Field Validation of a Modified HYDRUS Model for Simulating PFAS Leaching in the Vadose Zone

Jeff Silva, Ph.D. P.G.

Battelle 2024 Chlorinated Conference
June 05, 2017

Project Team

- Jeff Silva, Ph.D., P.G. (Arclight Research & Consulting)
  - *Project PI and Project/Modeling Lead*
- Mitch Olsen, Ph.D., Fritz Krembs, P.E., P.G., Mark Settembrino (Trihydro Corp)
  - *Site coordination/logistics, management, monitoring*
- John McCray, Ph. D. (Colorado School of Mines)
  - *Technical Consultant – Vadose Zone Hydrology*
- Jiri Simunek, Ph.D (University of California, Riverside)
  - *Technical Consultant – Vadose Zone Hydrology and HYDRUS modeling support*
- Charles Schaeffer, Ph.D (CDM Smith)
  - *Technical Consultant – Vadose Zone Hydrology and Source Term Characterization*

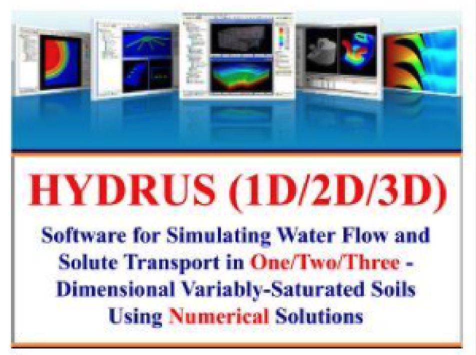
<u>AFCEC</u>

- Jeff Davis, Ernesto Perez, Kent Glover

Background

- SERDP Project ER18-1389 (Ongoing)
  - *Silva, McCray, Simunek*
  - *Modifying commercial version of HYDRUS unsaturated flow and transport simulator for PFAS leaching and transport within the vadose zone*
  - *Modifications Made to date:*
    - method of determining changes in air-water interfacial (AWI) areas with changes in moisture contents based on soil textural properties (thermodynamic method)
    - non-linear, concentration-dependent and ionic strength-dependent AWI adsorption.
    - multi-component, competitive AWI adsorption processes
    - concentration-dependent surface tension changes (competitive multicomponent)
    - pressure head - media wettability changes due to prior AFFF exposure
  - *Validating modifications made against controlled laboratory experiments*
- Current project seeks to validate model predictions at the field-scale at a former fire-training area.
- AFCEC-funded (Project: FA890322C0032)

HYDRUS Simulator



Silva et al., (2020). A modified HYDRUS model for simulating PFAS transport in the *vadose zone. Water*, 12, 2758.
Silva et al., (2021). Air-water interfacial adsorption coefficients for PFAS when present as a mixture. J. Contam. Hydrol., 236, 103731.
Silva et al., (2022). Comparison of methods to estimate air-water interfacial areas for evaluating PFAS transport, J. Contam. Hydrol., 237, 103984.
Vahedian et al. (2023). Impact of tension-driven flow on the transport of AFFF in unsaturated media. ACS ES&T Water, 4(2), 564.

Objectives

- Primary: Develop a practical and repeatable methodology for simulating PFAS leaching from source zones to the water table
- Evaluate the performance of PFAS-Modified HYDRUS simulator for field-scale application
- Evaluate minimum data requirements for HYDRUS model input parameterization
- Support establishing best practices for simulating PFAS leaching at the field scale

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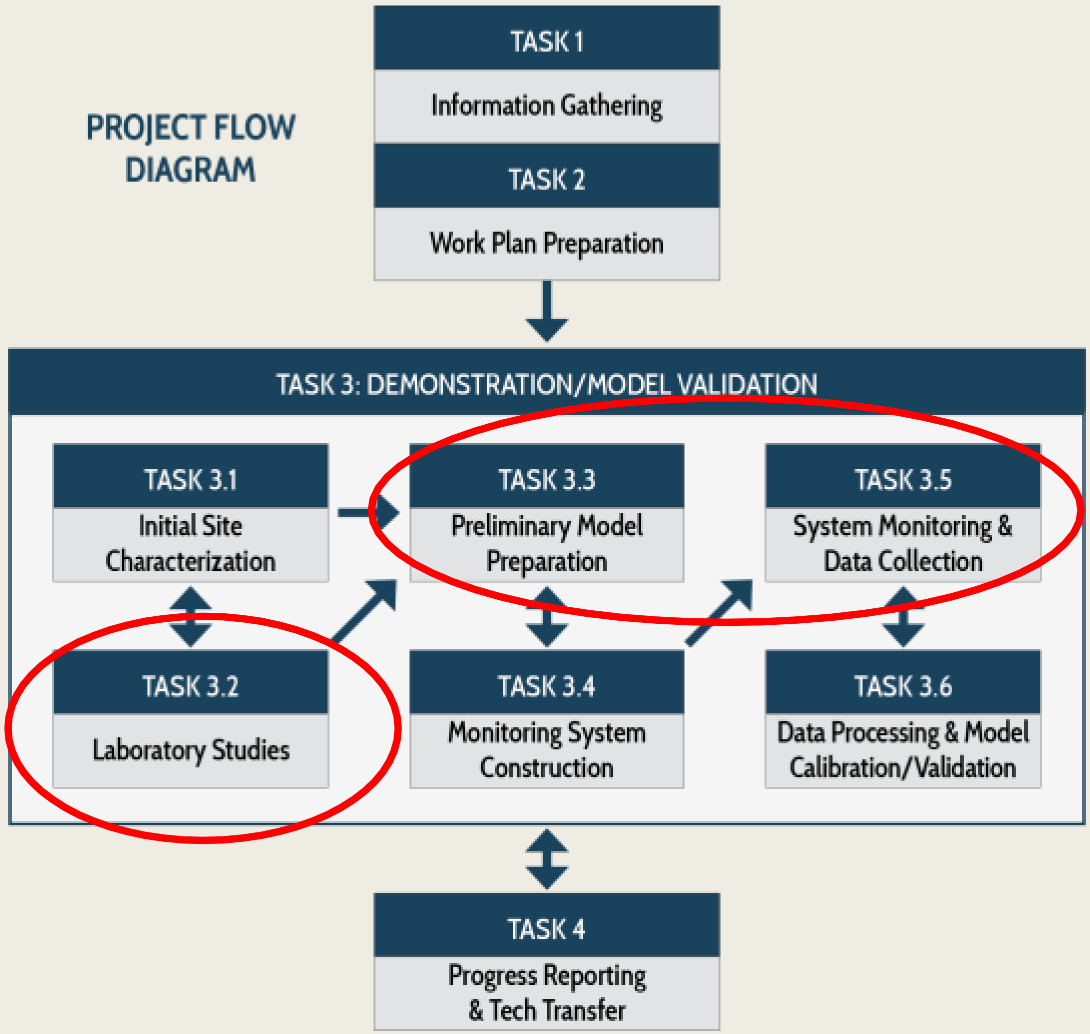
Project Execution



