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Application of the ASCEM Model to the SRS F-Area Seepage Basins:

Technical Advances in Long Term Monitoring of Groundwater

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The EM Challenge



107 major sites (1995) → 16 sites (2016)

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- Remediation of large complex groundwater plumes of metals and long-lived radionuclides (e.g., Tc, I)
- Transition from active remediation systems (P&T) to passive methods (Monitored Natural Attenuation)
- DOE sites (RL, SRS, Paducah, LANL, LM)

How do we do that?

 Enhanced attenuation -- In situ remedy that reduces mobility of contaminants to achieve goals that are sustainable for long time periods

Enhanced Attenuation Remedies

Monitored Natural Attenuation (MNA):

Let natural processes do the work and monitor progress

Enhanced Attenuation (EA):

Engineered remedy that increases attenuation capacity of aquifer

Attenuation-based remedies leave contaminants in subsurface

- Require a high burden of proof that contaminants will not re-mobilize and become a threat again
- Strategic design helps meet the burden of proof





The Problem: SRS F-area Basins

Groundwater plume resulted from 30 years of discharge of low activity wastewater from an industrial nuclear facility. Major contaminants of concern are metals, uranium, tritium, and radioactive iodine.





F-area Basins Remedial Timeline





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F-Area Basins Monitoring Network

Large number of point measurements

Small number of locations are required by regulatory agreement



Long Term Monitoring by Function

Baseline approach for LTM

- Quarterly monitoring of contaminant concentration
- Yield limited insight into the conditions and processes that control plume stability and contaminant migration

Long Term Monitoring by Function

Add inexpensive measurements of controlling processes such as boundary conditions and geochemical master variables to provide functional assessment to supplement analysis of a reduced number of groundwater samples

- Hydrologic Boundary Conditions
- Master Variables



Boundary Conditions

Overall physical and hydrological driving forces

Data types include meteorology, hydrology, geology, land use, operation/remediation history, e.g.

- changes in production of water from wells (process/potable/municipal/agricultural)
- changes in discharge of water to basins/streams, dams, etc.
- new infrastructure and construction
- discontinuation of active industrial processes

Generally easy to measure and often overlooked

Data Sources

- Precipitation Precipitation gauges and telemetry, satellite data, groundwater level monitoring
- Evapotranspiration Landsat satellite data
- Stream/River Flow USGS databases, stream flow gauges, satellite data
- Precipitation chemistry (Acid rain, Hg deposition) – NADP maps, point monitoring)
- Surface water (lakes, ponds, drainages, etc.)

 Army Corps of Engineers, local authorities, etc.
- Pumping Wells (New and existing wells) Local municipalities
- Discharges (Industry outfalls etc.) Local and government agencies
- Infrastructure/Construction -- Local and government agencies



Master Variables are the key variables that control the chemistry of the groundwater system

- -Redox variables (ORP, DO, chemicals)
- -pH
- -Specific Conductivity
- -Biological Community (Breakdown/decay products)
- -Temperature

Existing sensors and tools to measure these variables inexpensively are commercially available



Field Demonstration of Approach

Technical Problem

 How do you test a new paradigm for long-term monitoring without doing years of long-term monitoring?

Approach

- Use monitoring data from a waste site with a long history of data and well characterized changes to boundary conditions and master variables
- Identify key controlling variables and implement strategy at a well characterized test bed

Contaminants Through Time



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Complexities

Lots of "noise" in the measurements

Small water level changes cause significant changes in measurement of stratified plume.

Different areas of the plume exhibit fundamentally different behavior.

Time scale of change -- Daily, Seasonal, Climatic

What is a significant change? -- Determination of trigger levels.



How do you test a new paradigm for long term monitoring without doing years of monitoring?

- Use historical monitoring data from a waste site with a long history and documented changes to boundary conditions
- ✓ Develop a virtual test bed using 3D reactive flow and transport model



Prediction Capability: ASCEM

Advanced Simulation Capability for Environmental Management



New Paradigm of LTM

Big Data methods for real-time data analysis and early warning systems

• Data mining, machine learning (Kalman filters, artificial neural network) Virtual Test Bed: ASCEM modeling tool for predicting long-term performance New sensing technologies for automated remote continuous monitoring

• In situ sensors, geophysics, fiber optics, UAVs



F-Area Virtual Testbed

- Field Test Bed
 - -Historical datasets
 - \rightarrow Advanced statistical analysis
 - Data mining
 - Machine learning





Virtual Test Bed

- 3D reactive transport simulations
- Super computers

 \rightarrow System understanding, long-term predictions, testing different methods

