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Sensing and AI/ML Tools for Tracking Environmental Contamination

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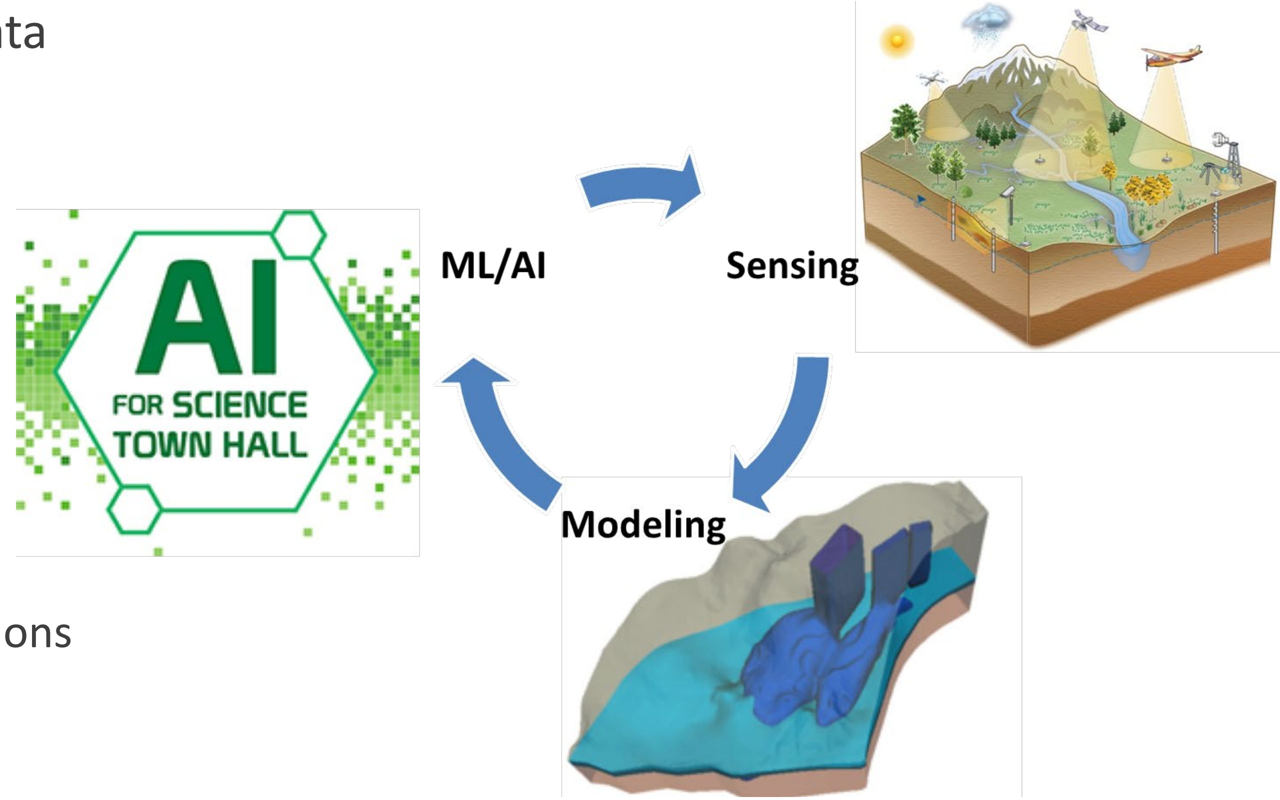
AI/ML Applied to Monitoring and Sensing of Complex Systems

- SRNL's portfolio of projects where AI/ML strategies have been used to fuse sensing/sampling/modeling data and extract signal or make predictions based on various data streams including:
  - Meteorological data,
  - Environmental contaminants/signatures,
  - Chemical/physical parameters (i.e., proxy variables)
  - Imagery
  - Characterization data



- Enabled Capabilities:
  - Spatiotemporal optimization of sensing/sampling locations for detection/prediction/estimation
  - Source quantification/attribution
  - Early detection with uncertainty quantification

ALTEMIS - Advanced Long-Term Environmental Monitoring Systems

- Remediation of DOE EM’s remaining complex plumes will take decades
- GAO estimates that EM’s liability for environmental cleanup across the country will exceed $550 billion
- Long term monitoring after sites have been cleaned up is a large component of that liability
- DOE-EM Technology Office is sponsoring SRNL-led program since 2020
    - Multi-lab and multi-agency team: SRNL, SRS-ACP, LBNL, PNNL, UC Berkeley, FIU/CRESP/MSIPP

ALTEMIS – The Approach

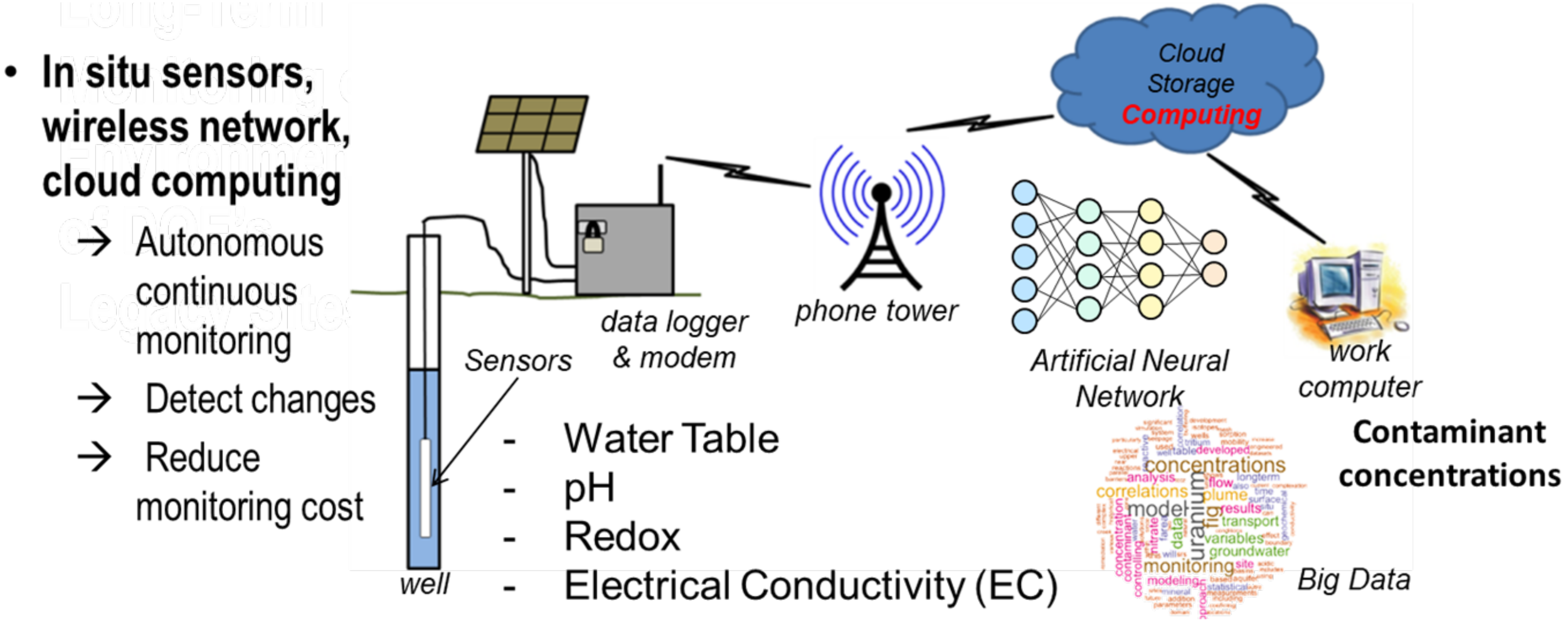
Identification of measurable in-situ variables that serve as proxies for contaminant measurements

Use of machine learning approaches to predict spatiotemporal concentrations across time, especially as environmental conditions evolve.

In this way, the monitoring system serves as an early warning system for unfavorable plume behavior in the dynamic environmental conditions.

ALTEMIS: Advanced Long-Term Environmental Monitoring Systems

- **Improve effectiveness and robustness of monitoring of contaminant plumes**
  - In situ monitoring approaches for monitoring master variables
  - Spatially integrative technologies including geophysics and contaminant detection
- **Use of master variables transforms the monitoring paradigm from *reactive* monitoring – respond after plume anomalies are detected – to *proactive* monitoring – detect the changes associated with the plume mobility before concentration anomalies occur.**

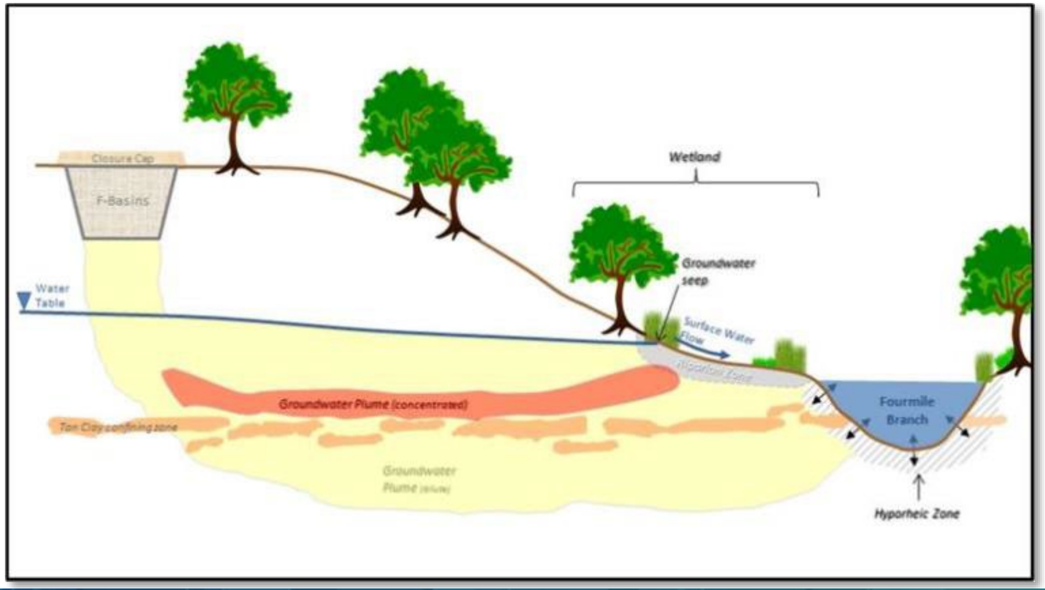


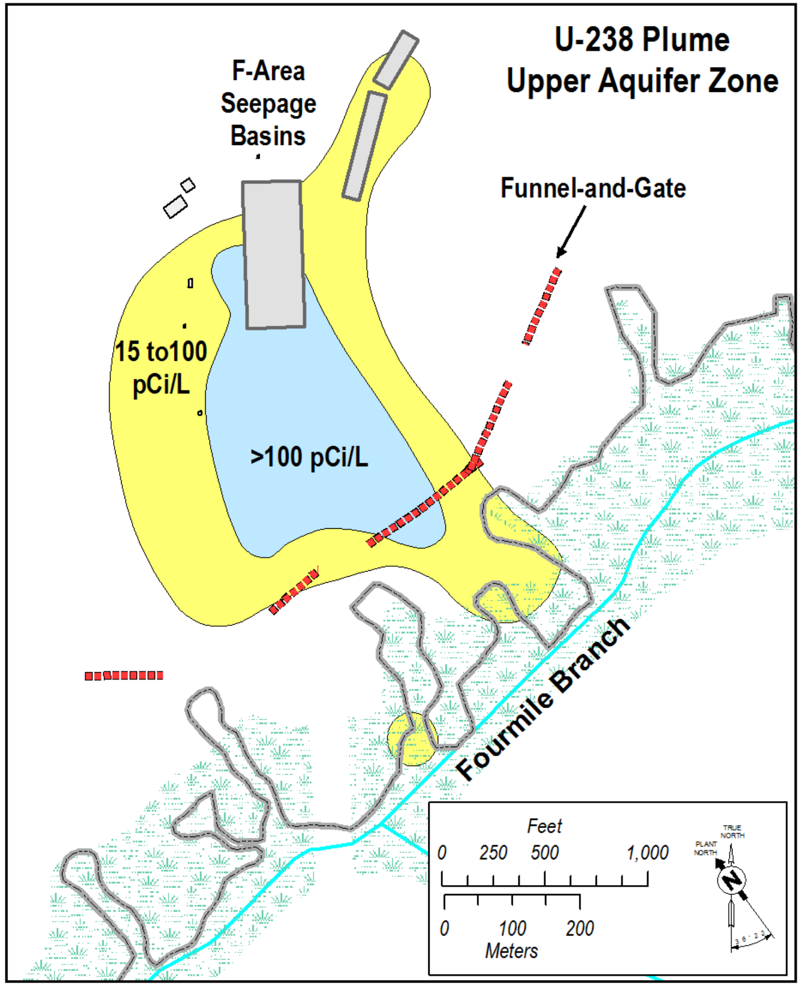
ALTEMIS Testbed – F-area Groundwater Plume, SRS

SRS F-area Groundwater Plume - 30 years of discharge of low activity wastewater. Major contaminants of concern are metals, uranium, tritium, and radioactive iodine.