Model Performance Evaluation Approach

- Preliminary Model Preparation
- 2-step Historical Validation Procedure
  - *monitoring changes in matric potential (flow model) and PFAS pore-water concentration (transport model)*
  - *2 seasonal cycles*
  - *Year 1 data used to calibrate the model*
  - *Year 2 data used to evaluate model performance*
- Looking at 1D model first
  - *Utility of 2D/3D model will be evaluated*

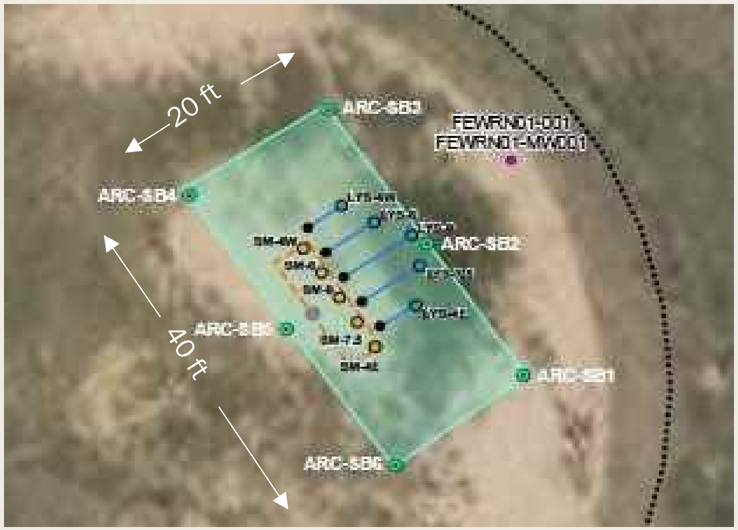
Project Site Selected

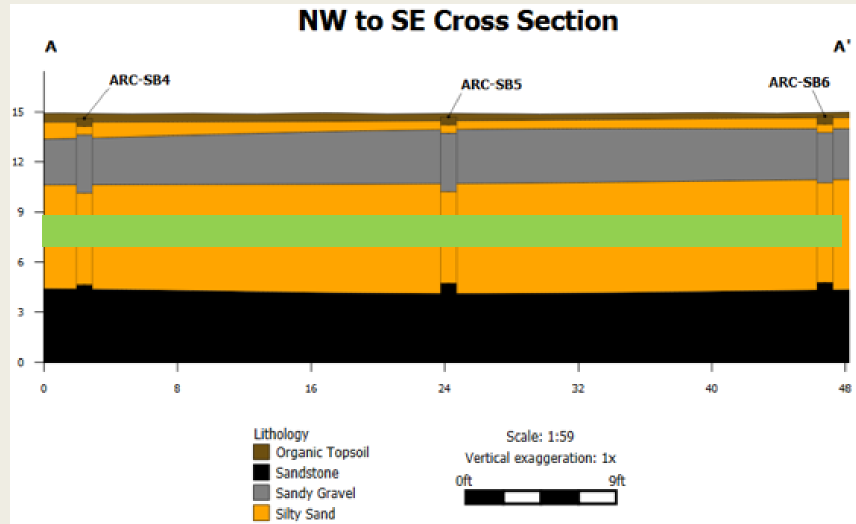
- F.E. Warren AFB, Cheyenne, WY – FFTA 2 (AFFF Area 1)
- Operated: 1965-1989, AFFF used 1974-1989
- PFAS Contamination: ~ 3,000 ug/kg PFBS/PFOS; 50,000 ug/kg PFOA

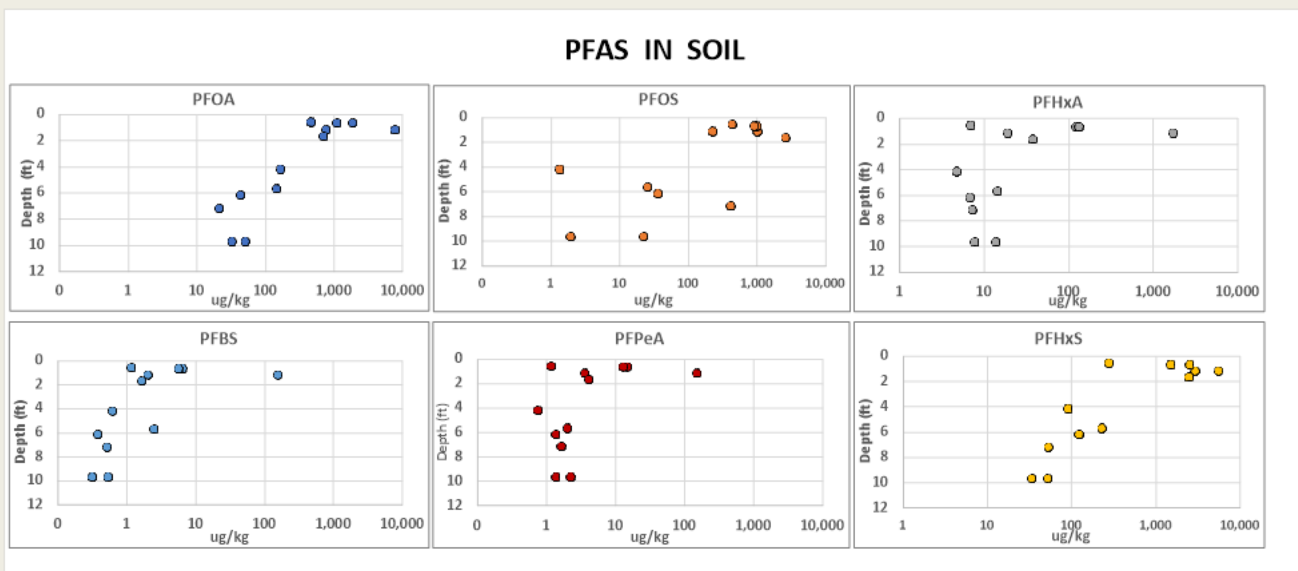
Initial Site Characterization

- Soil borings
  - *characterize site soil stratigraphy and initial condition for PFAS contamination*
  - *provide soil samples for laboratory characterization (modeling)*
- ER Surveys – Evaluate potential for preferential flow pathways

