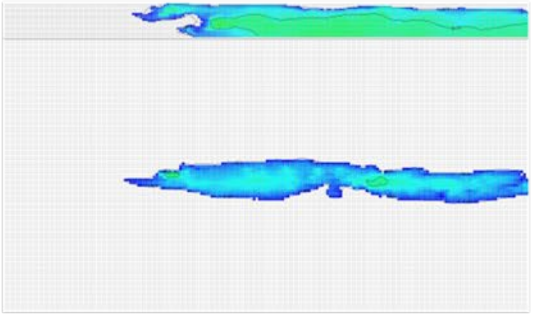
At 50+ years, plume extends beyond downgradient boundary

Significant plume remains at 75 years

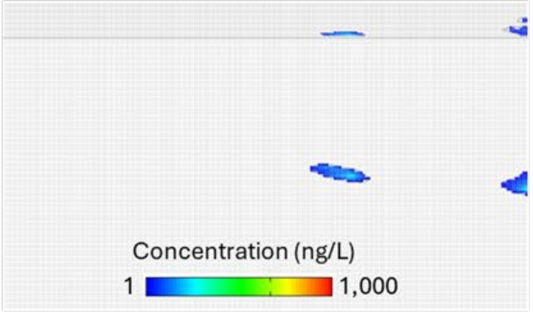
Scenario 2: PFOA Loading

After 25 years PFOA loading

- Same PFOA mass
- Very similar plume
- Similar maximum (780 ng/L)



Plume detached from source area after 50 years (25 years flushing)



Plume noticeably smaller than Scenario 1 plume at 75 years

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Simulations Thus Far Presented in *Groundwater*