Groundwater Testbed

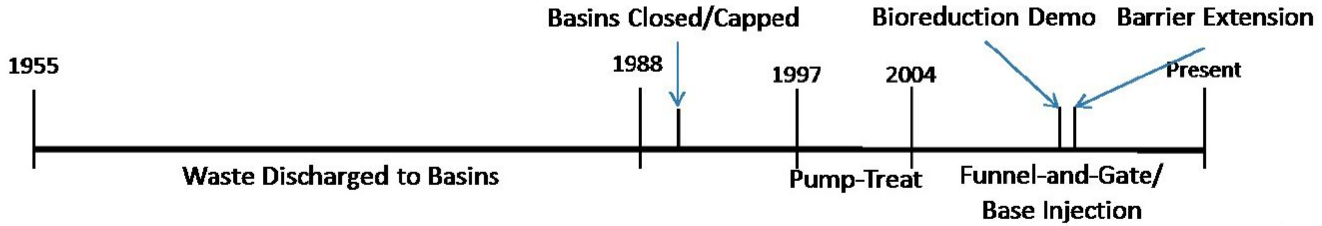
OS-Advanced Characterization (2008), ASCEM Reactive Transport modeling (2012), ALTEMIS (2020)



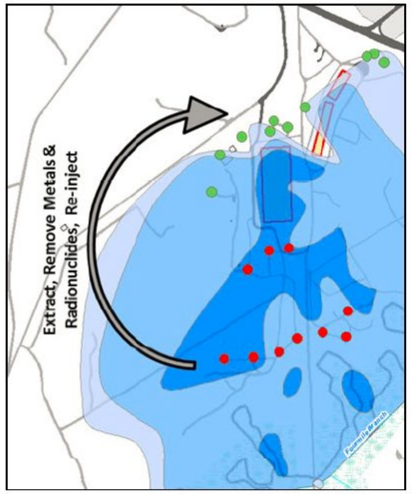


Altemis F-area Testbed – Remedial History

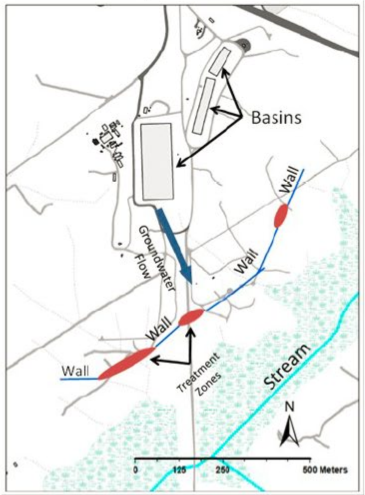
- Phased Remedial Strategy – Source Zone Isolation, Active Remediation, Enhanced Attenuation
- Enhanced attenuation strategies have improved remediation of low concentration plumes but have created the potential for creation of secondary source terms (e.g., I^{129}, U^{238}, Sr^{90})
- Require continuous monitoring over the course of the next several decades to ensure compliance with regulatory requirements



Basin Operation



Pump/Treat/Re-inject



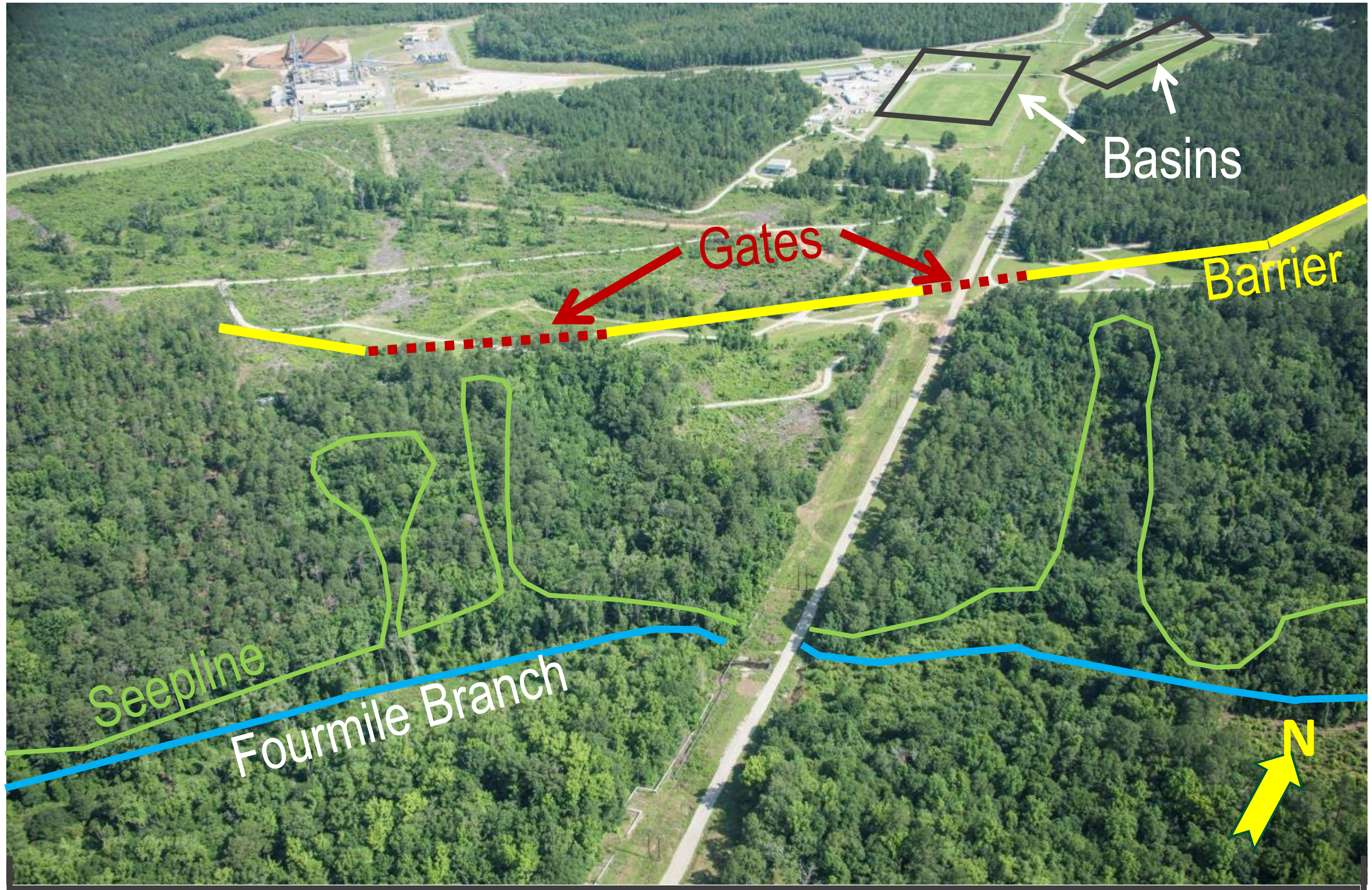
Funnel-Gate/Base Injection

LBNL 3D Uranium Plume Modeling/Analysis (1956-2050)

Reactive Transport Model (2012)

- Detailed stratigraphy from OS Advanced Characterization project
- Complex uranium geochemistry
  - sorption, cation exchange, pH dependency on U mobility
  - Adding strontium (2024)
- Key Remedial Dates
  - (1990, 1997-2004, 2011)

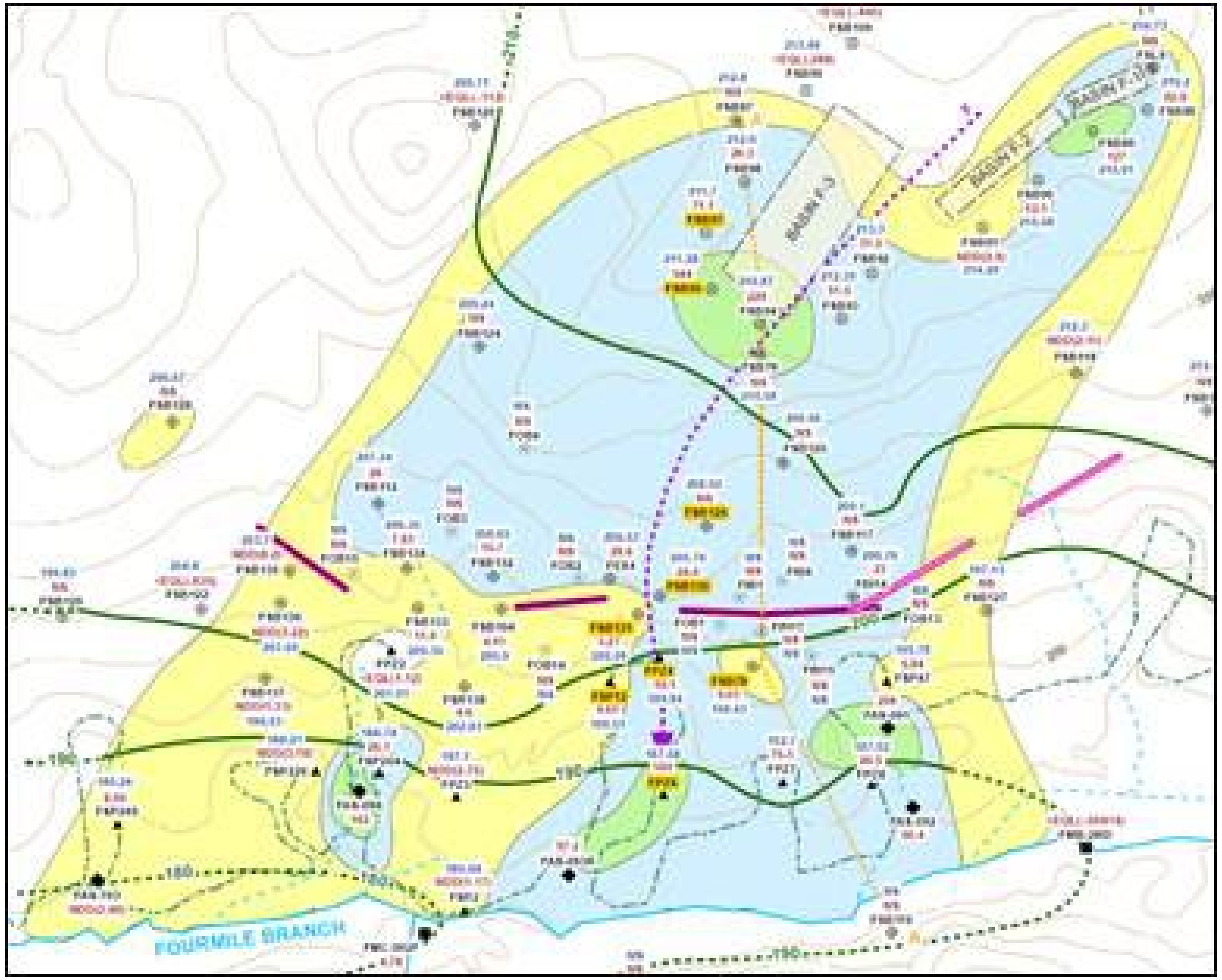
SRS F-Area Seepage Basins – Today



Approximately 1 Kilometer

Current Monitoring Well Map/Sampling Frequency

Frequency	Number of Wells at F-Area	Constituents Sampled at each Well
Quarterly	87	Cadmium, lead, nitrate, tritium, gross alpha, nonvolatile beta, pH, specific conductivity, groundwater elevation
Semi-Annually	54	17 inorganics, 7 organics, 24 radionuclides (Table A-2 to A-4)
Annually	93	17 inorganics, 7 organics, 24 radionuclides[1]
Annually	6	242 additional constituents to be sampled (Figure A-1)