Initial Site Characterization

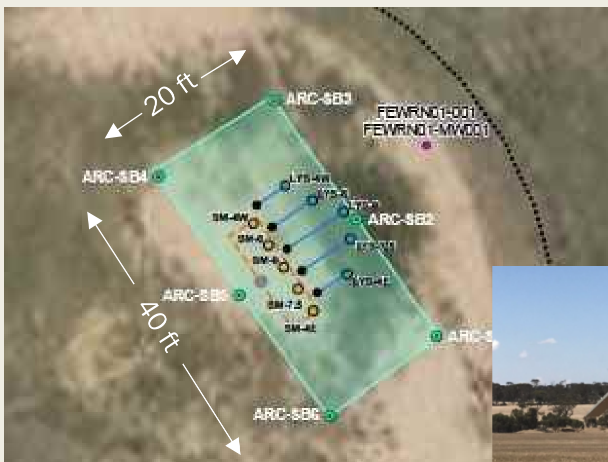




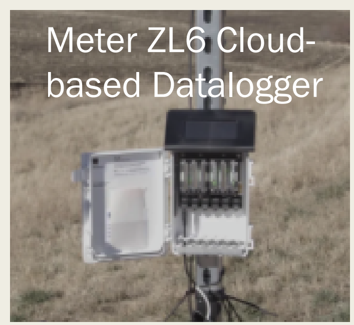


Monitoring System Installation

- Angled DPT tooling to install sampling lysimeters (45 degrees)
- Vertical 4-inch auger to install soil water potential sensors
- Coincident depth of installation along NW-SE transect




