BEM SYSTEMS

Derivation of Site-Specific Soil Standards Reflective of Mass Loading from PFAS Source Areas

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RESEARCH NEED & OBJECTIVES

EPA Standard SSL equation

$SSL = C_{gwt} \times DAF \times [K_d + ((\Theta_w + \Theta_a H)/\rho_b)]$

Where: $K_d = f_{oc} K_{oc}$

Objective: derive Site-Specific Soil Cleanup Values accounting for PFAS retention

$SSL = C_{gwt} \times \mathbf{DAF} \times [\mathbf{K_d} + \mathbf{K_{aw}\, A_{aw}} + ((\Theta_w + \Theta_a H)/\rho_b)]$

Where:

- *DAF accounts for site-specific properties*
- $K_d = \sum_{i=1}^{n} f_i \cdot K_i$
- ***$K_{aw}\, A_{aw}$ Accounts for PFAS adsorption at the air water interface***

BENEFIT:

Develop methodology to calculate actionable site-specific soil clean-up values from site data

→Prevent unnecessary remedial action that do not pose a risk to human health or the environment.

Processes such as adsorption at the air-water interface can significantly impact PFAS transport and should be considered in determination of SSLs

APPROACH

Source Area Selection

↓

Field Work (BEM & Arcadis)

Subsurface soil sampling	Lysimeter installation	Porewater sampling (5 rounds)

↓

Laboratory and Bench Analysis (UAZ)

Obtain high-resolution model input parameters	Inform proportion of PFAS retained by different sorptive domains

↓

Modeling (UAZ)

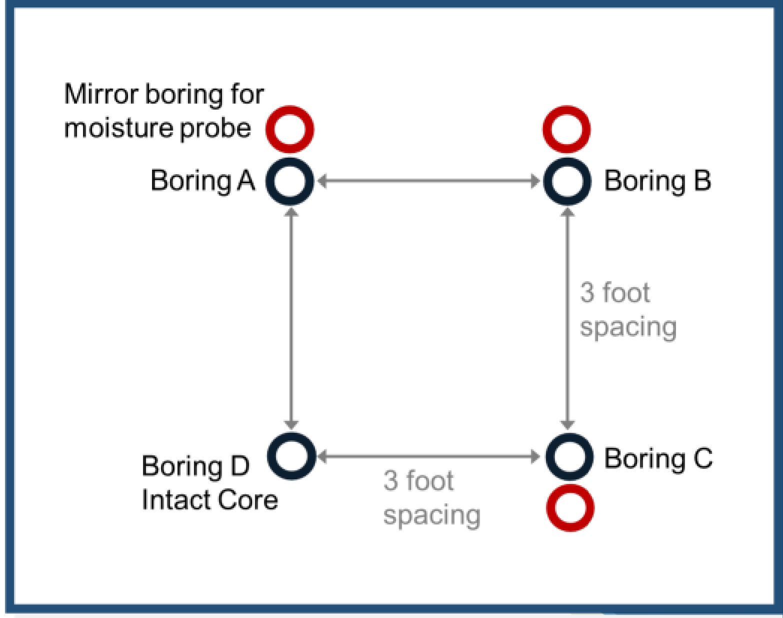
Tiered modeling approach	Simplest model evaluation	Calibration and Validation