Boundary Conditions/Master Variables

Monitor Boundary Conditions and Master Variables

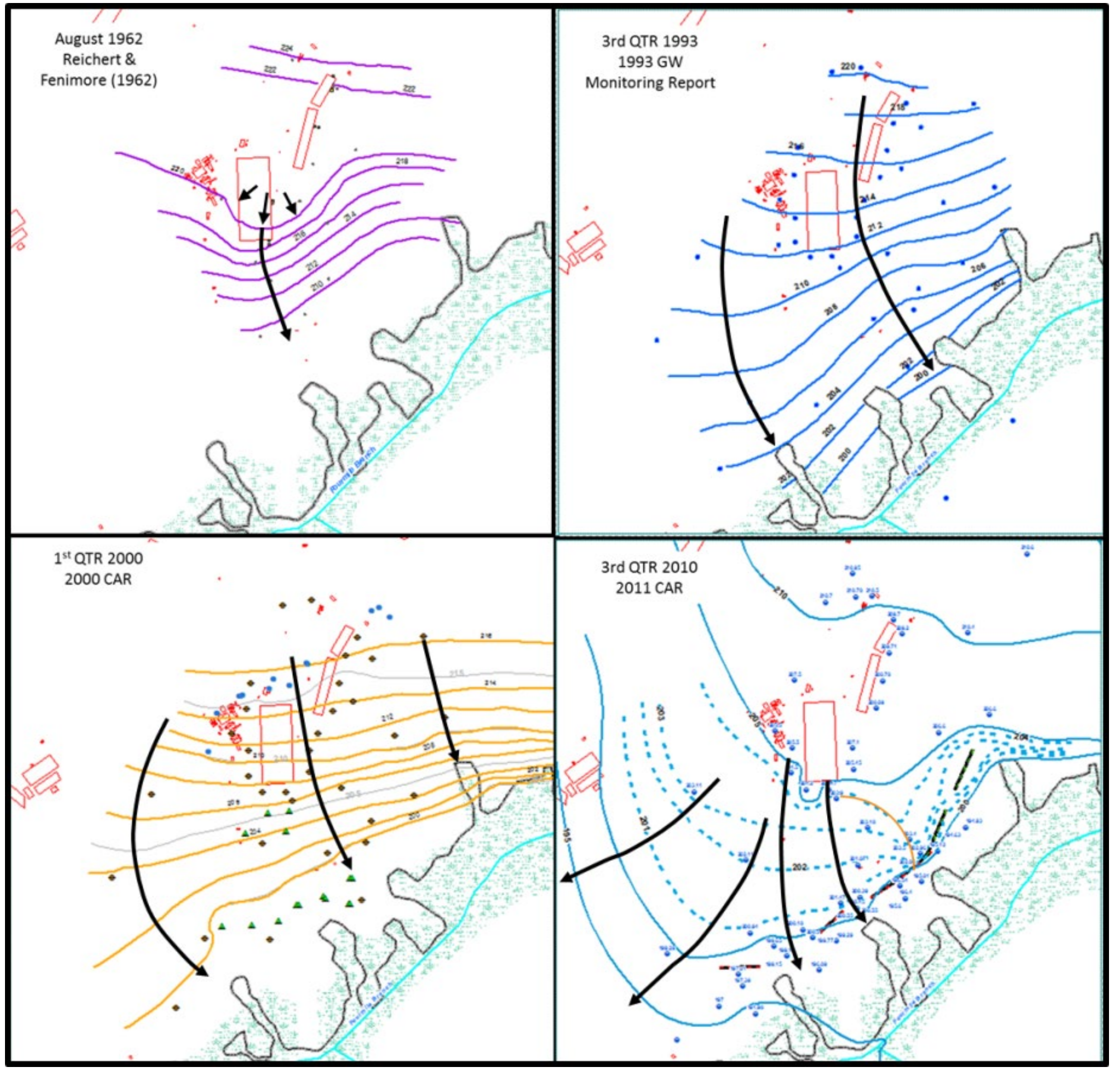
- Physical processes responsible for groundwater movement such as water level, rainfall, etc.

Groundwater always flows down gradient

- Water level measurements demonstrate distinct changes in flow pattern

Provides leading information

- Changes in stability of hydraulic/geochemical conditions signal potential remobilization of attenuated contaminants

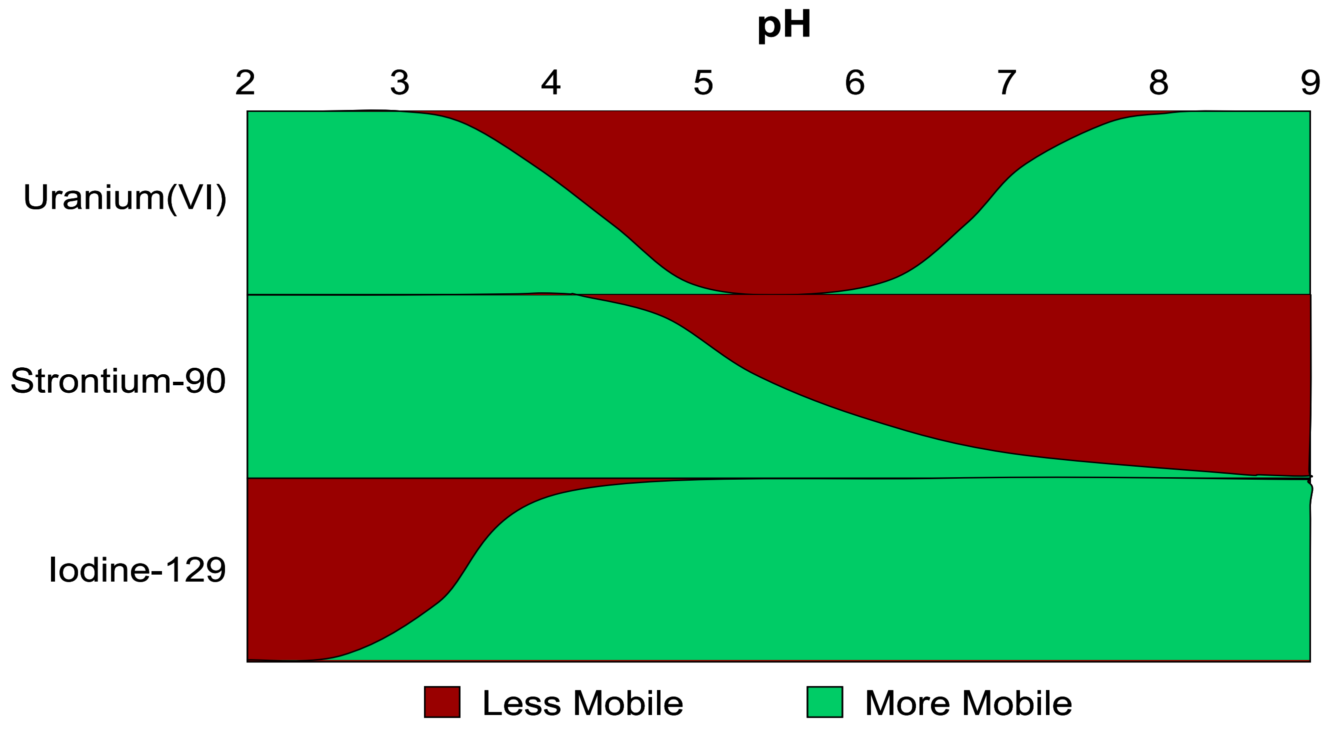


Plume Geochemistry

Primary objective is to monitor stability of attenuated contaminants

Monitor Master Geochemical Variables

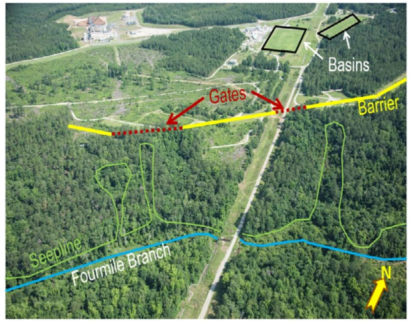
- Chemical processes (e.g., pH, redox, conductivity, etc.) responsible for attenuation of contaminants

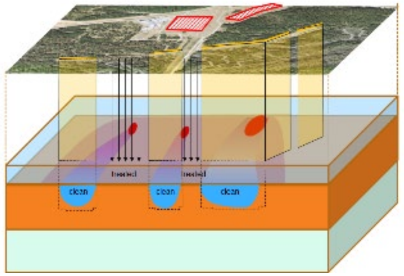


Zones of Vulnerability after 25+ years of Remediation

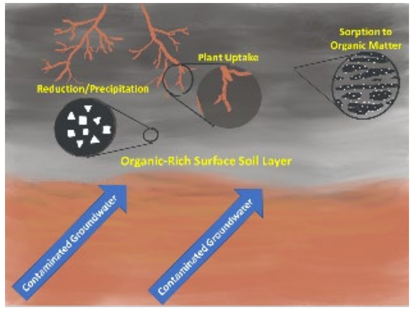
Basin Capping/Closure
- Contaminants remain in vadose zone soil
- Prevents infiltration that would drive contaminants deeper

Groundwater Contamination
Passive Treatment Zone Attenuated Contaminants
- U and Sr-90 attenuated by raising pH
- I-129 attenuated by precipitation of AgI

