Recognizing Critical Processes and Scales in Conceptual Site Models for Decision Support at Sites of Groundwater Contamination

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U.S. Geological Survey Toxic Substances Hydrology Program
Management Decisions at Sites of Groundwater Contamination

**Absolute Objectives:** Higher order community and societal (stakeholder) requirements (e.g., mitigate human and ecological adverse health effects, minimize disturbances to community, adherence to drinking water standards, etc.)

**Functional Objectives:** Operational goals that lead to successful achievement of absolute objectives (e.g., prevent off-site migration, source zone reduction/removal, reduction of concentrations to MCLs, etc.)

Functional objectives are the driving force for establishing & refining a Conceptual Site Model (CSM) and data collection to implement functional objectives...

Six-Step Process for Source Remediation

SCM = Site Conceptual Model

National Research Council, 2005
Functional objectives are like an elephant . . . they can appear to be large and cumbersome. . .

. . . require conceptualizing and synthesizing operational, physical, and biogeochemical processes over multiple spatial and temporal scales. . .
Functional objective: Mitigating off-site migration

- Source zone characterization. . .source zone architecture and fluxes, chemical phases, solid-phase reactions, biogeochemical process, etc. . . .

- Local and regional groundwater flow and contaminant transport. . .
  local and regional geologic controls, hydrologic & topographic controls, surface water drainages, chemical attenuation processes, etc. . . .
Conceptualization of Subsurface Contaminant Storage and Transport: Organic contaminants

14 - Compartment Model and Contaminant Fluxes between Compartments

(modified from Sale et al., 2008; Sale and Newell, 2011; ITRC 2011)
Functional objectives are like an elephant . . . they can appear to be large and cumbersome. . .


. . . identify those processes at spatial and temporal scales that dominate process outcomes. . .
Conceptualization of Subsurface Contaminant Storage and Transport: Organic contaminants

14 - Compartment Model and Contaminant Fluxes between Compartments

(modified from Sale et al., 2008; Sale and Newell, 2011; ITRC 2011)
An Example of Applying Functional Objectives

- Mitigating off-site contaminant migration in fractured rock

Discussions of the complexity of fractured rock aquifers (Site Characterization, Modeling, and Applications to Waste Isolation and Remediation)


An Example of Applying Functional Objectives

- Mitigating off-site contaminant migration in fractured rock

Fractures control groundwater flow.

... but, there are a lot of fractures.

... over dimensions of centimeters to kilometers.
What do we know about fractures and their capacity to transmit groundwater?

Fractures
Intersecting a Single Borehole

Hydraulic Conductivity of All Fractures

Few fractures control majority of groundwater flow
An Example of Applying Functional Objectives

- Mitigating off-site contaminant migration in fractured rock

**Critical Process and Scales:**

- Narrowed from looking at all fractures to only the most transmissive fractures & their connectivity
- Narrowed data collection and monitoring efforts
- Information critical to design of mitigation (e.g., hydraulic containment, constructed barriers, etc.)
Identifying Transmissive Fractures and Their Connectivity

Advances over 25+ years

• Local and regional tectonic and lithologic controls on fracturing

• Surface and borehole geophysical methods

• Multilevel monitoring equipment

• Design and interpretation of hydraulic and tracer tests

• Modeling groundwater flow and parameter estimation methods
Identifying Transmissive Fractures and Their Connectivity

Granite and Schist, Mirror Lake Watershed, New Hampshire

FSE Well Field Plan View

Distance (meters)

Distance (meters)

FSE Well Field Cross Section

30 meters

pumping

packer

Glacial drift
Identifying Transmissive Fractures and Their Connectivity

Clustering of drawdown records from different monitoring intervals during hydraulic tests provides evidence of transmissive fractures & fracture connectivity...
An Example of Applying Functional Objectives

- Mitigating off-site contaminant migration in fractured rock
  - Identify the most transmissive fractures & their connectivity
    
    One approach -> incorporating biogeochemical processes into groundwater flow path models. . .conceptually complex & computationally intensive to account for mobile and immobile groundwater. . . parameterization is highly uncertain . . .

- Accounting for source zone inputs and attenuation processes
An Example of Applying Functional Objectives

- Mitigating off-site contaminant migration in fractured rock
  - Accounting for source zone inputs and attenuation processes
    - *alternatively* -> conceptualize biogeochemical processes along representative flow paths and identify conditions that bound process responses.

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**Natural Attenuation Software**

- **REMChlor**
- **Matrix Diffusion Toolkit**
- **USGS Methodology for Estimating Times of Remediation Associated with Monitored Natural Attenuation**
- **EPA BIOCHLOR**
- **User’s Manual Version 1.0**

**USER’S MANUAL**

A Practical Approach for Modeling Matrix Diffusion Effects in REMChlor

ESTCP Project ER-201426

**ESTCP**
An Example of Applying Functional Objectives

- Mitigating off-site contaminant migration in fractured rock

Conceptual Site Model:

- **Critical process:** Chemical advection by most transmissive fractures

- **Bounding process outcomes:**
  - Source zone and attenuation processes along representative groundwater flow paths
  - Account for uncertainty in groundwater flow paths
An Example of Applying Functional Objectives

- Reduce/eliminate source zone contaminant mass

Evaluating efficacy of source zone remediation in fractured rock

what we hope to see... vs. the reality at many sites...