SOURCE AREA SELECTION

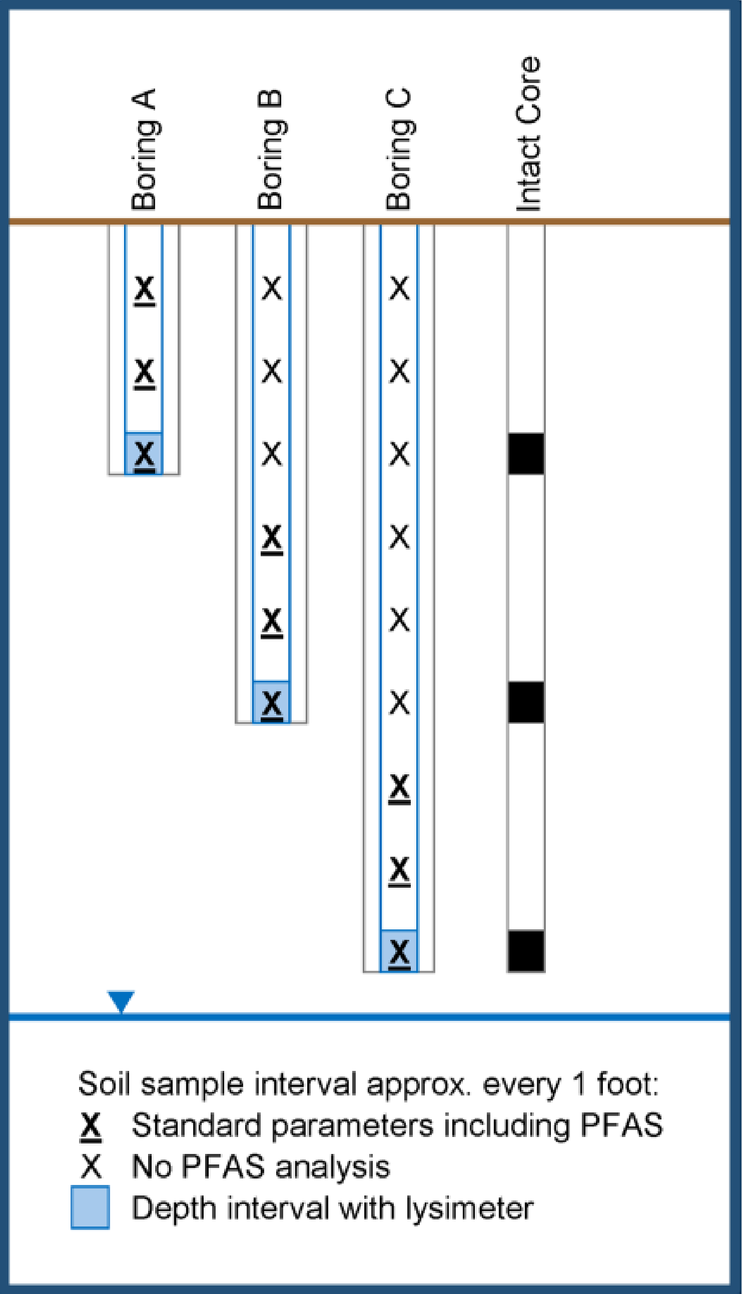
- Historical data (CSM), including PFAS analytical results (soil and groundwater) and boring logs.
- Range of PFAS concentrations
- Soil texture → avoiding gravelly sands
- Avoided asphalt (limits infiltration)

FIELD WORK

- 9 lysimeter clusters co-located with soil moisture monitors
- Intact core
- Porewater monitoring events → seasonal impacts on PFAS concentrations in PW



Plan view showing up to three lysimeters and *in-situ* soil moisture probes per location



Cross section schematic of lysimeters and soil borings

FIELD WORK

From the 9 lysimeter clusters one cluster was selected to validate the model based on:

- Availability of soil and porewater.
- PFAS analytical results (maximum soil concentrations and initial lysimeter porewater sample concentrations), and
- Soil moisture response to precipitation events
- Soil type (soil texture and particle size distribution).