In situ Variables vs Contaminants



→ Feasibility of In situ Monitoring



Automated QA/QC



- •ved) Remove outliers or noise using smoothing
 - Gap filling
 - Detect significant changes

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Flow/Transport Model



3D Mesh Development



Plume Visualization

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3D Mesh for Artificial Barriers





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Effect of Barriers on Tritium Plume



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Geochemistry Development

- Complex geochemistry
 - -pH Dependent
 - -Aqueous complexation
 - -Surface complexation
 - -Mineral dissolution/precipitation
 - -Cation exchange

-Decay

Surface complexation, cation exchange		log ₁₀ K (25° C)
(>SO)UO ₂ ⁺ ↔ >SOH - H ⁺ + UO ₂ ²⁺		-0.44
⁽²⁾ Cation Exchange		K (25 C)
$NaX \leftrightarrow Na^+ + X^-$ $CaX_2 \leftrightarrow Ca^{2+} + 2 X^-$		1.0 0.316
$A1X_3 \leftrightarrow A1^{3+} + 3 X^{-}$ $HX \leftrightarrow H^{+} + X^{-}$		1.71 0.025
Mineral dissolution/precipitation	log ₁₀ K (25° C)	Ref.
Quartz \leftrightarrow SiO ₂ (aq) Kaolinite \leftrightarrow 2A1 ⁺³ + 2SiO ₂ (aq) + 5H ₂ O - 6H ⁺	-3.7501 7.57	(2)
Goethite \leftrightarrow Fe ⁺³ + 2H ₂ O - 3H ⁺	0.1758	
Schoepite $\leftrightarrow UO_2^{+2} + 3H_2O - 2H^+$	4.8443	(1)
Gibbsite $\leftrightarrow Al^{+3} + 3H_2O - 3H^+$	7.738	(3)
Jurbanite $\leftrightarrow Al^{+3} + SO_4^{-2} + 6H_2O - H^+$	-3.8	(4)
Basaluminite $\leftrightarrow 4A1^{+3} + SO_4^{-2} + 15H_2O - 10H^+$	22.251	(4)
$Opal \leftrightarrow SiO_2(aq)$	-3.005	(5)
Aqueous complexation	log ₁₀ K (25° C)	
$OH^- \leftrightarrow H_2O-H^+$	13.99	
$AIOH^{2+} \leftrightarrow AI^{3+} + H_2O - H^+$	4.96	
$Al(OH)_2^+ \leftrightarrow Al^{3+} + 2H_2O - 2H^+$	10.59	
$Al(OH)_3(aq) \leftrightarrow Al^{3+} + 3H_2O - 3H^+$	16.16	
$Al(OH)_4^- \leftrightarrow Al^{3+} + 4H_2O - 4H^+$	22.88	
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3D Plume Evolution



First-Order Effective Decay Rates

• Effective decay rates given by first-order decay equation

$$C_t = C_0 \times e^{-kt}$$

- Incorporate all attenuation mechanisms
- If contaminant concentration vs. time follows firstorder behavior, time to reach MCL can be calculated
- Spatial variations in time to reach MCL can guide monitoring strategy for different areas of plume
- Sharp changes in effective decay rate indicate change in controlling mechanism
 - Highlights need to understand controlling mechanism
 - May even allow trigger levels to be established



Environmental Data Management



Geophysical Subsurface Imaging

- Electrical Resistivity Tomography
- Autonomous data collection and streaming
- Bulk electrical conductivity \rightarrow Plume migration etc



Fiber Optics Technologies

- Autonomous
 Distributed sensing
 - Temperature
 - Soil moisture
 - Acoustic properties
 - Chemistry (e.g., pH)



Permafrost Thaw Detection



We put schipe Franklin et al

Drone-based Sensing Technologies

2014Oct09_Ortho.tif 2014Mar08 DEM.ti Courtesy to Dafflon et al.

Soil Moisture/Surface Drainage Mapping

Fukushima Gamma Source Mapping



Courtesy to Kai Vetter et al.

- Microtopography
- Surface deformation
- Vegetation dynamics/characteristics
- Surface temperature
- Radioactive contamination

Summary

Real/Virtual Test Bed at SRS F-Area

- Data analysis confirmed the feasibility of in situ monitoring
- ASCEM 3D flow and transport simulations quantified the correlations (spatially and temporally variable) but also the future trajectory
- UQ/sensitivity analysis: the long-term feasibility of monitoring

Cost-effective strategies for long-term monitoring of contaminants (incl. Tritium)

- In situ sensors, data streaming and data analytics for automated continuous monitoring
- Advanced technologies: geophysics, fiber optics, UAVs
- Data Analytics: QA/QC, correlations between master variables and contaminant concentrations
- Integrated approach (data + modeling) for system understanding/estimation