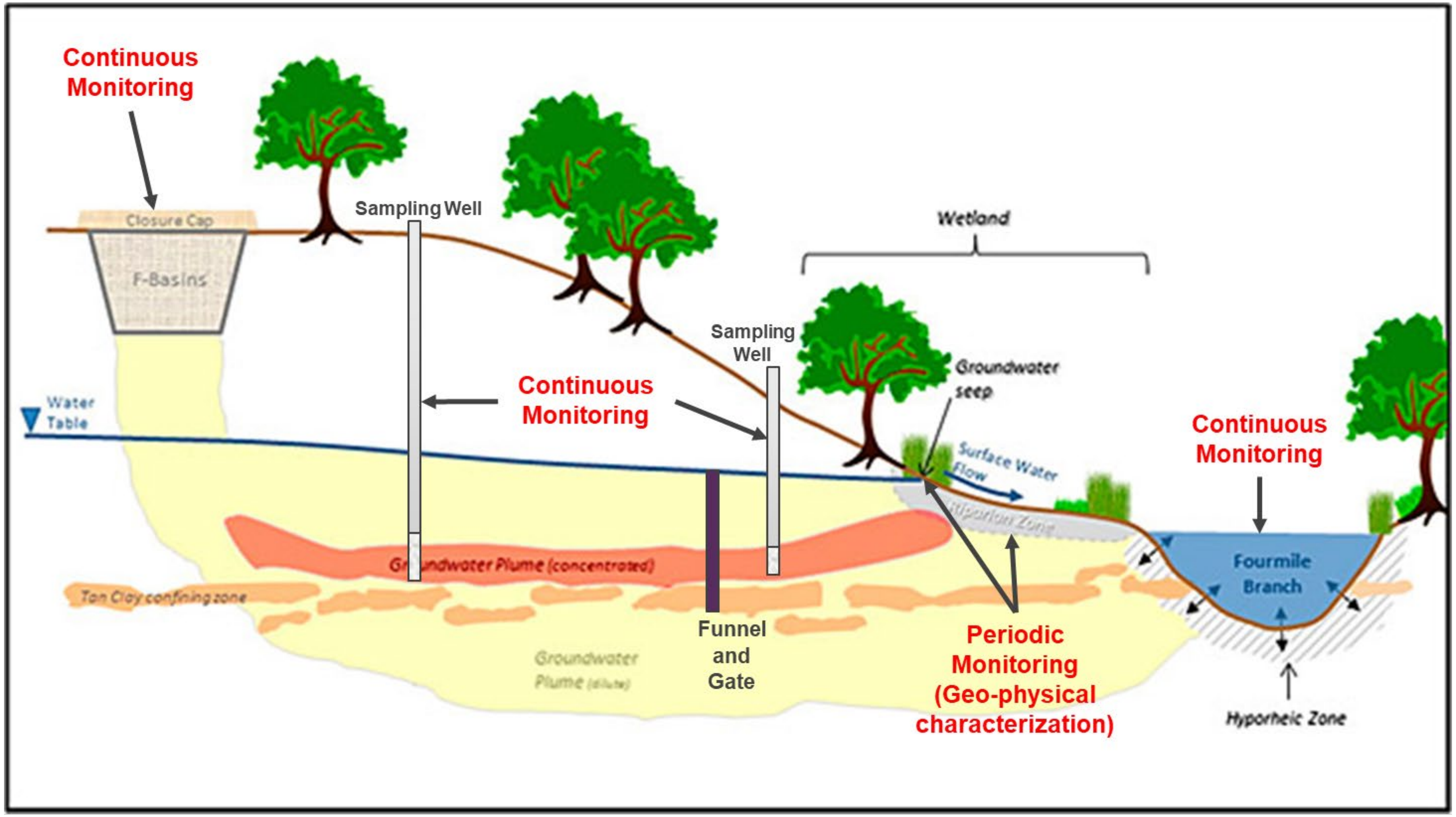




Wetlands
- Contaminants attenuated by processes in organic-rich soils
- Sorption to organic matter, plant uptake, reduction/precipitation for some contaminants

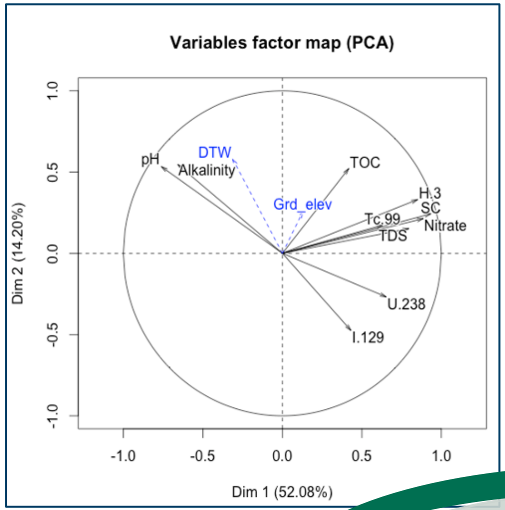


Conceptual Model and Data Paradigm



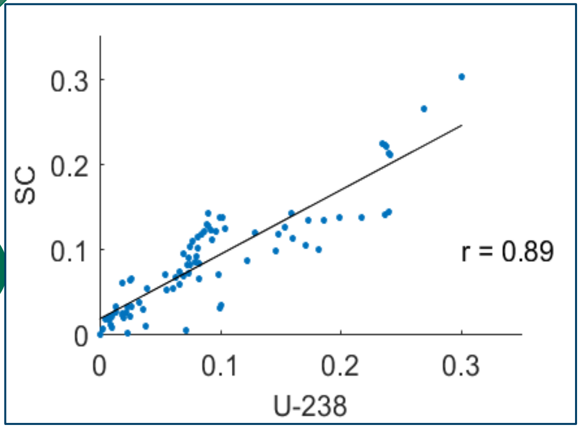
Eddy-Dilek, et al. 2016

ALTEMIS AI/ML Overview – Principal Component Analysis



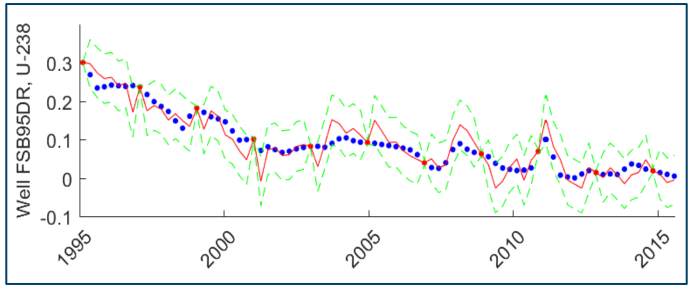
Exploratory Data Analysis

Quantification of Correlations



Contaminant Concentration Estimation

Kalman Filter



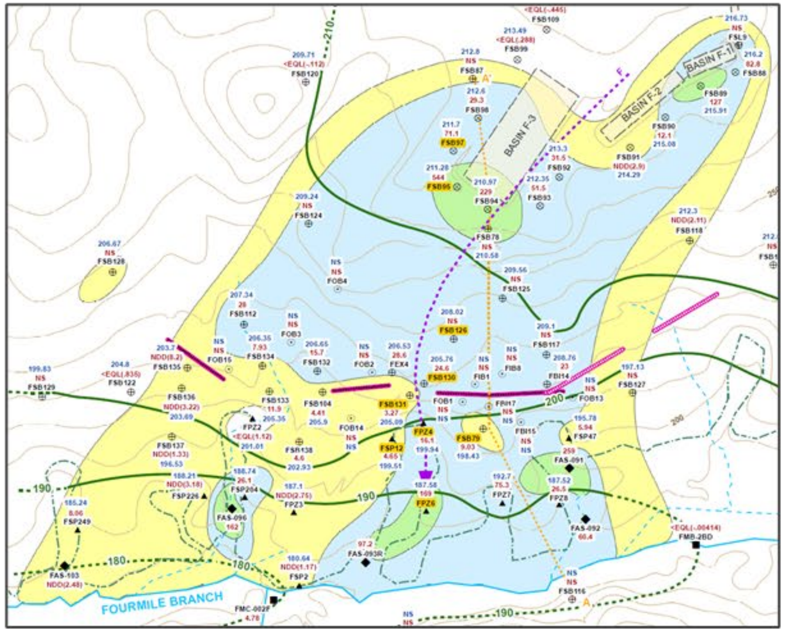
ALTEMIS AI/ML Goals:

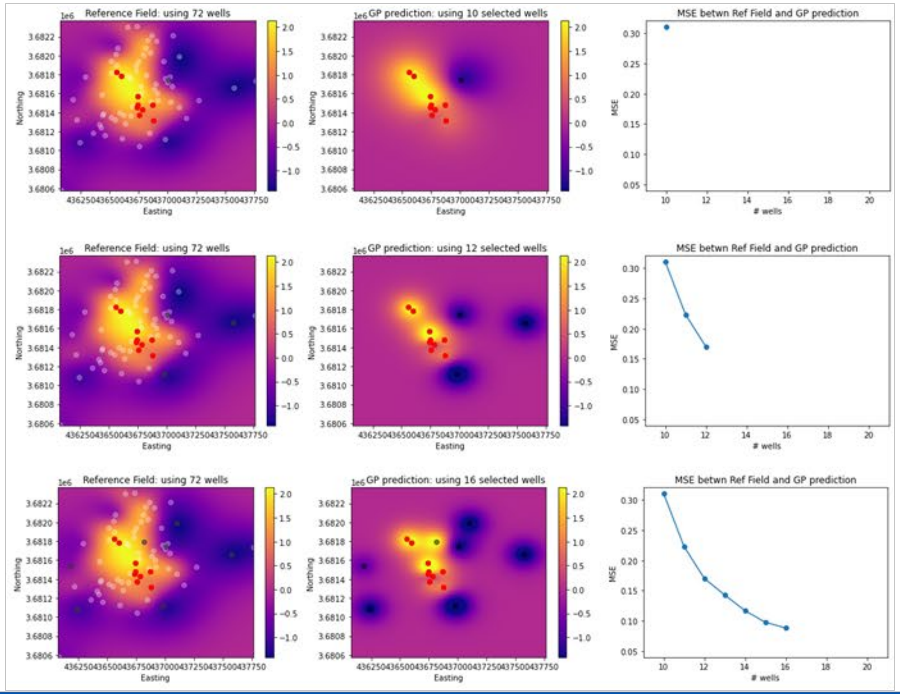
- Identify spatiotemporal patterns of contaminant concentrations
- Optimize the placement of in situ real-time monitoring networks to capture contaminant concentration distributions and measure proxy variables
- Estimate spatiotemporal contaminant concentrations using proxy variables
- Quantify responses to climate disturbances such as flooding or drought

Sensor Network Optimization

Monitoring locations are optimized across space, time, and all contaminants of interest