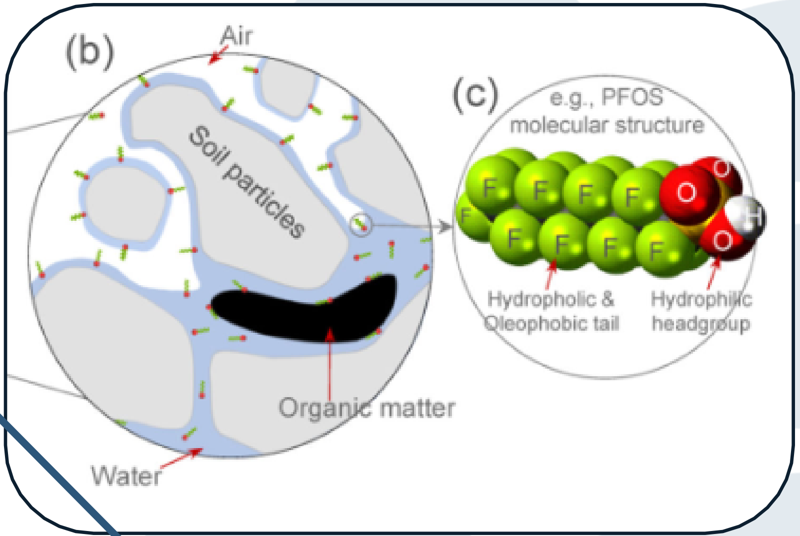
Example soil core and stainless steel lysimeter

Direct push drilling near the runway ramp and fire station

LABORATORY AND BENCH ANALYSIS: PARAMETERIZATION

Measurement (Soil)	Classification	Availability
PFAS	Tier 1	Specialized commercial lab
Bulk density	Tier 1	standard commercial lab
Porosity	Tier 1	standard commercial lab
Soil texture (gravel, sand, silt, clay)	Tier 1	standard commercial lab
Particle size distribution (PSD)	Tier 1	standard commercial lab
Soil pH	Tier 1	standard commercial lab
Cation exchange capacity (CEC)	Tier 1	standard commercial lab
Anion exchange capacity (AEC)	Tier 1	standard commercial lab
Soil electrical conductivity (EC)	Tier 1	standard commercial lab
Soil organic carbon content (OC)	Tier 1	standard commercial lab
Soil total carbon (TOC)	Tier 1	standard commercial lab
Metal oxides	Tier 2	specialized commercial lab
Clay mineralogy	Tier 2	specialized commercial lab
Solid surface area (SSA)	Tier 2	specialized commercial lab
Saturated hydraulic conductivity (Ksat)	Tier 2	specialized commercial lab
Soil water characteristic curve (SWC)	Tier 2	specialized commercial lab
Air-water interfacial area (A_{aw})	Tier 3	UAZ lab
Sorption measurement (K_d)	Tier 3	UAZ lab
Air-water interfacial adsorption coefficient (K_{aw})	Tier 3	UAZ lab

Measurement (Porewater)	Classification	Availability
Bromide	Tier 1	commercial lab
PFAS	Tier 1	commercial lab
Electrical conductivity (EC)	Tier 1	commercial lab
Total dissolved solids (TDS)	Tier 1	commercial lab
pH	Tier 1	commercial lab
Oxidation-reduction potential (ORP)	Tier 1	commercial lab
Ionic composition	Tier 2	UAZ lab

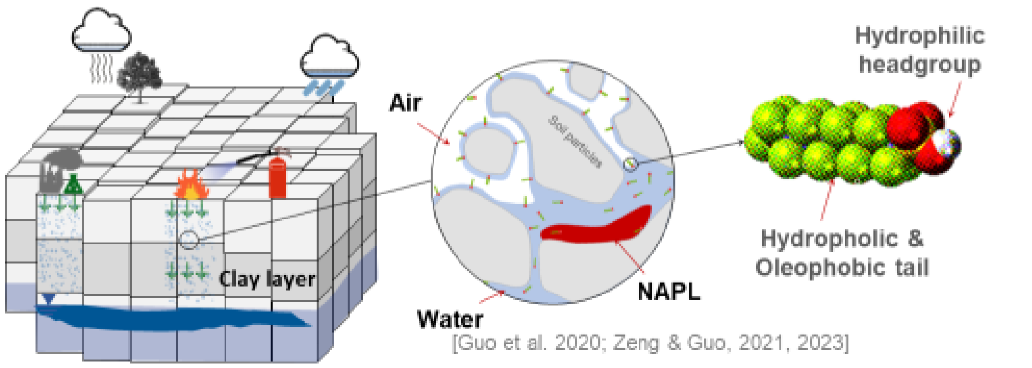


$$SSL = C_{gwt} \times \mathbf{DAF} \times [\mathbf{K_d} + \mathbf{K_{aw}}\ \mathbf{A_{aw}} + ((\theta_w + \theta_a H)/\rho_b)]$$

