Application of the ASCEM Model to the SRS F-Area Seepage Basins:
Technical Advances in Long Term Monitoring of Groundwater

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107 major sites (1995) → 16 sites (2016)
The EM Challenge

• 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
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

- **1955**: Waste Discharged to Basins
- **1988**: Basins Closed/Capped
- **1991**: Pump-Treat
- **1997**: Funnel-and-Gate/Base Injection
- **2003**: Present
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

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

**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

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
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.
Virtual Testbed

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
    → Advanced statistical analysis
  – Data mining
  – Machine learning

• Virtual Test Bed
  – 3D reactive transport simulations
  – Super computers
    → System understanding, long-term predictions, testing different methods
In situ Variables vs Contaminants

Feasibility of In situ Monitoring
Automated QA/QC

- Remove outliers or noise using smoothing
- Gap filling
- Detect significant changes
F-Area Virtual Testbed

• **Field Test Bed**
  – Historical datasets
    → Advanced statistical analysis
  – Data mining
  – Machine learning

• **Virtual Test Bed**
  – 3D reactive transport simulations
  – Super computers
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Flow/Transport Model

Bea et al. (2013)
3D Mesh Development

Surface Seismic Method

Wainwright et al. (2014)
Plume Visualization
3D Mesh for Artificial Barriers

Meshing by LAGriD
Effect of Barriers on Tritium Plume
Geochemistry Development

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

### Surface complexation, cation exchange

<table>
<thead>
<tr>
<th>Reaction</th>
<th>log₁₀ K (25°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(SO)UO₂⁺ ↔ SO⁻H⁺ + UO₃²⁺</td>
<td>-0.44</td>
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</table>

### Cation Exchange

<table>
<thead>
<tr>
<th>Reaction</th>
<th>K (25°C)</th>
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<tbody>
<tr>
<td>NaX ↔ Na⁺ + X⁻</td>
<td>1.0</td>
</tr>
<tr>
<td>CaX₂ ↔ Ca²⁺ + 2 X⁻</td>
<td>0.316</td>
</tr>
<tr>
<td>AlX₃ ↔ Al³⁺ + 3 X⁻</td>
<td>1.71</td>
</tr>
<tr>
<td>HX ↔ H⁺ + X⁻</td>
<td>0.025</td>
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</tbody>
</table>

### Mineral dissolution/precipitation

<table>
<thead>
<tr>
<th>Reaction</th>
<th>log₁₀ K (25°C)</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartz ↔ SiO₂ (aq)</td>
<td>-3.7501</td>
<td>(1)</td>
</tr>
<tr>
<td>Kaolinite ↔ 2Al³⁺ + 2SiO₂ (aq) + 5H₂O - 6H⁺</td>
<td>7.57</td>
<td>(2)</td>
</tr>
<tr>
<td>Goethite ↔ Fe⁺⁺ + 2H₂O - 3H⁺</td>
<td>0.1758</td>
<td></td>
</tr>
<tr>
<td>Sceopeite ↔ UO₂²⁺ + 3H₂O - 2H⁺</td>
<td>4.8443</td>
<td>(3)</td>
</tr>
<tr>
<td>Gibbsite ↔ Al³⁺ + 3H₂O - 3H⁺</td>
<td>7.738</td>
<td>(3)</td>
</tr>
<tr>
<td>Jarvanite ↔ Al³⁺ + SO₄²⁻ + 6H₂O - H⁺</td>
<td>-3.8</td>
<td>(4)</td>
</tr>
<tr>
<td>Basaluminite ↔ 4Al³⁺ + SO₄²⁻ + 15H₂O - 10H⁺</td>
<td>22.251</td>
<td>(4)</td>
</tr>
<tr>
<td>Opal ↔ SiO₂ (aq)</td>
<td>-3.005</td>
<td>(5)</td>
</tr>
</tbody>
</table>

### Aqueous complexation

<table>
<thead>
<tr>
<th>Reaction</th>
<th>log₁₀ K (25°C)</th>
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<tbody>
<tr>
<td>OH⁻ ↔ H₂O - H⁺</td>
<td>13.99</td>
</tr>
<tr>
<td>AlOH₂⁺ ↔ Al³⁺ + H₂O - H⁺</td>
<td>4.96</td>
</tr>
<tr>
<td>Al(OH)₂⁺ ↔ Al³⁺ + 2H₂O - 2H⁺</td>
<td>10.59</td>
</tr>
<tr>
<td>Al(OH)₃(aq) ↔ Al³⁺ + 3H₂O - 3H⁺</td>
<td>16.16</td>
</tr>
<tr>
<td>Al(OH)₄ ↔ Al³⁺ + 4H₂O - 4H⁺</td>
<td>22.88</td>
</tr>
</tbody>
</table>

(And more)
3D Plume Evolution

Low-pH plume

U plume
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 first-order 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

- **QA/QC methods developed for**
  - Pressure transducer data to measure water levels
  - Temperature data in vadose zone and groundwater
  - Meteorological data

- **QC flagging method to identify**
  - and correct erroneous data outside a reasonable range and occurrence of anomalous spikes (due to perturbations during water sampling events from monitoring wells).

- **QA/QC of location coordinates,**
  - elevations and top of casings
Geophysical Subsurface Imaging

- Electrical Resistivity Tomography
- Autonomous data collection and streaming
- Bulk electrical conductivity → Plume migration etc
Fiber Optics Technologies

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

Permafrost Thaw Detection

Ajo-Franklin et al.
Drone-based Sensing Technologies

Soil Moisture/Surface Drainage Mapping

Fukushima Gamma Source Mapping

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

Courtesy to Kai Vetter et al.

Courtesy to Dafflon et al.
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