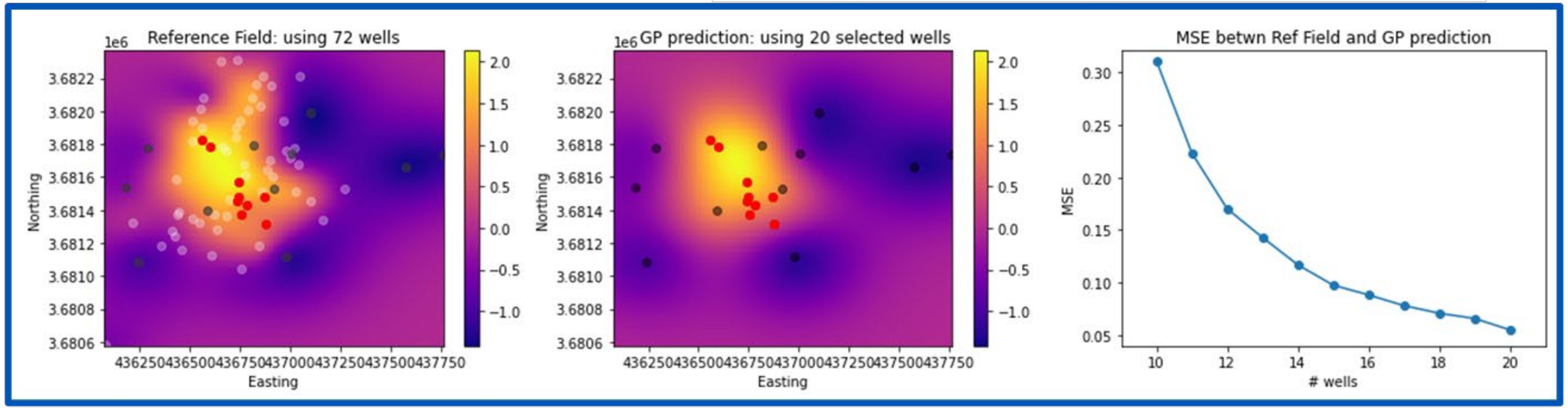
Existing Well Locations



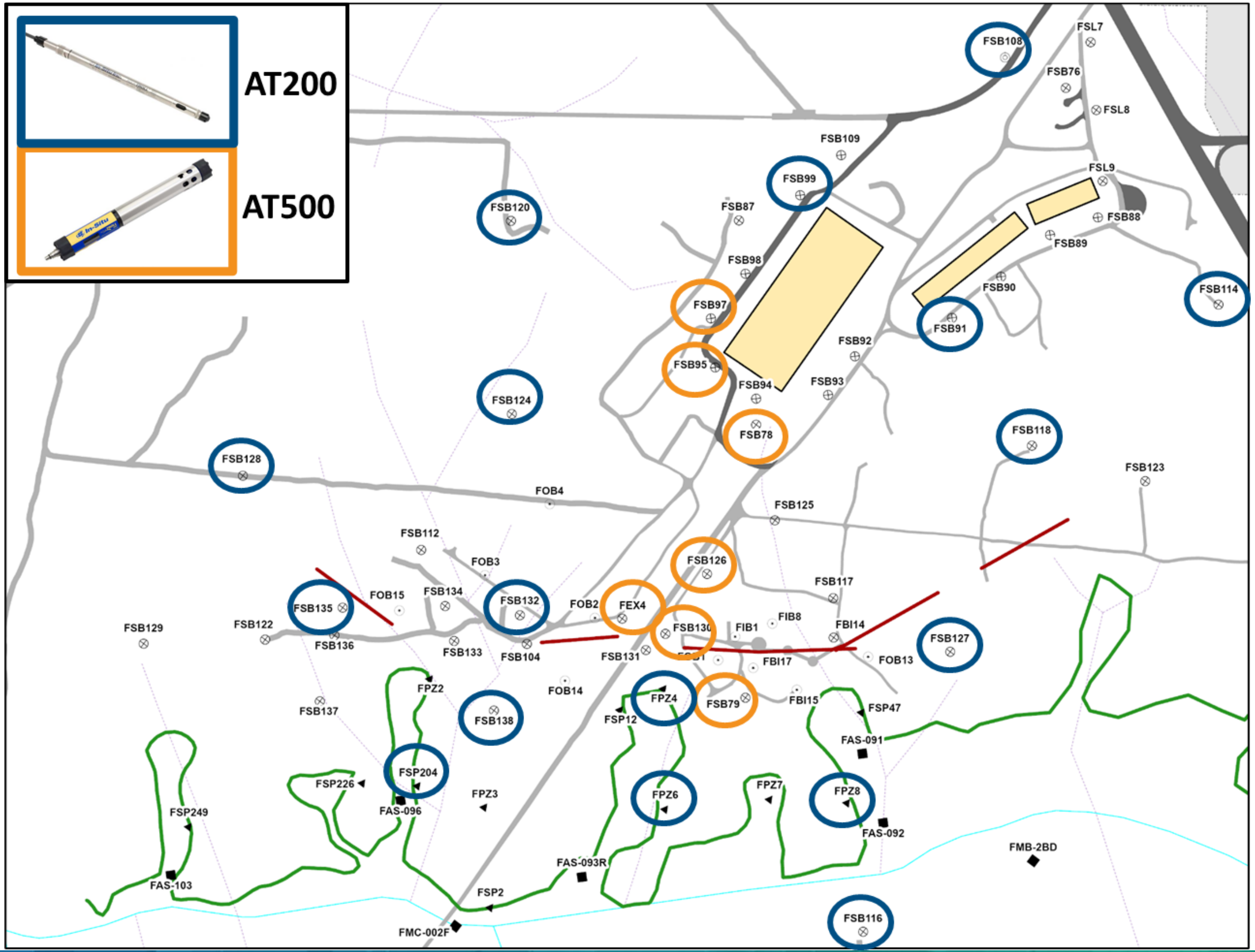


Iterative Refinement

Optimized Layout



Optimized Sensor Network Layout



Zones of Vulnerability after 25+ of Remediation

Basin Capping/Closure

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- Prevents infiltration that would drive contaminants deeper

Subsurface Barrier w/Treatment Zones

- U and Sr-90 attenuated by raising pH
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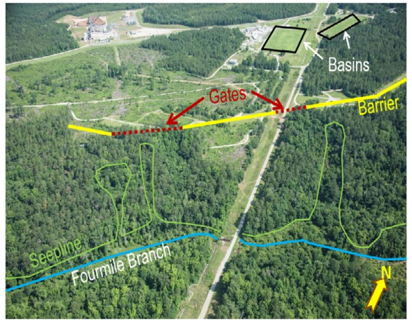

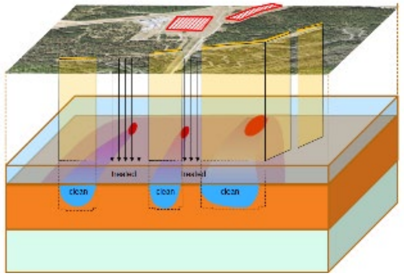

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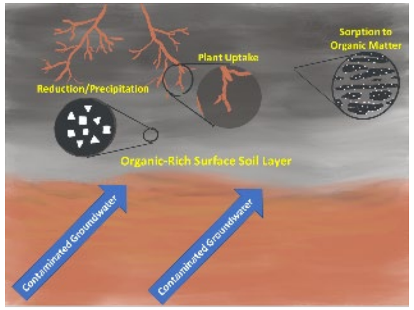
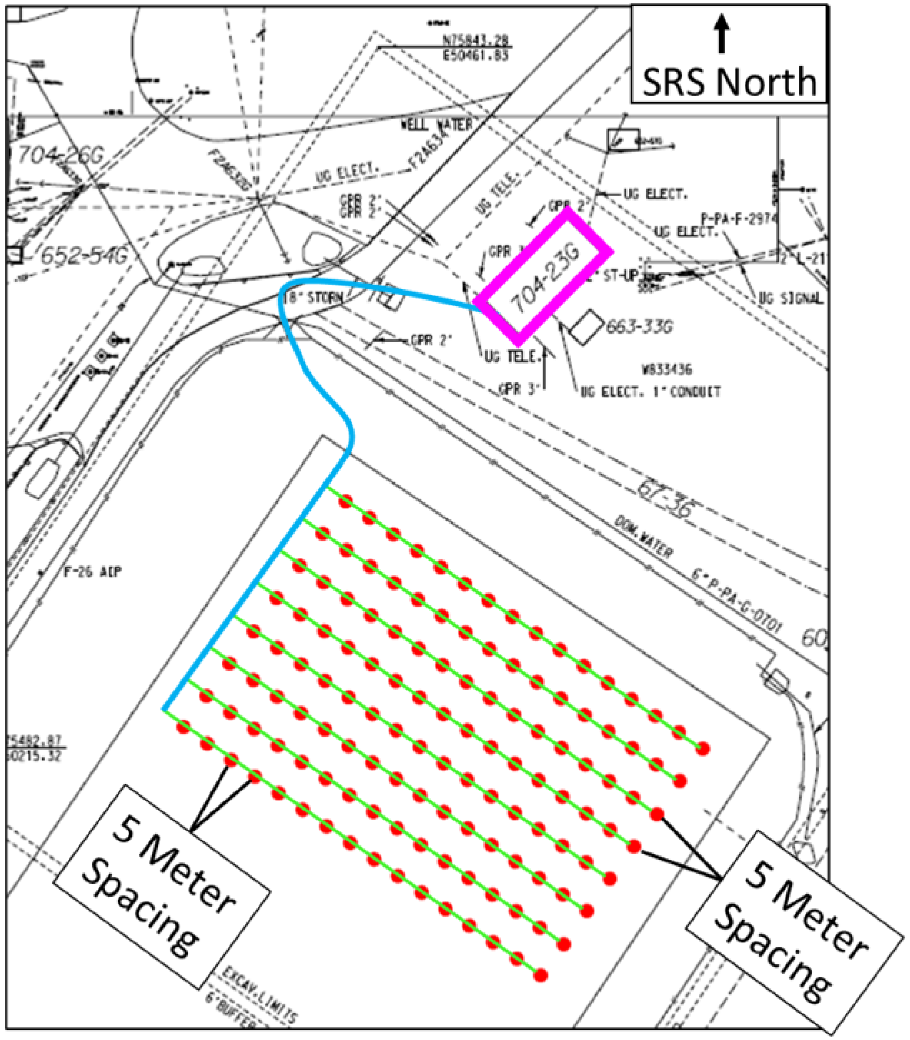
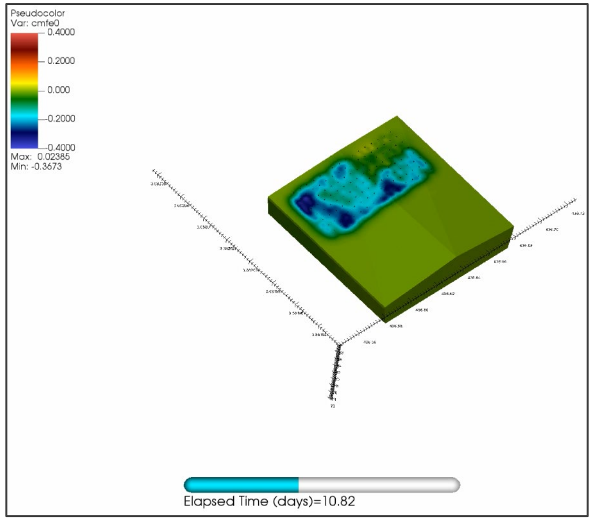
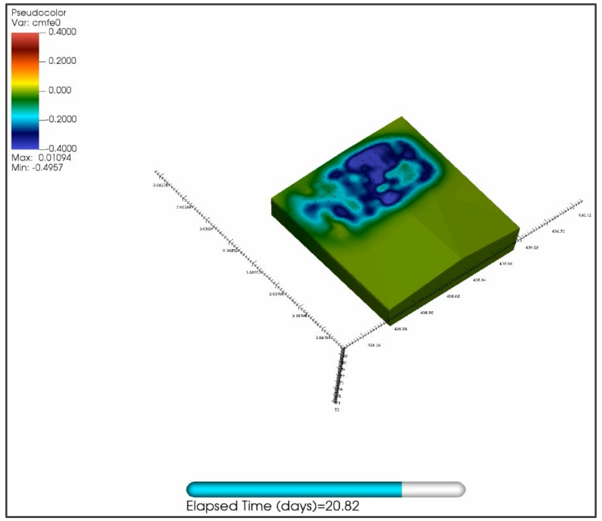