TIER 1 – PFAS-LEACH-COMP-GW

Features: Full-process model in 3D

- *Anticipated application:* Sites with sufficient data; complex spatial heterogeneity and/or source conditions



Attenuation Treatment

- Transient variably saturated flow
- Surfactant-induced flow
- Nonlinear and kinetic sorption
- Nonlinear and kinetic air-water interfacial adsorption

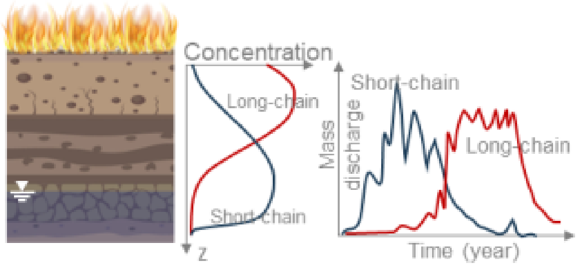
$$h = \frac{\sigma}{\sigma_0} h_0$$

$$C_s = K_f C^N$$

$$C_{aw} = A_{aw}\Gamma = A_{aw}K_{aw}C$$

(Zeng et al., 2021; Guo et al., 2020)

TIER 2 – PFAS-LEACH-HYDRUS-GW



Features: Implemented in HYDRUS-1D GUI

- *Anticipated application:* Insignificant lateral heterogeneity; uncertainty quantification

[Zeng et al. 2021]

Attenuation Treatment

- Transient variably saturated flow
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$$h = \frac{\sigma}{\sigma_0} h_0$$

$$C_s = K_f C^N$$

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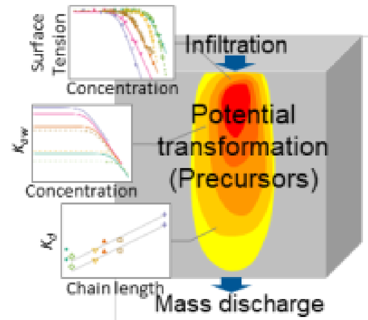
(Guo et al., 2020)

TIER 3 – PFAS-LEACH-ANALYTICAL-GW



Features: Implemented in Excel

- Mode 1: Analytical solutions of linearized 1D transport equation
- Mode 2: Simple compartment model to compute source attenuation and mass discharge

Anticipated application: Limited data; early stage of site management; order-of-magnitude estimate.

[Guo et al. 2022

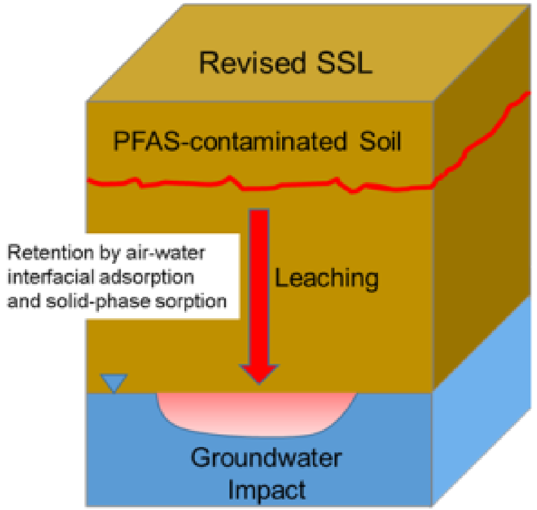
$$DF = 1 + \frac{U_{gw}\delta_{gw}}{I_f W}$$

Attenuation Treatment

- Steady-state water infiltration
- Linear, kinetic sorption
- Linear, equilibrium air-water interfacial adsorption
- Homogenous & uniformly saturated vadose zone

(Guo et al., 2022)