Atmos 41 Weather Station

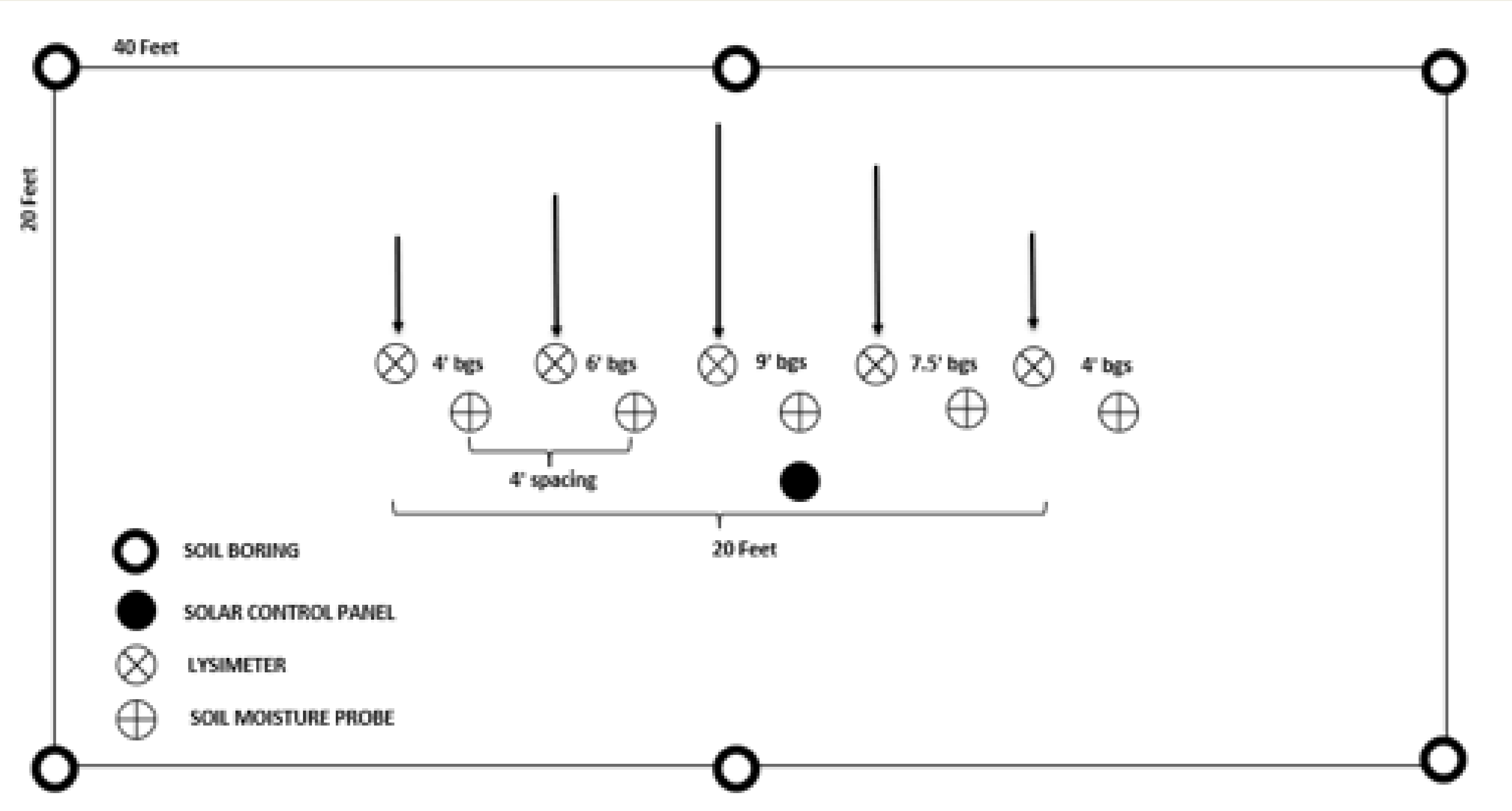

Meter ZL6 Cloud-based Datalogger


Terros 21 Matric Potential Sensor


Single-Chamber SMS Lysimeter

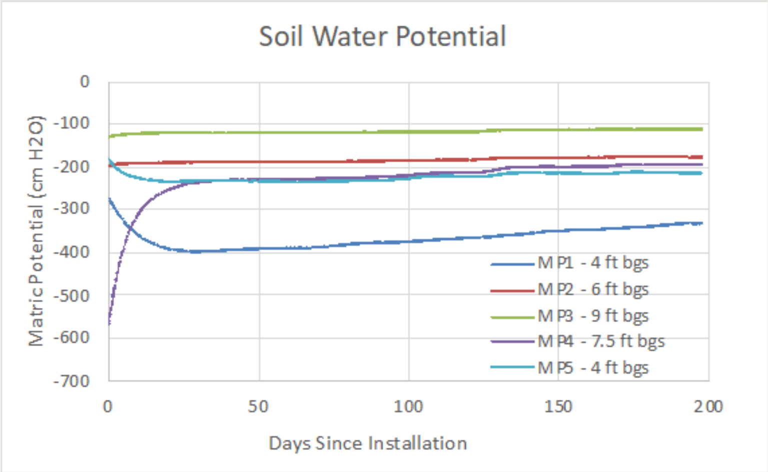
07-09 Nov 2023

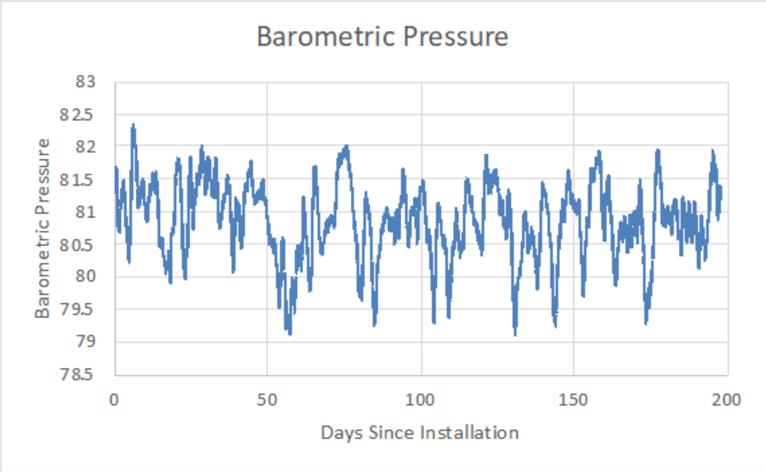
Monitoring System Installation

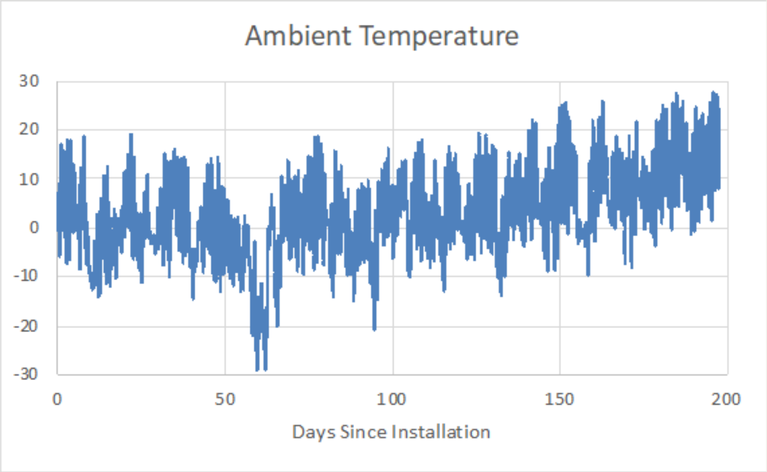


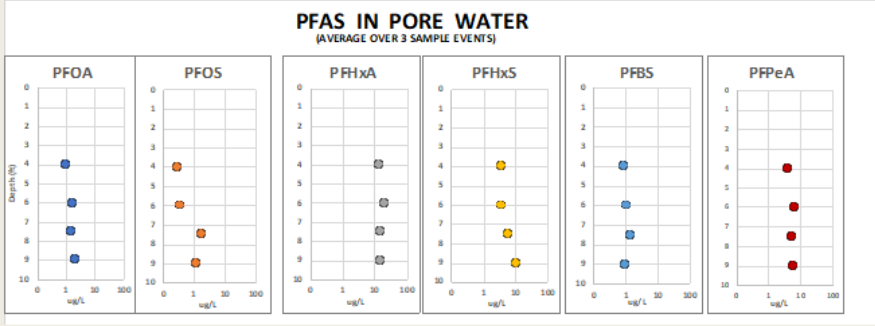
Installation completed: 11/9/2023

System Monitoring



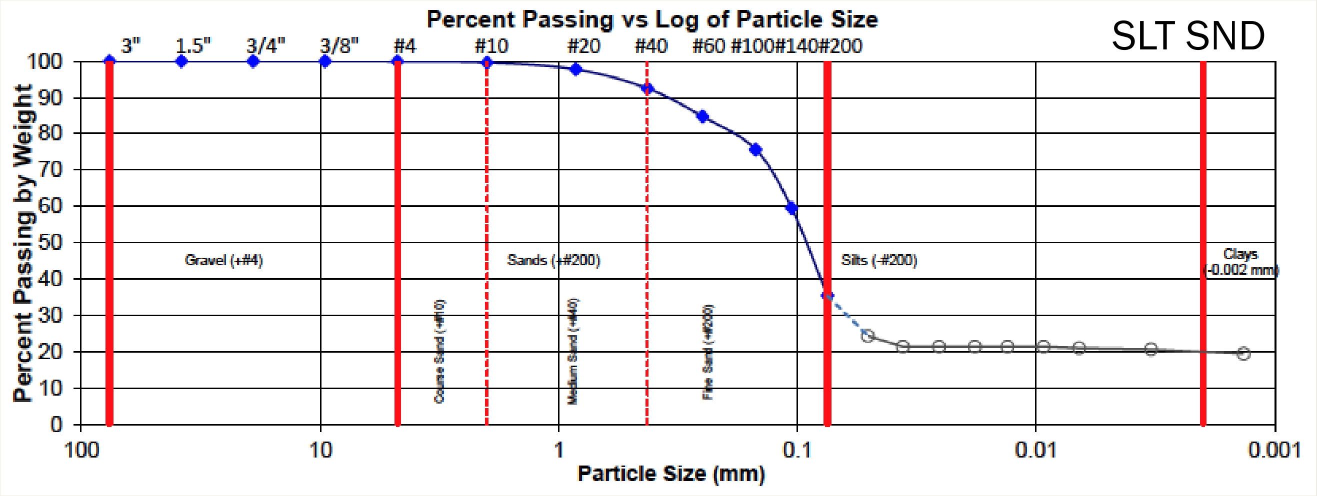






Laboratory Studies

- Particle Size Analysis (Primary Soil Types)
  - *ASTM D 2487 – Sieve Analysis & Hydrometer*