Volume 60, No. 1 - January-February 2021

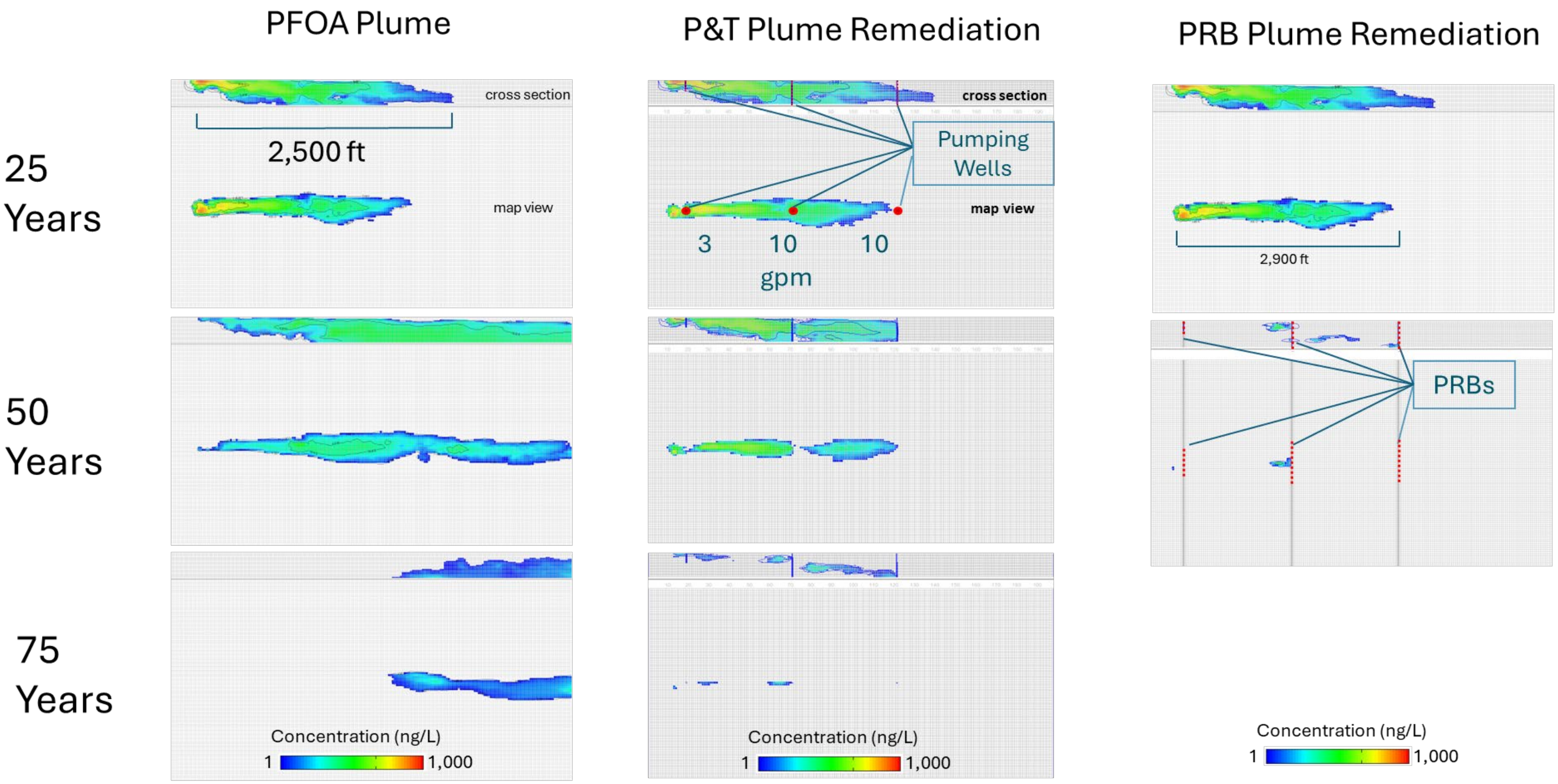
Groundwater

Rapid Communication/

Modeling PFAS Fate and Transport in Groundwater, with and Without Precursor Transformation

by Michael J. Gefell[1,2], Hai Huang[3], Dan Opdyke[4], Kyle Gustafson[1], Dimitri Vlassopoulos[3], John E. McCray[5], Sam Best[6], and Minna Carey[1]

Results – PFOA Plume Remediation



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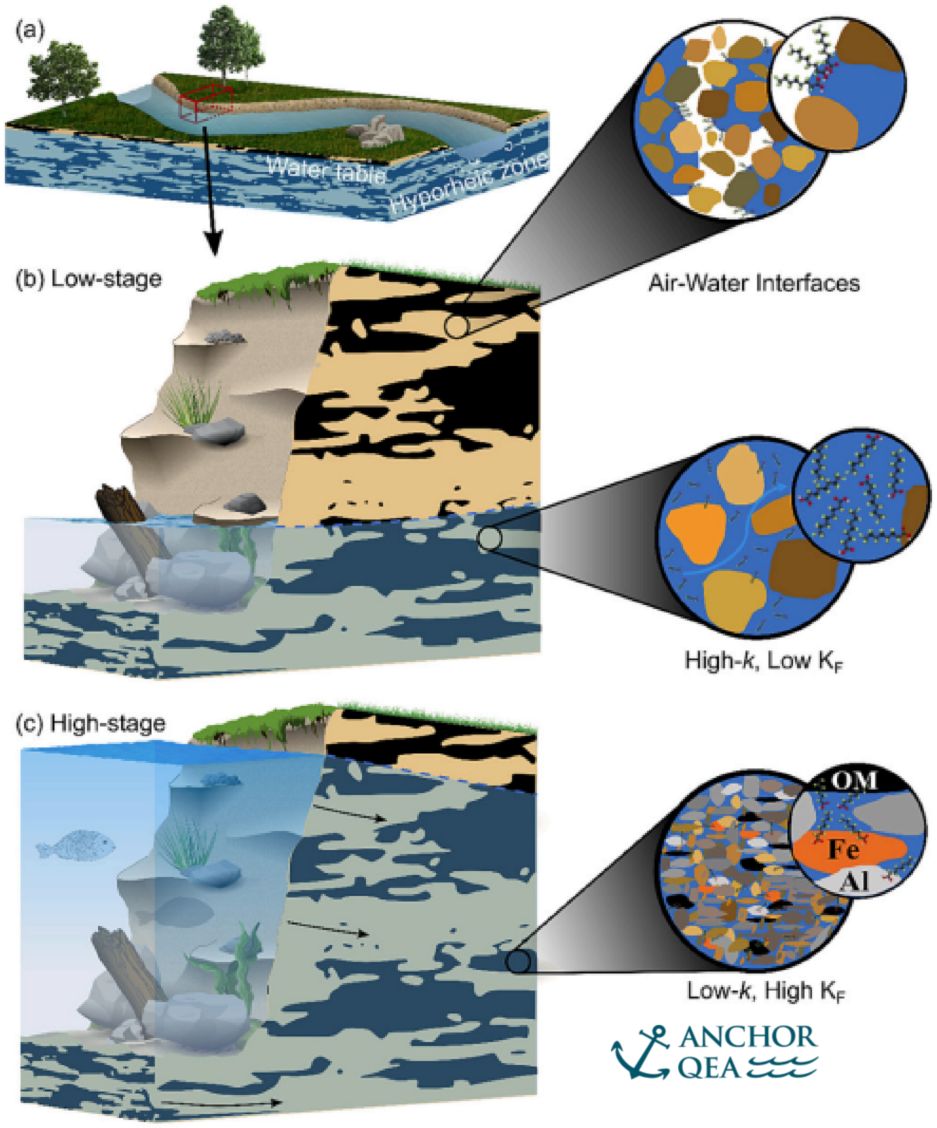
Observations