TIER 4 – PFAS-LEACH-DAF



Features: Revised EPA dilution-attenuation model

- Simplified mass-balance calculations

Anticipated application: Initial screening of sites

[Brusseau & Guo, 2023]

$$DAF = 1 + \frac{k\,i\,d}{I\,L}$$

Attenuation Treatment

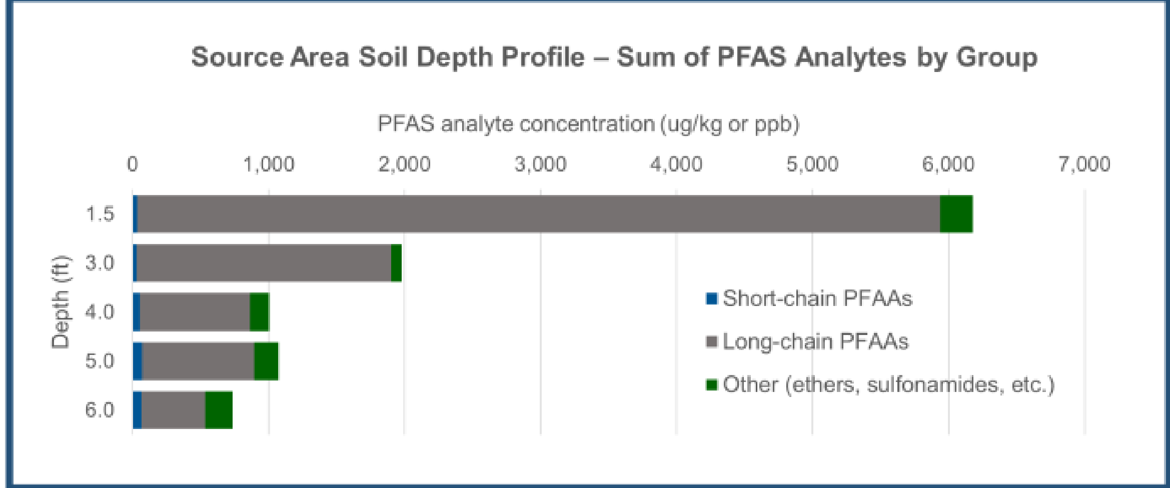
- Dilution in groundwater
- No attenuation in the vadose zone

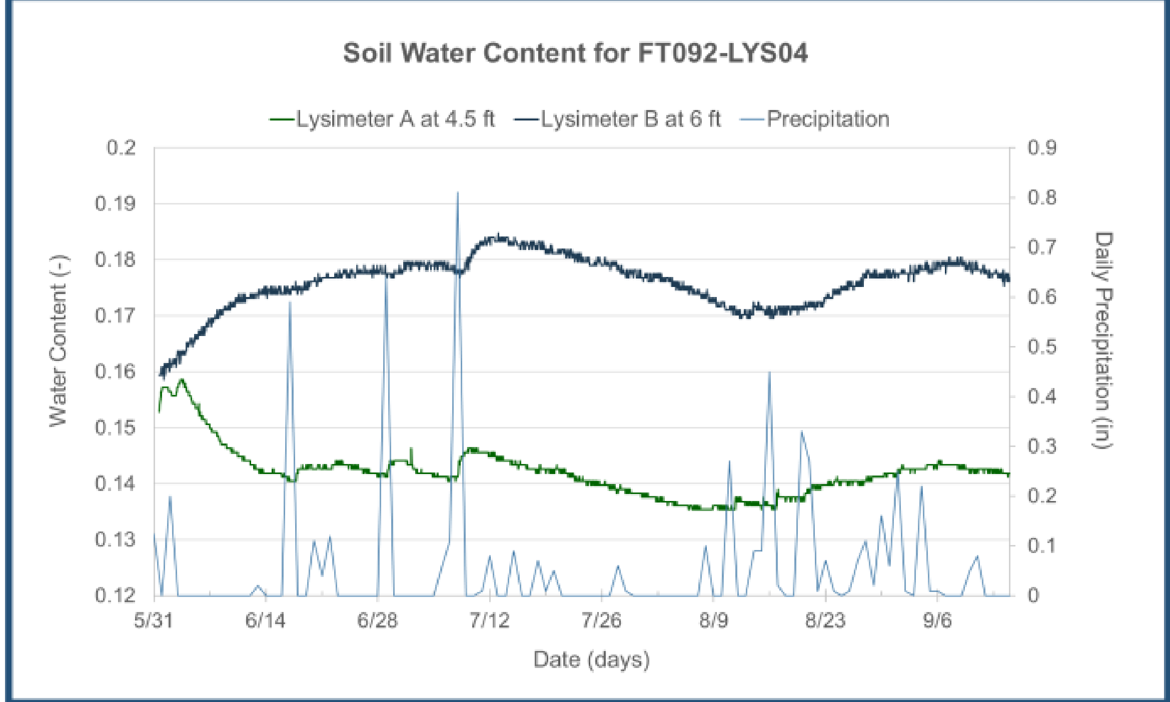
(Brusseau and Guo, 2023; Smith et. al, 2024)