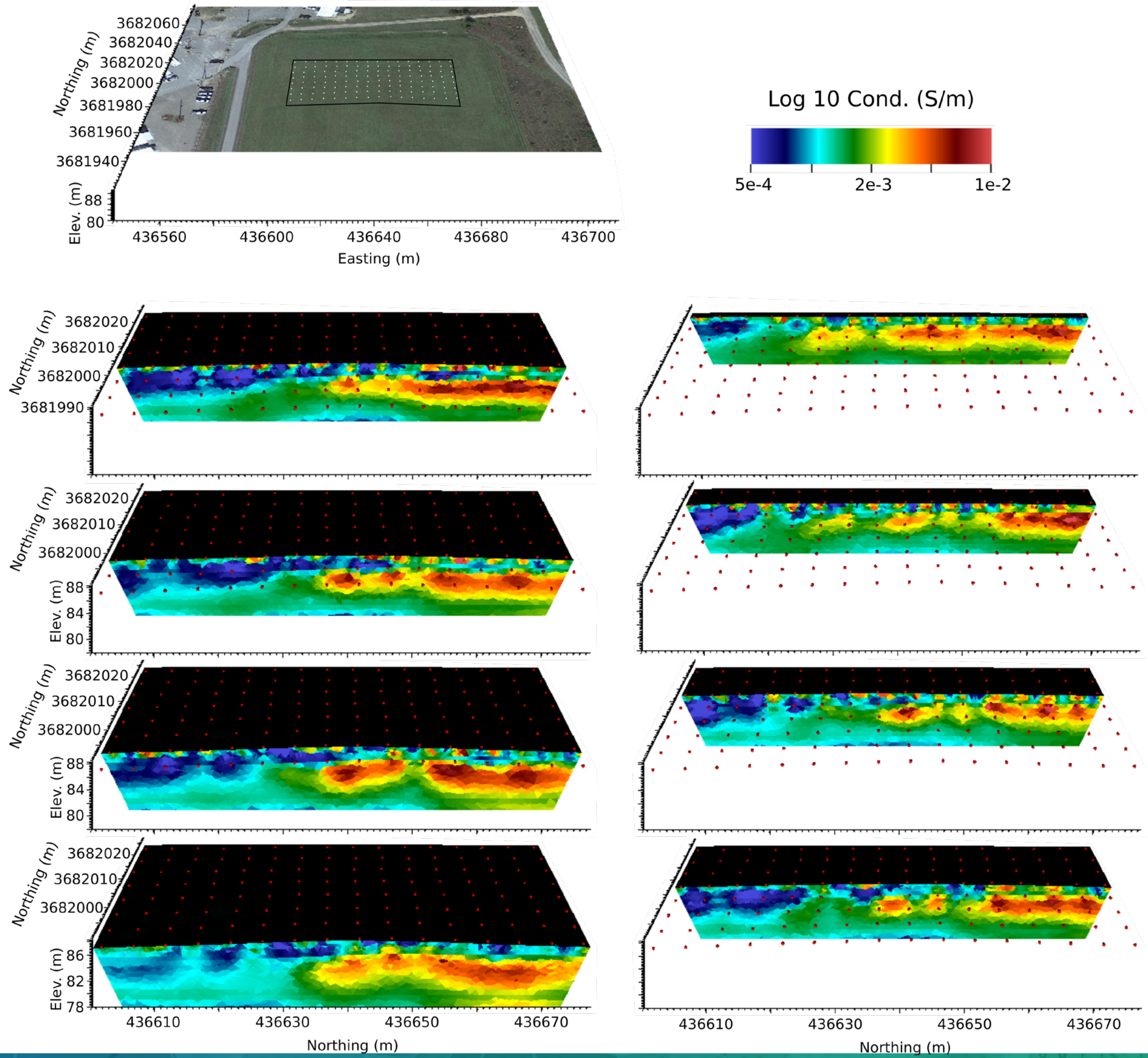
Electrical Resistance Tomography



Monitoring Basin Soils Beneath Low Permeability Cap







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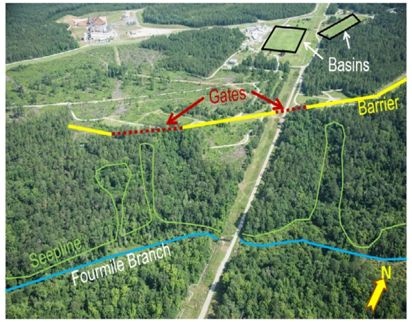
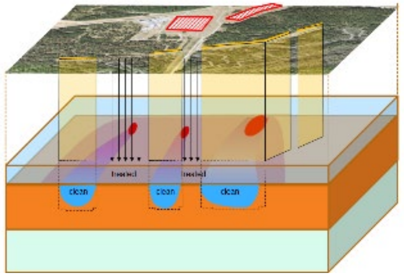
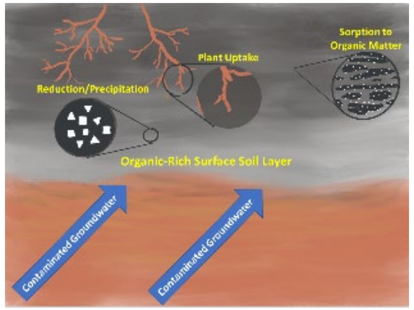




Wetland/Hyporheic Zone

- Contaminants attenuated by processes in organic-rich soils
- Sorption to organic matter, plant uptake, reduction/precipitation for some contaminants



Wetland/Seepline monitoring

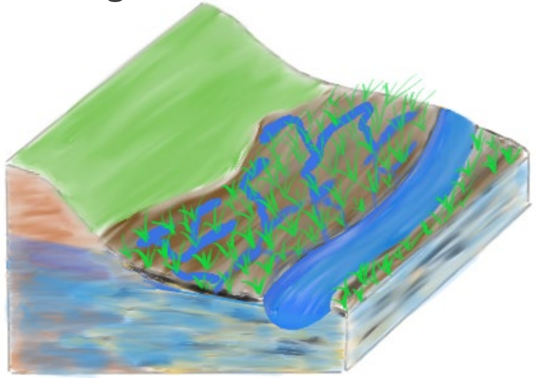
<u>Vulnerability:</u> Physical and chemical conditions change, releasing dissolved and/or particulate-bound contaminants

<u>Objective:</u> Monitor wetlands to ensure no remobilization of attenuated contaminants

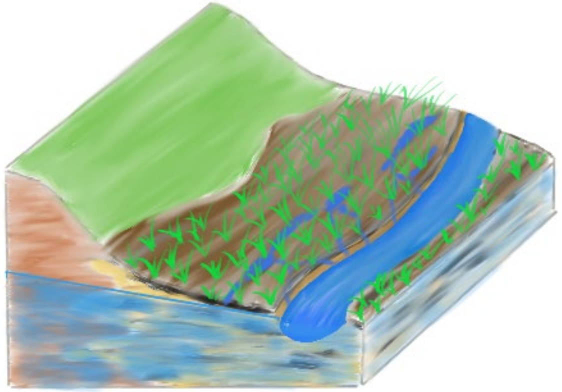
<u>Monitoring Tools/Technologies:</u>

- Spatially Integrative Tools
  - ➢ Periodic UAV surveys: LiDAR, gamma, photogrammetry
    - Topography, vegetation, contaminant distribution, springs distribution, etc.
  - ➢ Distributed Temperature Sensors
    - Temperature, soil moisture
- Point Source Measurements
  - ➢ Sensors in surface water

High Water Table



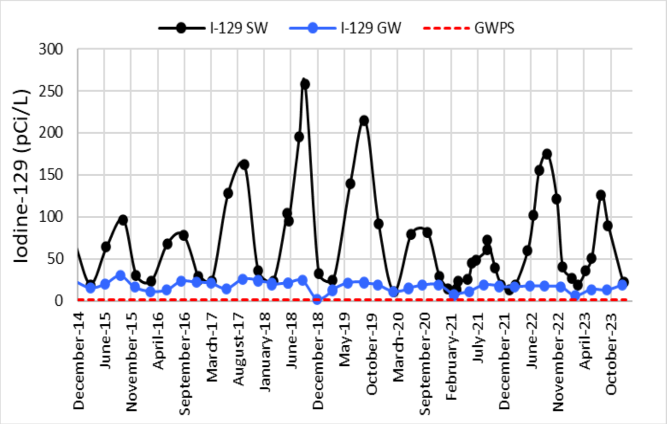
Low Water Table



F-Area Wetlands: Seasonal Variations of I-129

Installation of wetland sensor network

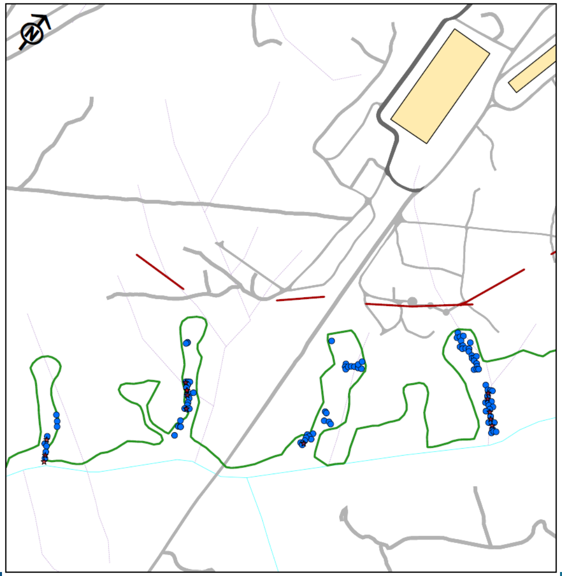
- Sensors deployed in 6 shallow piezometer wells and 6 surface water monitoring points.
- Monitoring changes in groundwater/surface-water chemistry that could potentially remobilize contaminants.



F-Area Wetlands: Groundwater-Surface Interaction

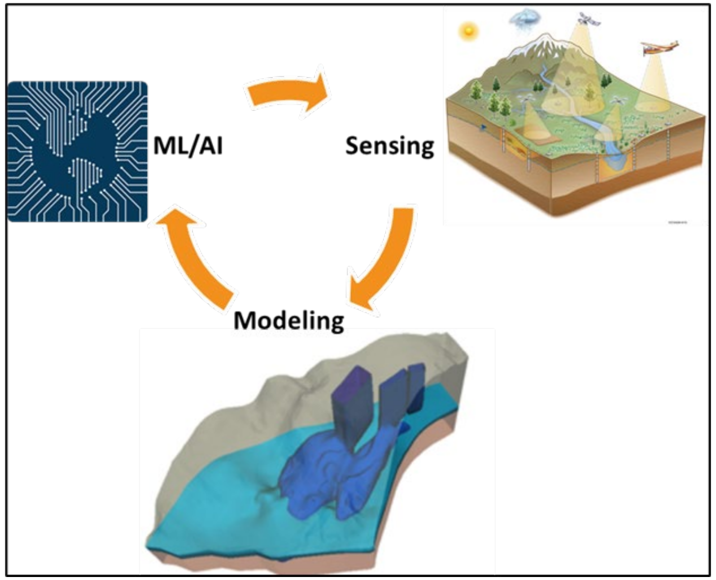
<u>Temperature Sensor Network</u>

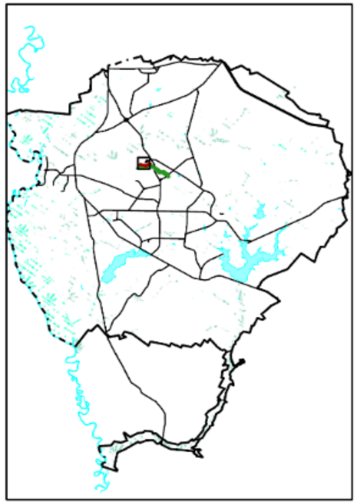
- Depth discrete temperature probes at 97 locations in the wetlands.
- High spatial resolution measurements (10 cm) of temperature with depth.