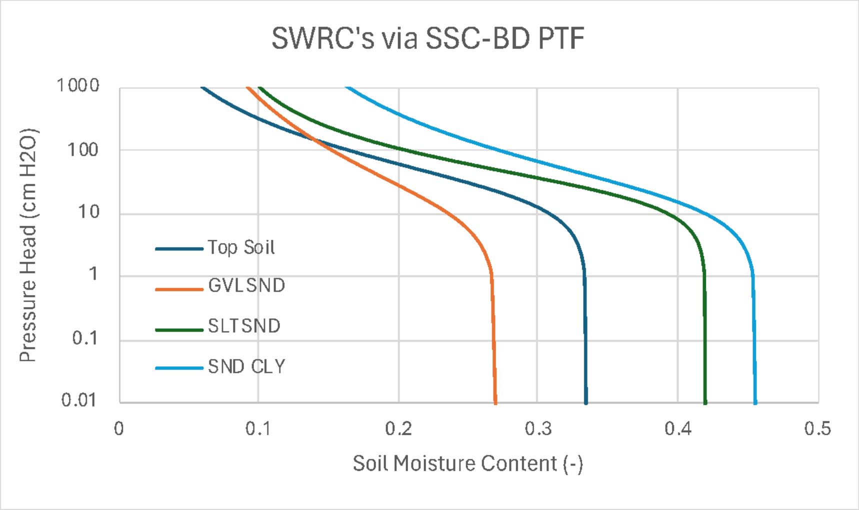


Soil Category	%CLAY	%SILT	%SAND	Dry Bulk Density (g/cm^3)
TOP SOIL	15	52.3	32.7	1.65
GVL SND	1.1	53.8	45.1	1.85
SLT SND	19.8	64.5	15.7	1.4
SND CLY	49.3	18.7	32	1.4

Laboratory Studies

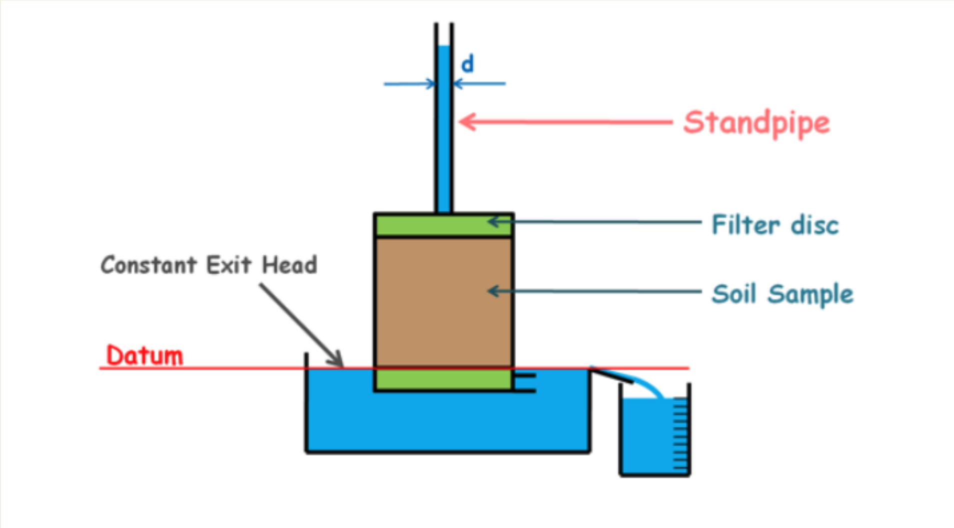
- Hydraulic Properties (Primary Stratigraphic Units)
  - Soil-water retention curves (van Genuchten equation)
    - *measured vs. predicted based on pedotransfer functions*

	Rosetta - SSC-BD Pedotransfer Function			
VGM Parameter	**TOP SOIL**	**GVL SND**	**SND SLT**	**SND CLY**
Qr	0.001	0.070	0.002	0.083
Qs	0.334	0.419	0.270	0.455
Alpah (1/cm)	0.010	0.005	0.053	0.018
n	1.462	1.280	1.280	1.380
Ksat (cm/d)	20	17.33	13.24	22.18



Laboratory Studies

- Hydraulic Properties (Primary Stratigraphic Units)
  - Saturated Hydraulic Conductivities
    - *Falling Head Permeameter Method (finer media)*



	Ksat (cm/d)			
Soil Category	**1**	**2**	**3**	**Predicted Rosetta SSC-BD**
Organic topsoil	18	18.2	TBD	20.0
sandy Gravel	19.4	19.1	TBD	17.3
silty Sand	15.3	15.3	TBD	13.2
clayey Sand	20.2	21	TBD	22.2

Laboratory Studies

- Source Term Characterization (CDM Smith)
  - Batch desorption kinetic tests (each primary soil type)
  - Batch desorption isotherm tests (sequential dilution approach)
  - Methods: Schaeffer et al (2022)*
- Goal is to:
  - *characterizing desorption of PFAS from source media*
    - rates – fast/slow fractions
  - *aid in selection of solid phase sorption/desorption model*
  - *PFAS types (EPA Method 1633)*
- Porewater geochemistry and soil total organic carbon (TOC) also analyzed for site characterization soils

Check for updates

ASCE

Desorption Isotherms for Poly- and Perfluoroalkyl Substances in Soil Collected from an Aqueous Film-Forming Foam Source Area

Charles E. Schaefer[1]; Dung Nguyen[2]; Emerson Christie[3]; Stefanie Shea[4]; Christopher P. Higgins, A.M.ASCE[5]; and Jennifer Field[6]