MODEL CALIBRATION

Calibration → determine the most representative input parameters

- Simulations will first be conducted using the initial input parameters determined from the independent soil characterizations
- Simulation results will be compared to measured soil moisture and soil PFAS concentration data
- Performed iteratively until the match between simulated and measured results improves

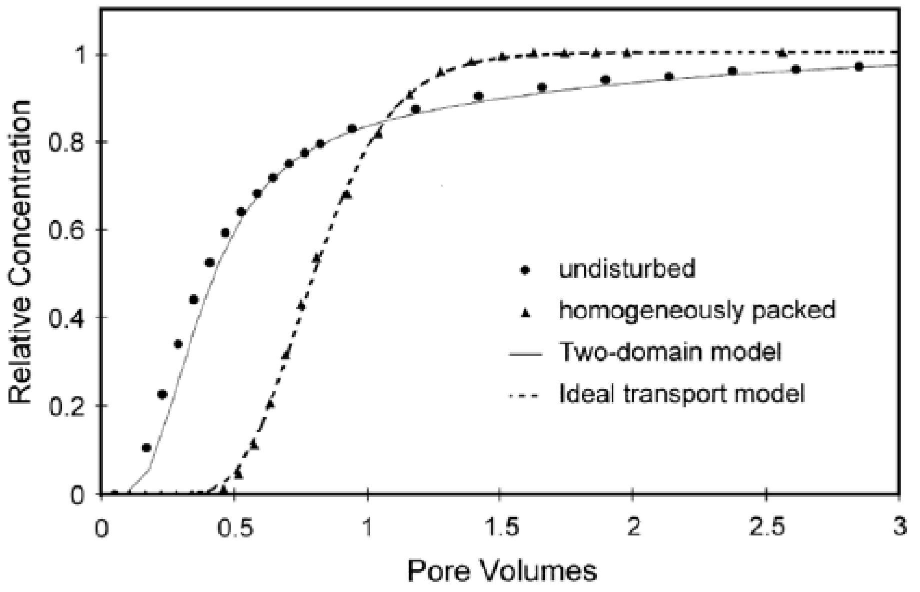




MODEL VALIDATION

Intact core experiments

- Characterize the change in porewater concentrations and the magnitude of PFAS leached under realistic but controlled conditions.
- Compare leaching test results to interfacial -tracer tests
- Inform amount and proportion of PFAS retained by the PFAS-specific sorption processes
- Impact of physical heterogeneity (soil structuring) on PFAS leaching



Nonreactive Tracer Breakthrough Curve

(Johnson et al, 2003)

ILLUSTRATIVE APPLICATION OF THE DAF MODEL

Parameter	Parameter Source	PFOS		PFOA	
		Standard Model	Revised Model	Standard Model	Revised Model
Dilution Factor (DF)	ADEC default	3.3	3.3	3.3	3.3
Attenuation Factor (AF)		4	4	4	4
Dilution-Attenuation Factor (DAF)		13.2	13.2	13.2	13.2
Soil-Water Partitioning Term	Calculated	2.1	37.8	1.1	3.5
Target groundwater concentration (C_{gw}, µg/L)[a]	Assumed	0.1	0.1	0.1	0.1
Soil Screening Level (SSL, µg/kg)	Calculated	2.8 [ADEC=3.0]	49.9	1.5 [ADEC=1.7]	4.6