Comprehensive Sensor Network F-area

- Multiple sensing modalities at various "zones of vulnerability"
- Refining AI/ML approaches to automate data processing, make predictions, and detect anomalous behavior
- Feedback loop between sensing, AI/ML, and deterministic models





Locations of Sensor Network Installed at the F-Area Seepage Basins

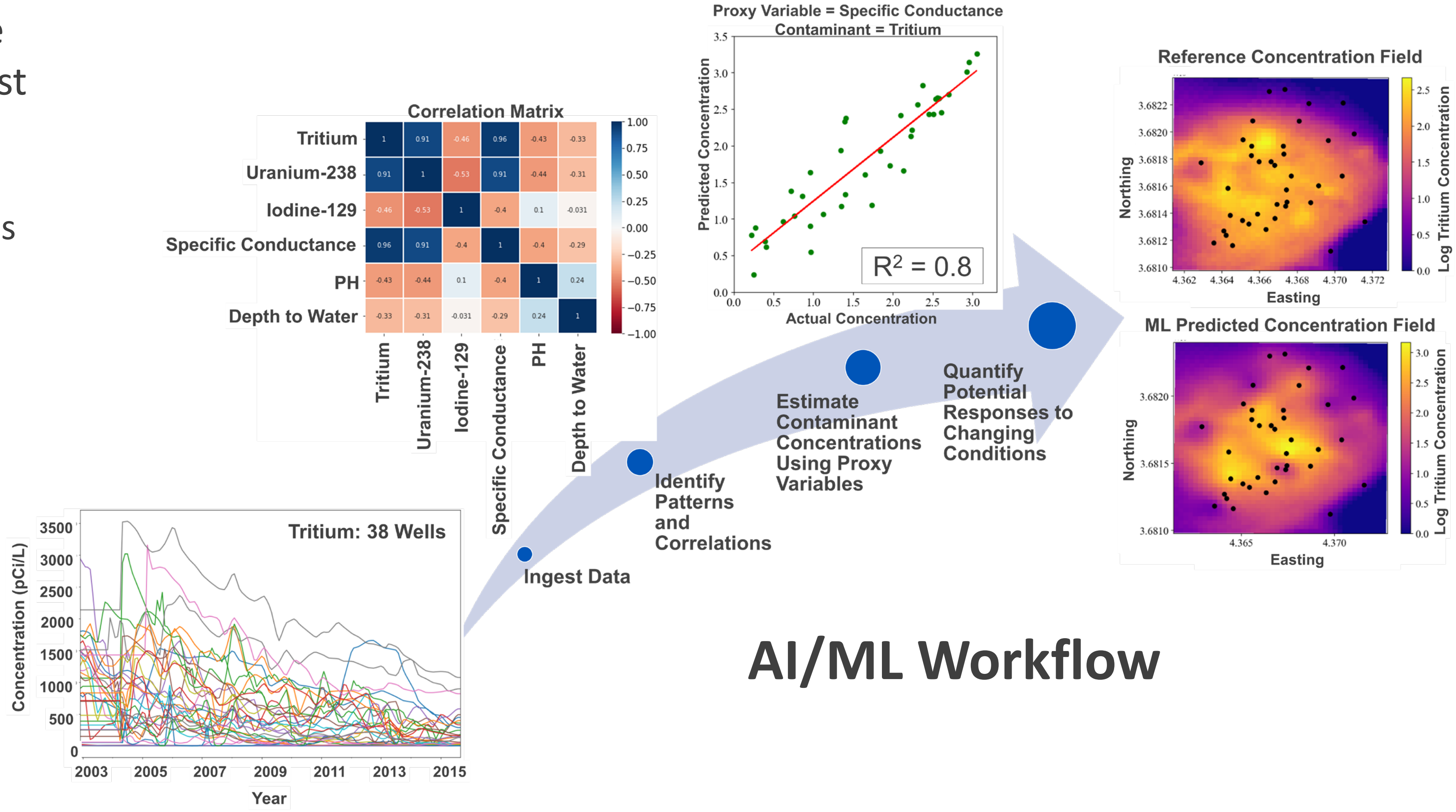
Path Forward – ALTEMIS

- Sensor network installation at the F-Area completed
- Current activities have shifted towards monitoring and maintenance of sensors.
- Development of a data management system to house the transmittal, storage, and access of the continuous sensor data.
- Use of statistical tools to optimize monitoring.
- Use of AI/ML approaches to automatize data process, make predictions and anomaly detection.

- Meetings with regulators, stakeholders
- Application to arid sites/problems

Outstanding Challenges

- Environmental datasets are messy, but AI/ML works best with clean data
  - Missing values, different analysis techniques across time, etc.
  - Geophysical/chemical considerations (environmental discontinuities)
  - Poor spatio-temporal coverage across time
- Accessibility to non-AIML experts

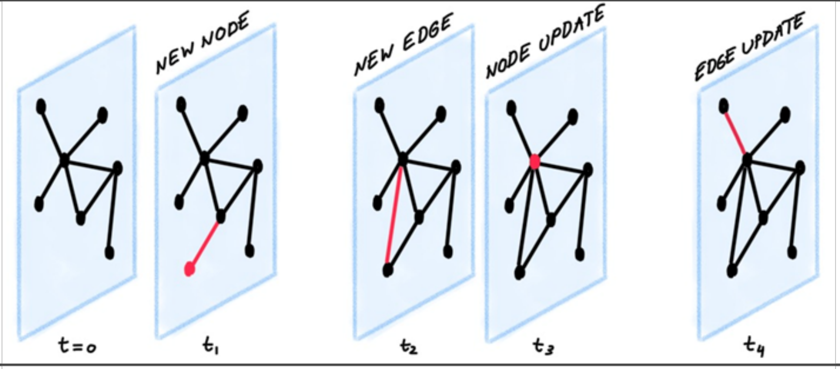


AI/ML Workflow

Overcoming Challenges

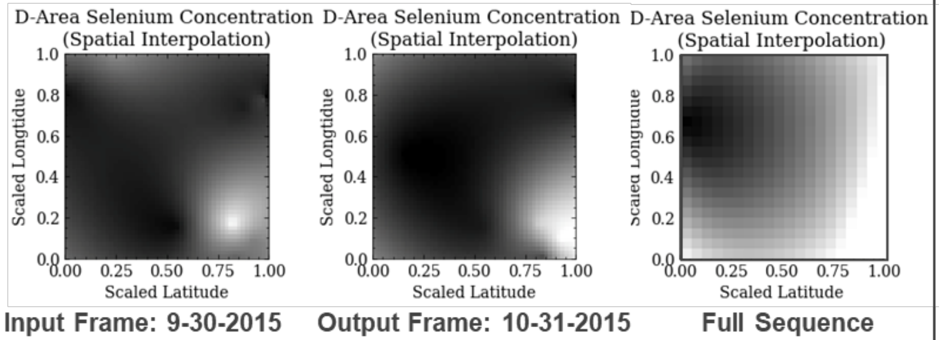
Graph Neural Networks

- Specialize in learning relationships between nodes in a network (e.g., wells)
- Can accommodate temporal changes in graph structure (e.g., links between nodes may not be static)



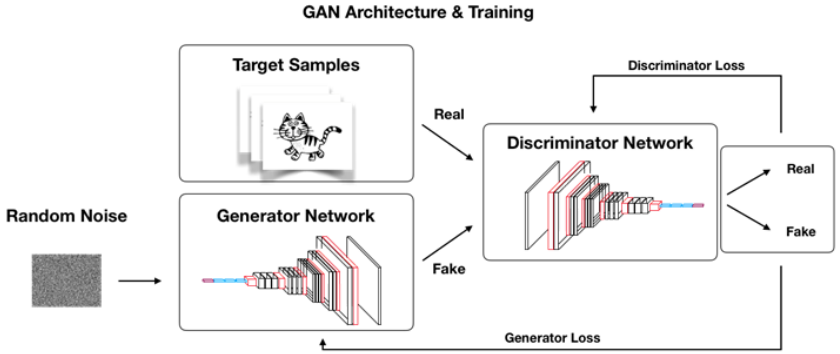
ConvLSTM

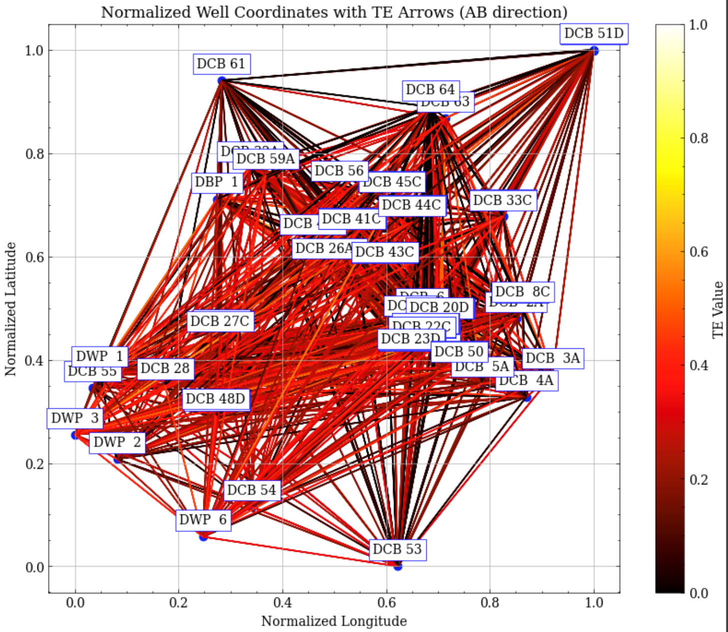
- Ability to learn across space and time in a single pass
- Automatically performs interpolation due to the nature of the input and out



Generative Adversarial Networks

- Can be used to generate synthetic datasets
- Overcomes challenges associated with locations that have small datasets