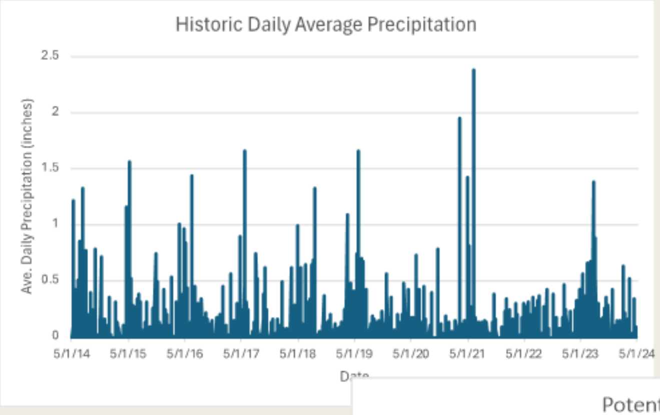
*Schaeffer et al. (2022) J. Environ. Eng., 148(1), 04021074

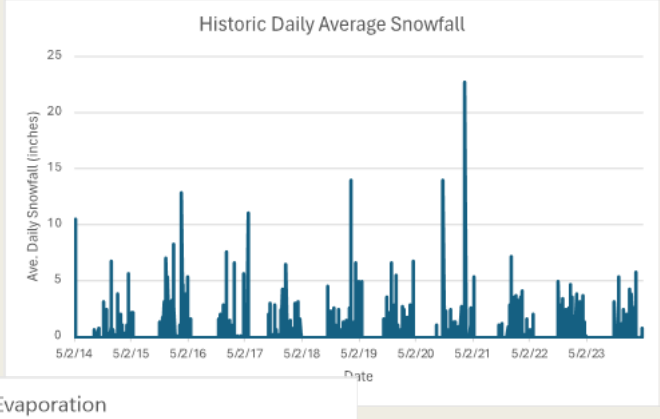
Parameterizing HYDRUS

- Preliminary Model Development
  - *Historic meteorological data (precipitation, evaporation potential)*
    - establish upper atmospheric boundary conditions.
  - *Soil stratigraphic data*
    - Construct representative soil textural model
  - *Representative hydraulic data (K_{sat}, SWRC parameters)*
    - Assign hydraulic parameters to soil textural categories.
    - Condition flow model to represent current moisture condition
  - *PFAS contamination (soil and porewater)*
    - Establish current condition for PFAS contamination
  - *PFAS source term characteristics*

Preliminary Model Preparation

- Meteorological Input
  - *10-year historic daily precipitation, evaporation potential*
    - *snowmelt model*
  - *Use historic data to establish initial condition for soil moisture content.*





Preliminary Model Preparation

- Soil Stratigraphic Model

	Rosetta - SSC-BD Pedotransfer Function			
VGM Parameter	**TOP SOIL**	**GVL SND**	**SND SLT**	**SND CLY**
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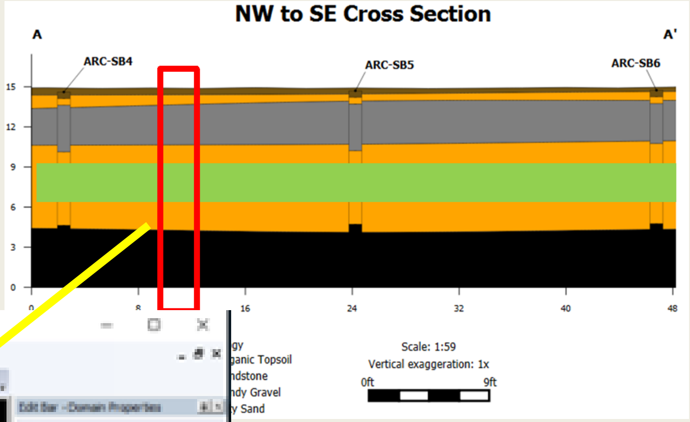
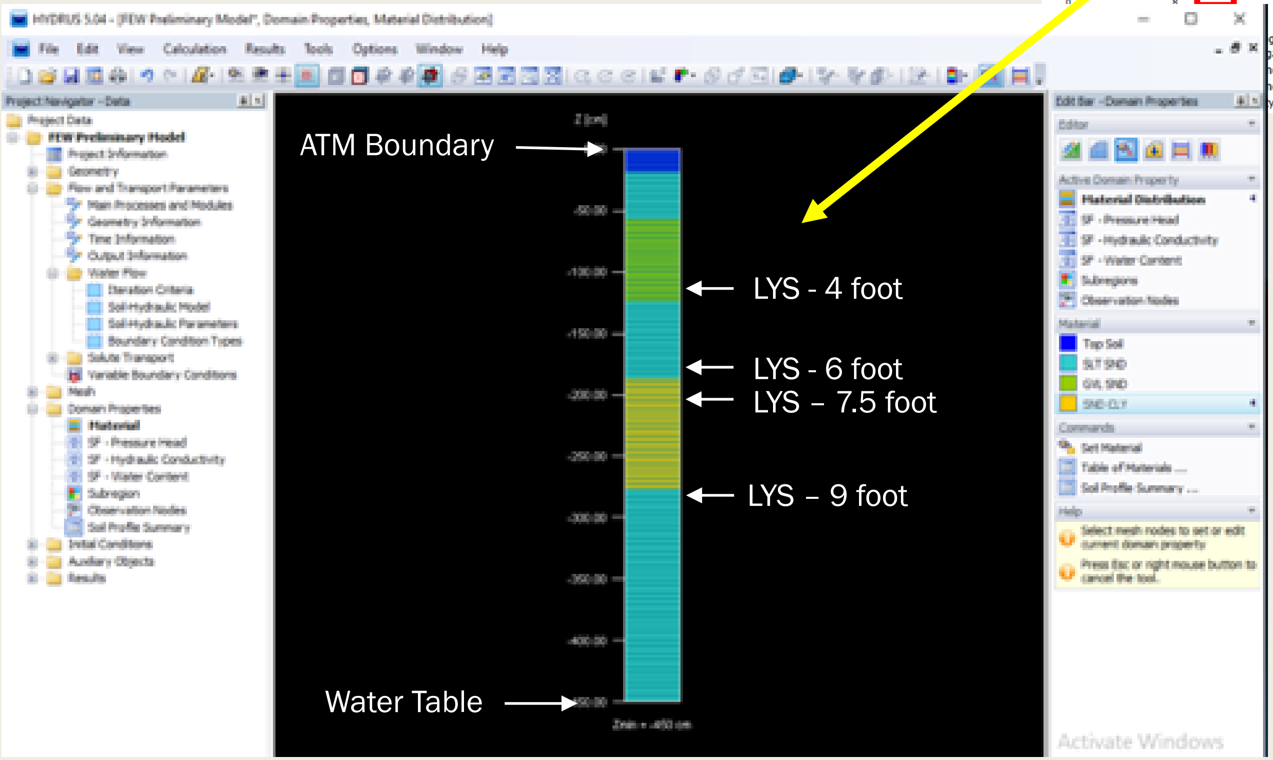
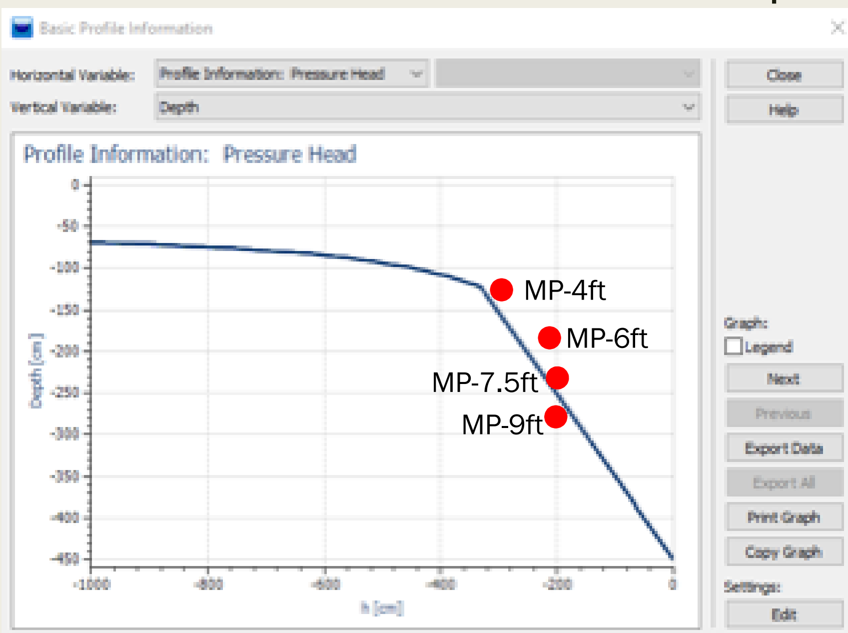
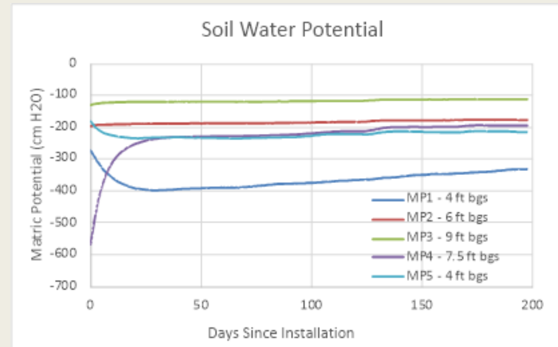


