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Use of an Alternative Paradigm to Support Optimization of In Situ Remedies at Metal and Radionuclide Contaminated Sites

'The Virtual Test Bed'

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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



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





F-Area Basins Monitoring Network

Large number of well/sampling locations where groundwater is sampled and analyzed

Only a small number of locations are required by regulatory agreement



Baseline approach

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

Monitoring by Function

Add inexpensive measurements of controlling processes such as boundary conditions and geochemical_{mas} ter 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



Technical Problem

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

Approach

- Use monitoringdata from a waste site with a lon ⁹histor ^y 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



Groundwater Flow Through Time

Water level measurements indicate distinct changes in flow pattern

Precipitation predictive of water level in some wells





Sensor Installation









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Contaminants Through Time



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Specific Conductance as a Surrogate





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15

Lots of "noise" in the measurements

- Small water level changes cause significant changes in measurement of stratified plume.
- Time scale of change Daily, Seasonal, Climatic ...
- Different areas of the plume show different trends
- Surrogate measurements seem to be robust but calibration issues with sensors an issue

How do you determine what is a significant change?

Determination of trigger levels for action

Yikes !!! – What to Do?

Advanced Simulation Capability for Environmental Management



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

✓ Develop a virtual test bed using 3D reactive flow and transport model



Flow/Transport Model



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3D Mesh Development



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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

		(25° C)
⁽¹⁾ Equilibrium Surface Complexation		
$(>SO)UO_2^+ \leftrightarrow >SOH - H^+ + UO_2^{2+}$		-0.44
⁽²⁾ Cation Exchange		K (25 C)
$NaX \leftrightarrow Na^+ + X^-$		10
$CaX_2 \leftrightarrow Ca^{2+}+2X^{-}$		0.316
$A1X_3 \leftrightarrow A1^{3+} + 3 X^{-}$		1.71
HX↔H ⁺ + X ⁻		0.025
Mineral dissolution/precipitation	log10 K (25° C)	Ref.
Quartz \leftrightarrow SiO ₂ (aq)	-3.7501	(1)
Kaolinite $\leftrightarrow 2\text{Al}^{+3} + 2\text{SiO}_2(\text{aq}) + 5\text{H}_2\text{O} - 6\text{H}^+$	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 $\leftrightarrow AI^{+3} + 3H_2O - 3H^+$	7.738	(3)
Jurbanite $\leftrightarrow Al^{+3} + SO_4^{-2} + 6H_2O - H^+$	-3.8	(4)
Basaluminite $\leftrightarrow 4Al^{+3} + SO_4^{-2} + 15H_2O - 10H^+$	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	
$A10H^{2+} \leftrightarrow AI^{3+} + H_2O - H^+$	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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New Paradigm

Big_{Da} ta methods for real-time data analysis and early_{Wa} rning systems **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



Virtual test bed



Developing specific strategy for F-area

- Master variables and sensor/well locations through time for different contaminants
- Change in absorption/mobility for contaminants in system as pH evolves
- Establish trigger levels for boundary conditions
- Test hypotheses using virtual test bed
- Develop recommendations for key geochemical events for complex plumes of metal and radionuclides
- Investigate new methods for monitoring_{that} are multidimensional to focus on measurement of changes.



Environmental Data Management



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Geophysical Subsurface Imaging

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



Fiber Optic Technologies

Autonomous Distributed sensing

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



Permafrost Thaw Detection





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Ajo-Franklin et al

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Drone-based Sensing Technologies

Soil Moisture/Surface Drainage Mapping



Fukushima Gamma Source Mapping



• Microtopography

Courtesy to Kai Vetter et al.

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



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