- Microbial Dechlorination of TCE
- in situ biostimulation and bioaugmentation

results of microcosm experiment
Bloom et al., ES&T, 2000

Shapiro et al., Groundwater, 2018

Decisions... how long and how much?... next steps?...
.additional treatments or continued hydraulic containment?
Challenges in Evaluating Source Zone Remediation in Fractured Rock

- Majority of contamination likely to reside in rock matrix in sedimentary rocks

TCE contamination in mudstone

After 20 years of continuous pumping, TCE remains orders of magnitude above MCL... “back diffusion” from rock matrix...

- Monitoring conducted by sampling water extracted from permeable fractures

- Monitoring sparsely distributed boreholes may not provide an accurate distribution of contaminant mass

- Residual remediation amendments in boreholes may bias interpretation of the robustness of the remediation

“challenges”... may limit our capacity to characterize processes at a given scale...
Conceptualization of Subsurface Contaminant Storage and Transport: Organic contaminants

(modified from Sale et al., 2008; Sale and Newell, 2011; ITRC 2011)
TCE Contamination in a Fractured Mudstone

Former Naval Air Warfare Center, West Trenton, NJ

- Aircraft engine test facility operating between 1950’s-1990’s
- Dipping mudstone units characterized by different depositional conditions
- Groundwater flow dominated by bedding plane partings along rheologically weak, carbon-rich, mudstone units
- Pump-and-treat
Pilot Study: Biostimulation and Bioaugmentation

Accelerate reductive dechlorination

Inject electron donor (emulsified soybean oil) & microbial consortium known to degrade TCE

TCE ➔ \textit{cis}-DCE ➔ VC ➔ Ethene

Amendment distribution

Continuous pumping
Characterizing the Groundwater Flow Regime

Groundwater flux through cross-bed fractures:
- 4% From Lower-K zone
- 96% From along strike

- amendment concentrations diluted at up-dip monitoring wells
- long residence time in treatment zone (low-permeability)
Biostimulation & Bioaugmentation: Results
Amendments injected into lower permeability strata have long residence time.

\[ Q_A + Q_B + Q_S - Q_{15BR} - Q_{45BR} = 0 \]

Flux from overlying unit

Flux to 45BR

Flux from along strike of bedding

Flux from underlying unit

Flux to 15BR
Monitoring and Evaluating the Bioremediation

Sources of CE in \( V \) . . . Diffusion out of rock matrix, desorption, dissolution of NAPL TCE

\[
V \frac{dC_{CE}}{dt} = -(Q_{15BR} + Q_{45BR})C_{CE} + Q_A C_A + Q_B C_B + Q_S C_S + V F_{CE}
\]

\( C_{CE} \) – molar sum of chloroethene and ethene, concentrations representative of \( V \)

\( C_A, C_B, C_S \) – molar sum of chloroethene and ethene concentrations of fluxes into \( V \)

Flux from overlying unit

Flux to 45BR

Flux from along strike of bedding

Flux from underlying unit

Flux to 15BR
**Chloroethene Mobilization Rate**

\[
V \frac{dC_{CE}}{dt} = -(Q_{15BR} + Q_{45BR})C_{CE} + Q_AC_A + Q_BC_B + Q_SC_S + VF_{CE}
\]

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<tr>
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<th>CE Mobilization Rate ( V_F F_{CE} ) (kg TCE/yr)</th>
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<tbody>
<tr>
<td>Before start of</td>
<td>4.2 - 7.3</td>
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<tr>
<td>remediation</td>
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CE mobilized from rock matrix, desorption, dissolution of NAPL TCE

Biostimulation and bioaugmentation increase CE mobilization rate out of treatment zone by 5X – 10X

Shapiro et al., *Groundwater*, 2018
[https://doi.org/10.1111/gwat.12586](https://doi.org/10.1111/gwat.12586)

Tiedeman et al., *Groundwater*, 2018
[https://doi.org/10.1111/gwat.12585](https://doi.org/10.1111/gwat.12585)
Significance of the Chloroethene Mobilization Rate

Estimate of CE in Rock Matrix (BlkFis-233) from CE analyses of Rock Core

~1000 kg TCE

Significance of the Chloroethene Mobilization Rate

Rock core collected from 70BR and analyzed for CE

Goode et al., Journal of Contaminant Hydrology, 2014
https://doi.org/10.1016/j.jconhyd.2014.10.005

CE Mobilization Rate

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Minimum of 30+ yrs and repeated treatments for source zone removal

~1000 kg TCE
An Example of Applying Functional Objectives

- Reduce/eliminate source zone contaminant mass

Evaluating efficacy of source zone remediation in fractured rock

Conceptual Site Model:

- **Critical process:**
  Chemical fluxes into and out of treatment zone

Chloroethene mobilization from rock matrix

Chloroethene mass in rock matrix
Recognizing Critical Processes and Scales in Conceptual Site Models for Decision Support at Sites of Groundwater Contamination

Summarizing...

Beneficial to have understanding of all processes and scales that affect contaminant fate and transport...

To address specific functional objectives...all processes and scales do not need to translate into a forecasting/predictive model...

Recognize critical processes and fluxes – constrains data collection efforts, couple less complex models to bound process outcomes...

Recognize critical processes and fluxes – address spatial and temporal scales consistent with limitations of complexity and data availability...