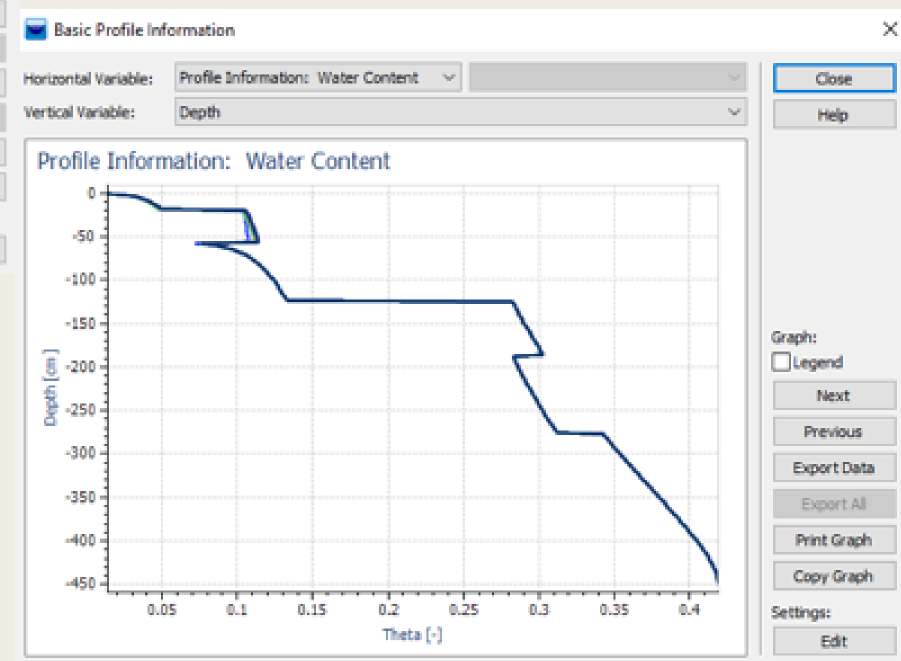


Preliminary Model Preparation

- Condition flow model to represent current moisture condition







Waiting for Source-Term characterization data to condition transport model.

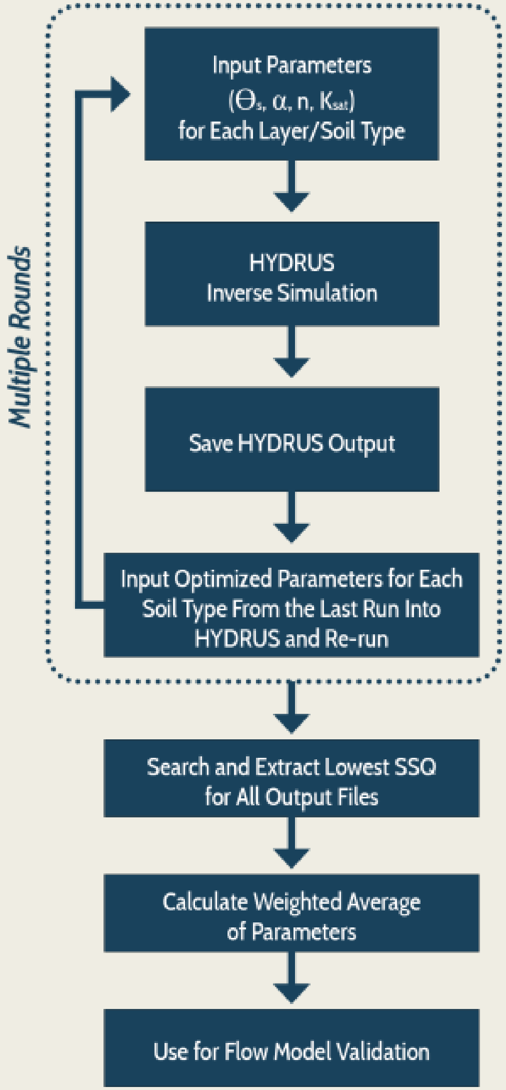
Simulated Observations

- Evapoconcentration

  - *Relevant to non-reactive solute*
  - *Less impactful for PFOS (i.e., more surface active PFAS)*
  - *Should be more impactful for less surface active PFAS*