[a]*Target groundwater concentration is an arbitrary value for illustration purposes only.*

Input Parameter Values:

- Porosity = 0.4,
- Water content = 0.2,
- Air content = 0.2,
- Bulk density = 1.5,
- K_d = 2(PFOS)/1(PFOA),
- **K_{aw} = 1.2(PFOS)/0.008(PFOA),**
- **A_{aw} = 446**

Note that the K_d and A_w values are measured for a surrogate vadose zone soil

$$SSL = C_{gwt} \times \mathbf{DAF} \times [\mathbf{K_d} + \mathbf{K_{aw}}\, \mathbf{A_{aw}} + ((\Theta_w + \Theta_a H)/\rho_b)]$$

(Brusseau and Guo, 2023)

CONCLUSIONS AND FUTURE WORK

- PFAS-specific sorption processes can significantly impact PFAS transport and should be considered in determination of SSLs
- Impact to prioritization of sites for remedial action

What requires a rigorous approach?

- If soil concentrations exceed the DAF SSL → pursue a sites-specific SSL is required
- Very deep depth to GW→ER24-8160 Framework for Site Specific Source Strength and Leaching at AFFF Sources

BEM

THANK YOU

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(ER21-5041)

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EXTRA SLIDES

Parameter	Symbol	Units	Tier 1	Tier 2	Tier 3	Tier 4
Air-water interfacial area	A_{aw}	cm^{-1}	✓	✓	✓	✓
Saturated hydraulic conductivity tensor	K_s	cm/sec	✓	✓	✓	
Saturated water content	θ_s	(-)	✓	✓	✓	
Residual water content	θ_r	(-)	✓	✓	✓	
Porosity	Φ	(-)	✓	✓	✓	
Bulk density	ρ_b	g/cm^3	✓	✓	✓	
van Genuchten parameter (alpha)	α	cm^{-1}	✓	✓	✓	
van Genuchten parameter (n)	n	(-)	✓	✓	✓	
van Genuchten parameter (m)	m	(-)	✓	✓	✓	
Aqueous diffusion coefficient	D_0	cm^2/s	✓	✓	✓	
Solid-phase adsorption parameters	K_f, N	$(\mu mol/g)/(\mu mol/cm^3)^N$	✓	✓		
Parameters for kinetic solid-phase adsorption	Fs, α_s	(-), /s	✓	✓		
Parameters for kinetic air-water interfacial adsorption	Faw, α_{aw}	(-), /s	✓	✓		
Szyszkowski parameters for PFAS	a, b, σ_0	various	✓	✓		
Dispersivity	α_L, α_T	cm	✓	✓		
Air-water interfacial adsorption coefficient	K_{aw}	(-)			✓	✓
Parameters for kinetic solid-phase adsorption	Fs, α_s	(-), /s			✓	
Average groundwater velocity	U_{gw}	cm/s			✓	
mixing zone depth	δ_{gw}	cm			✓	
vertical dispersivity	α_v	cm			✓	
lateral width of the contaminated site	W	cm			✓	
net infiltration rate	I_f	cm/s			✓	
Actual water content	θ	(-)			✓	
Sorption coefficient	K_d	(-)			✓	
Longitudinal dispersity	α_L	cm			✓	
Target concentration in groundwater	C_{gw}	µg/L or ng/L				✓
Hydraulic gradient	i	m/m				✓
Aquifer thickness	d	m				✓
Infiltration or recharge	I	m/yr				✓
Source zone length	L	m				✓
Dilution-attenuation factor	DAF	(-)				✓
Sorption coefficient	K_d	(-)				✓
Water-filled soil porosity	θ_w	(-)				✓
Air-filled soil porosity	θ_a	(-)				✓
Henry's law constant	H	(-)				✓
Bulk density	ρ_b	g/cm^3				✓
Hydraulic conductivity	Ks	m/yr				✓