- Numerical modeling can be useful for simulating PFAS fate and transport to test “what if” scenarios
- Same PFOA plume can be calibrated using different source assumptions
  - With or without precursor(s)
- Precursors increase PFOA plume longevity, so precursor presence or absence should be carefully considered
- P&T can expedite downgradient plume remediation, but beware of stagnation zones
- PRBs may remediate PFOA plumes more quickly than P&T

PFAS Sorption and Soil or Sediment Variability

PFAS Sorption and Soil or Sediment Variability

- Subsurface heterogeneity is critical to PFAS transport and retention.
- Two primary sorption mechanisms
  - Solid-phase sorption
  - Air-water interface (AWI) sorption
- Recent studies show AWI sorption is a major factor contributing to PFAS retention in the vadose zone (over 70% of PFAS mass can accumulate in some cases)
- Study Goal: Understand PFOA fate and transport in the hyporheic zone, focusing on the effects of physical and geochemical sediment heterogeneity
- Using transient flow and reactive transport models



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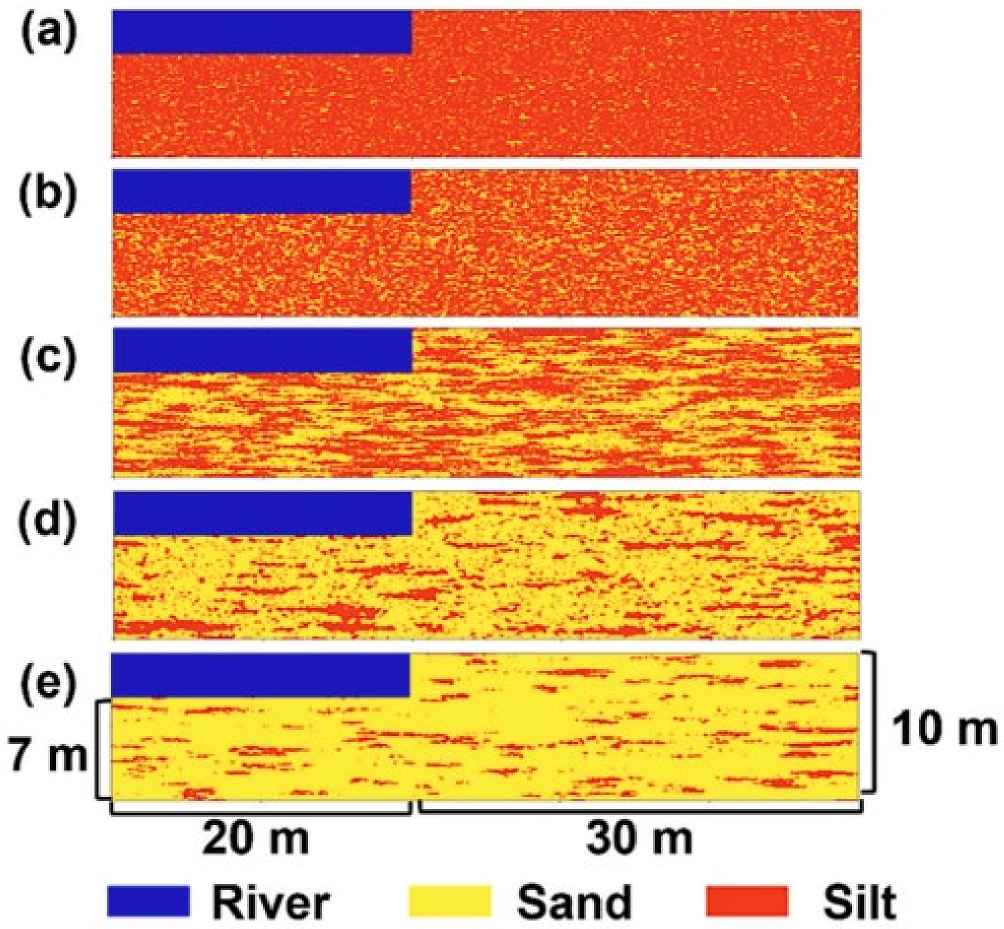
Fate and Transport Modeling