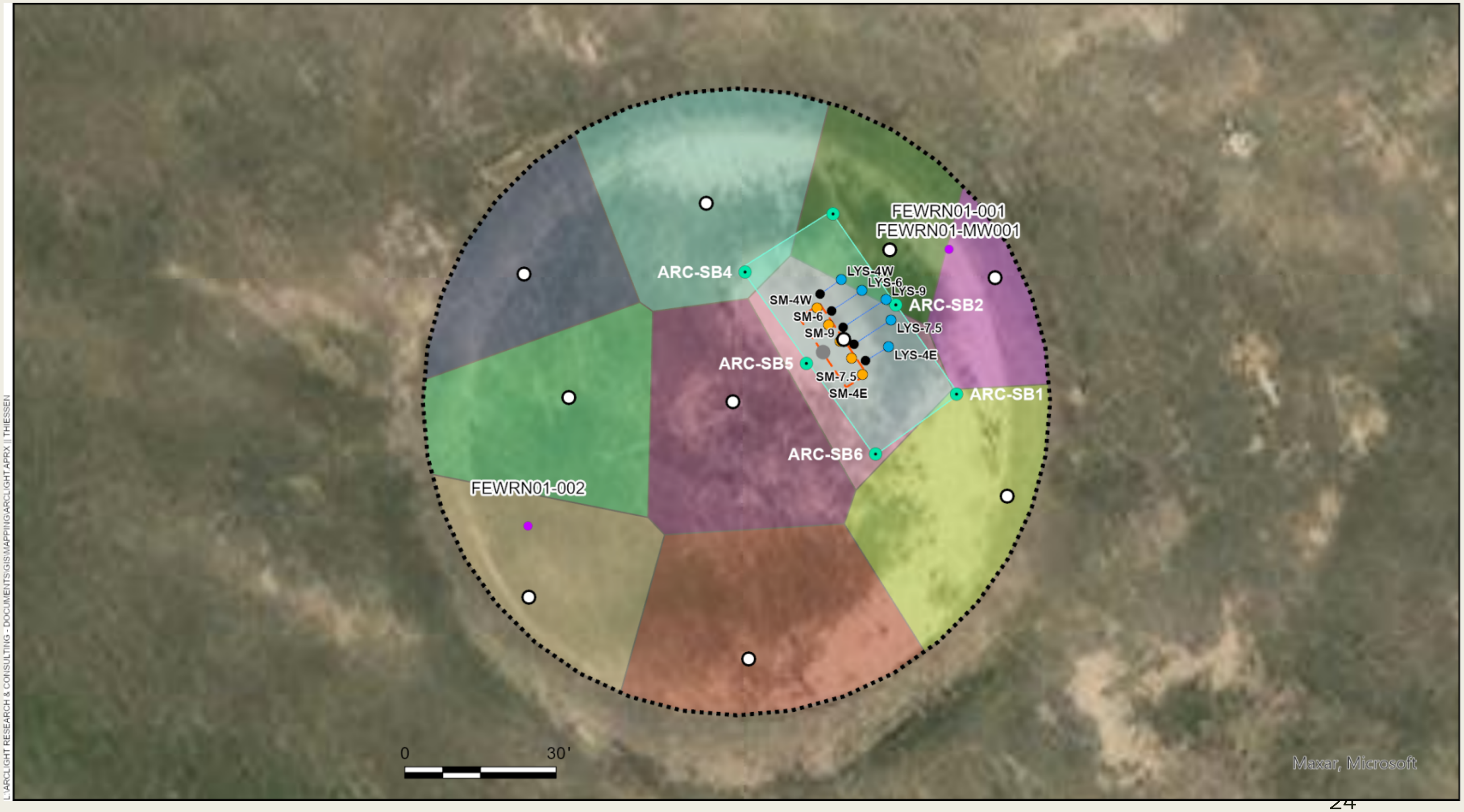
Model Performance Evaluation

- 2-Step Historical Validation
  - *1st-year monitoring data – conditioning*
  - *2nd-year – performance evaluation*
- Flow Model Conditioning
  - *Inverse Modeling*
  - *non-linear least squares (SSQ) parameter optimization*
  - *time-series data = objective function*
- Transport Model Conditioning
  - *Less straightforward*
  - *More complex – multiple processes*
  - *Fix AWI adsorption parameters (best estimate based on data collected)*
  - *Inverse modeling to minimize error in solid-phase interaction parameters*
  - *Multiple inverse runs to optimize select solid-phase parameters to time-series pore-water concentration data*
  - *step out – repeat as sensitivity analysis on AWI adsorption parameters.*



Modeling Approach

- Potential 1-D Model Extension to Whole Site Modeling
  - *Thiessen polygon or other spatial clustering-type approach delineate FTA segments sharing similar conditions*



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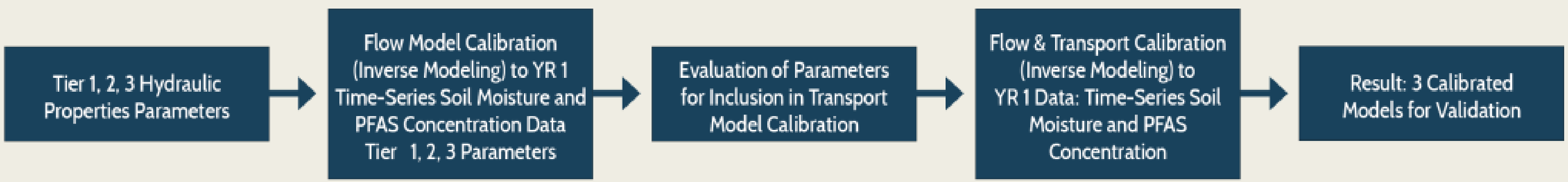
Model Performance Evaluation

- Process flow diagrams

Calibration Process Flow Diagram



Validation Process Flow Diagram