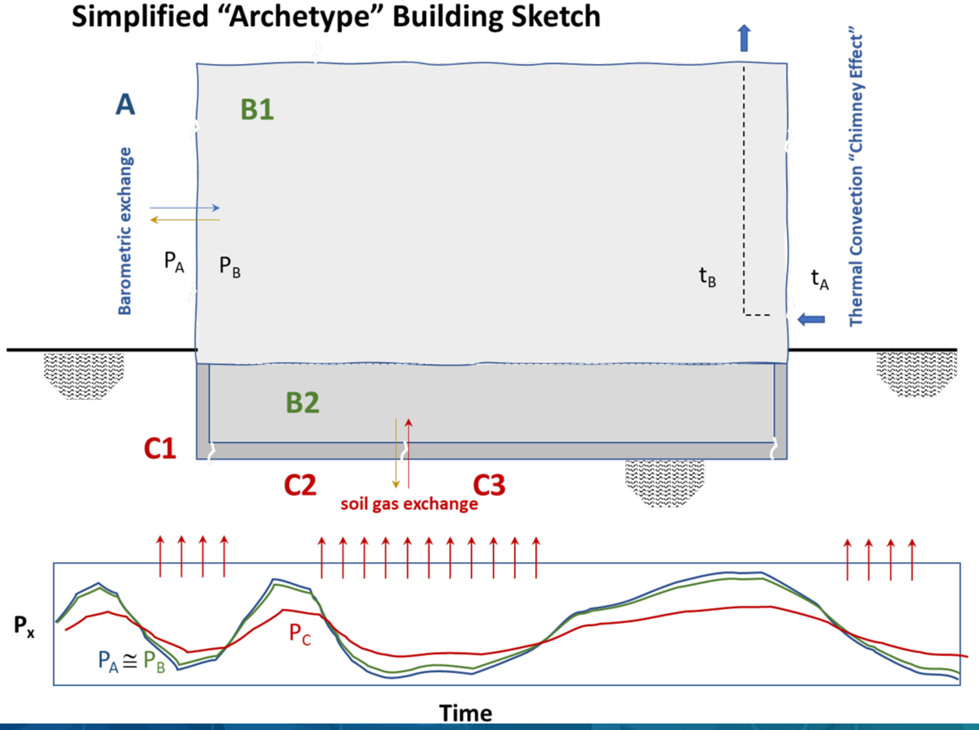


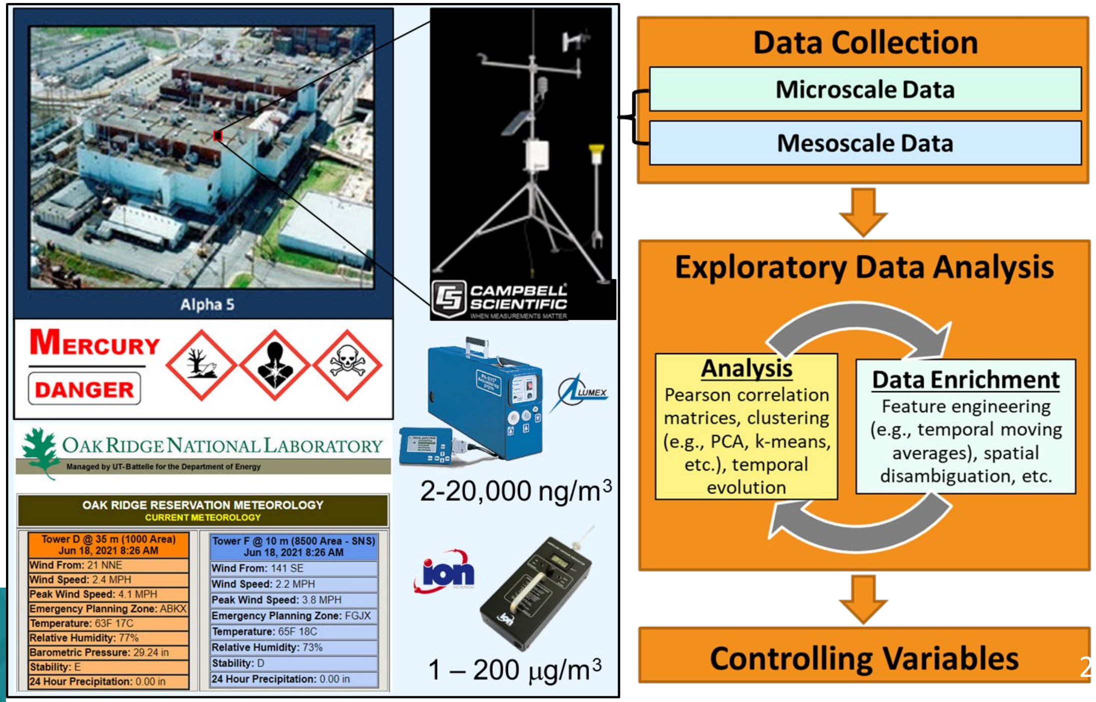
Transfer Entropy

- Enhance per-well prediction by considering potential causality
- Non-parametrically produces matrix of directed connections

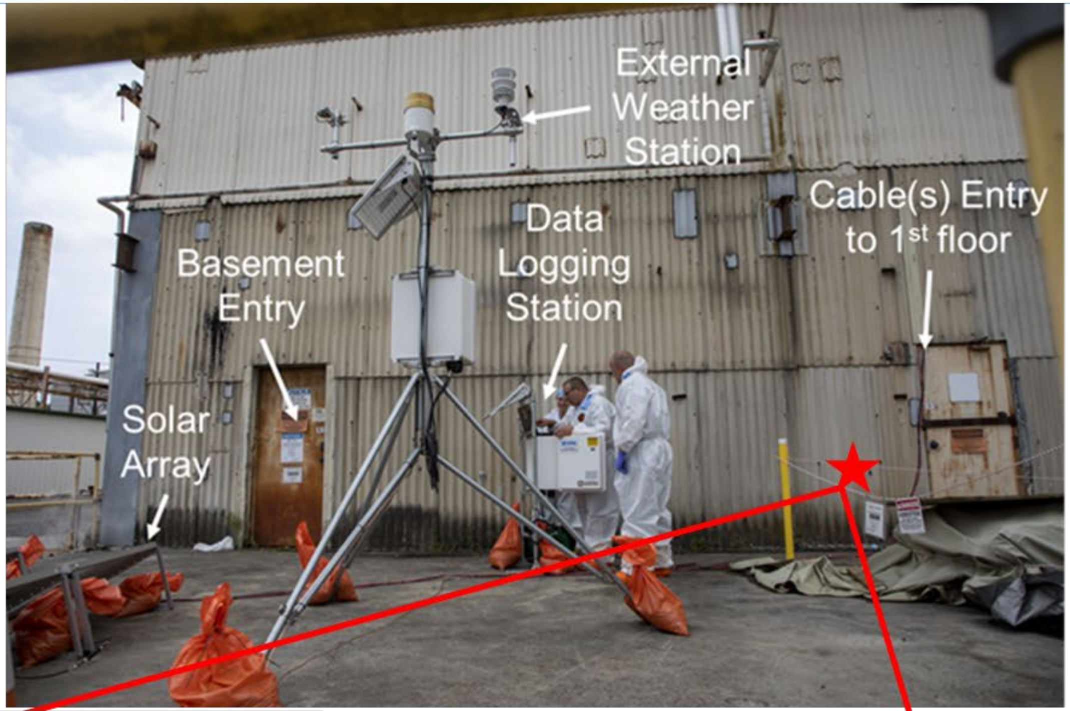
SRNL Activities at Y-12 Mercury Use Facilities

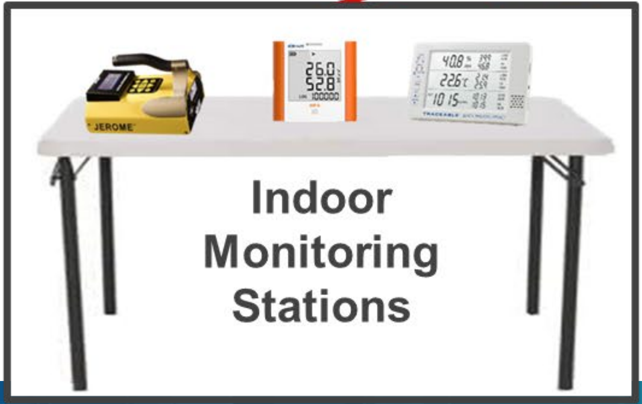
- **Y-12's legacy mercury-use facilities**
  - Significant levels of mercury present in equipment, piping systems, facility sumps, drain fields, and structures
- **Challenge for D&D**
  - Presence of intermittent, variable, and high levels of mercury vapor distributed through the interior of the building
  - Periodically exceeds established OSHA exposure limits for mercury
  - Controlling mechanisms for the release of mercury vapors is poorly understood

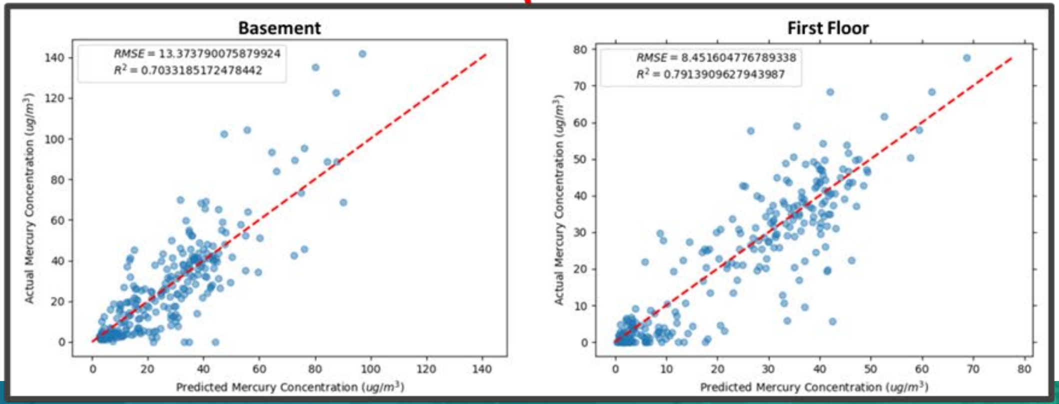




SRNL Activities at Y-12 Mercury Use Facilities



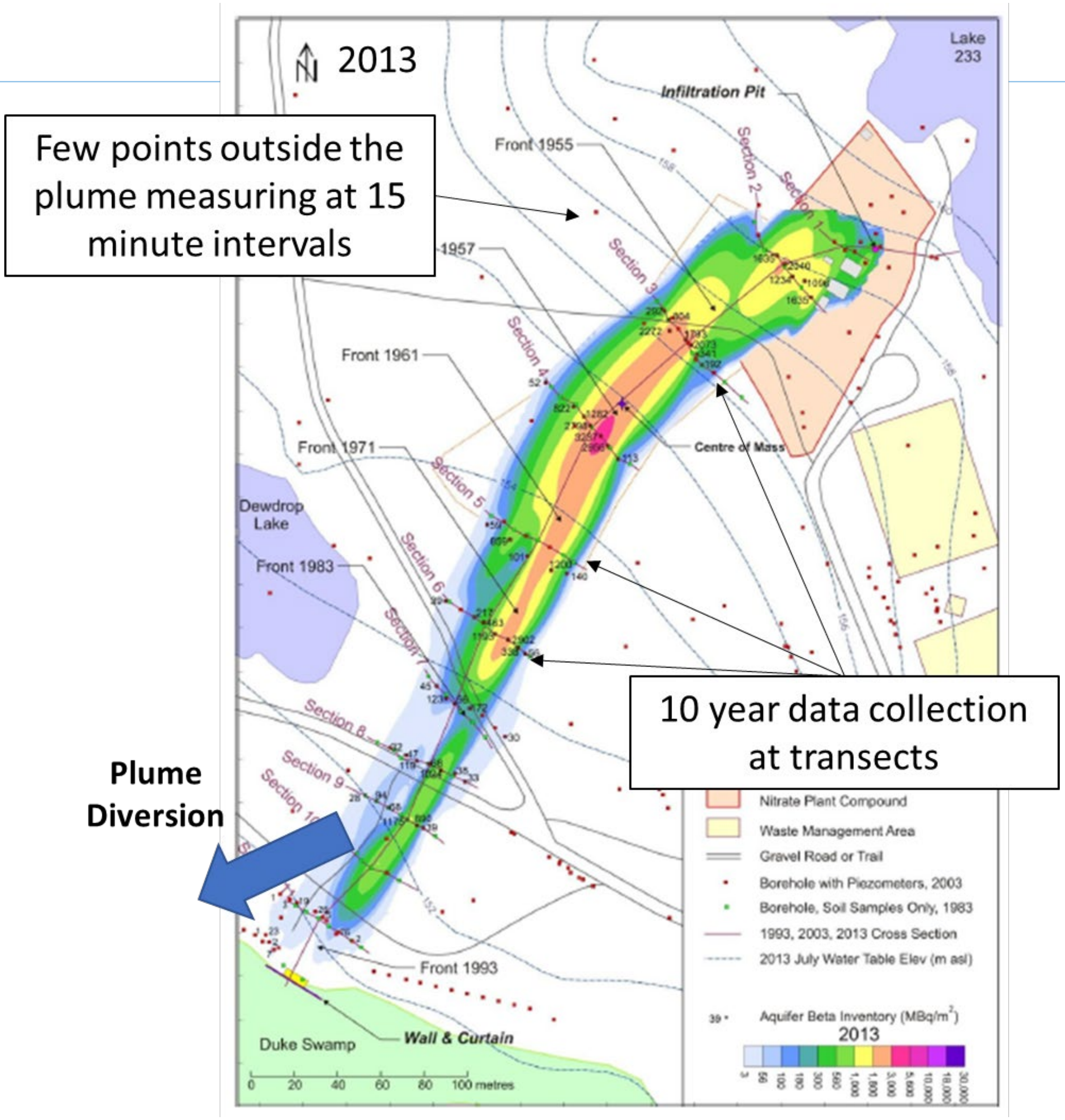




ALTEMIS Applied at Chalk River

- Plume anomalies have appeared in the plume across time – e.g., beaver dam failure, followed by plume diversion **(environmental discontinuity)**

- 10-year facility characterization updates – how can we monitor for anomalies in the interim periods? **(sparse temporal data)**



Concluding Remarks

- With guidance from a strong conceptual model, installation of sensor networks enhances environmental datasets and improves robustness of models
- Sensors coupled with AI/ML provides an opportunity to capture environmental shifts and guide-decision making process
- **End Result**: Safer, more proactive, and cost-effective approach to long-term monitoring and cleanup activities

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- Joanna Szornel

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Pacific Northwest National Laboratory

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Florida International University

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- Aubrey Litzinger
- Phuong Pham

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