- PFLOTRAN numerical modeling (saturated/unsaturated)
- The river was set to be the PFOS source and water level fluctuates with time
- The sand volume proportion varied between 10%, 25%, 50%, 75%, and 90%
- As the sand proportion increases, the sand facies connectivity also increases
- All solute transport simulations were run for 48 hours



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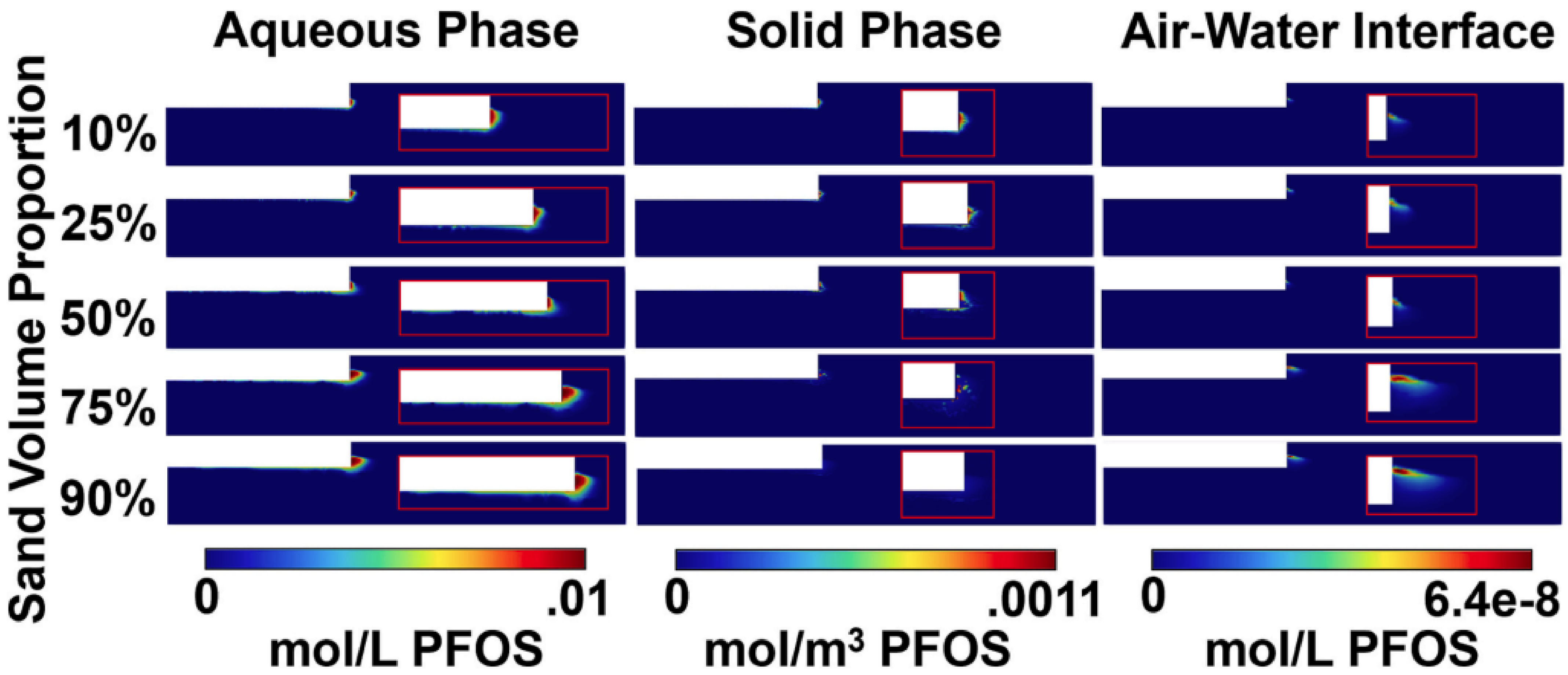
Results



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Observations

- Sensitivity analyses have shown sediment grain size exerts strongly influences PFAS fate and transport
  - Groundwater flow rate
  - AWI sorption
  - Solid phase sorption
- Thus, sedimentary architecture and the resulting facies connectivity plays a crucial role in the fate and transport of PFAS

Conclusions

- PFAS fate and transport is highly complex, but modeling tools are available to estimate PFAS behavior in the environment.
- A PFOA plume could be from a precursors source or a PFOA source; the source type would influence plume longevity.
- PRBs made remediate a PFOA plume more quickly than P&T in some cases.
- PFAS sorption to AWI is important and should not be neglected.

Thank you for your attention!