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

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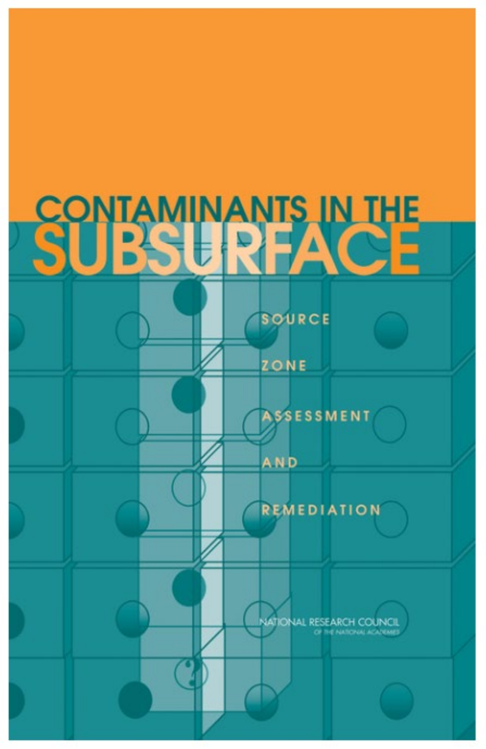
Acknowledgements:

U.S. Geological Survey Toxic Substances Hydrology Program

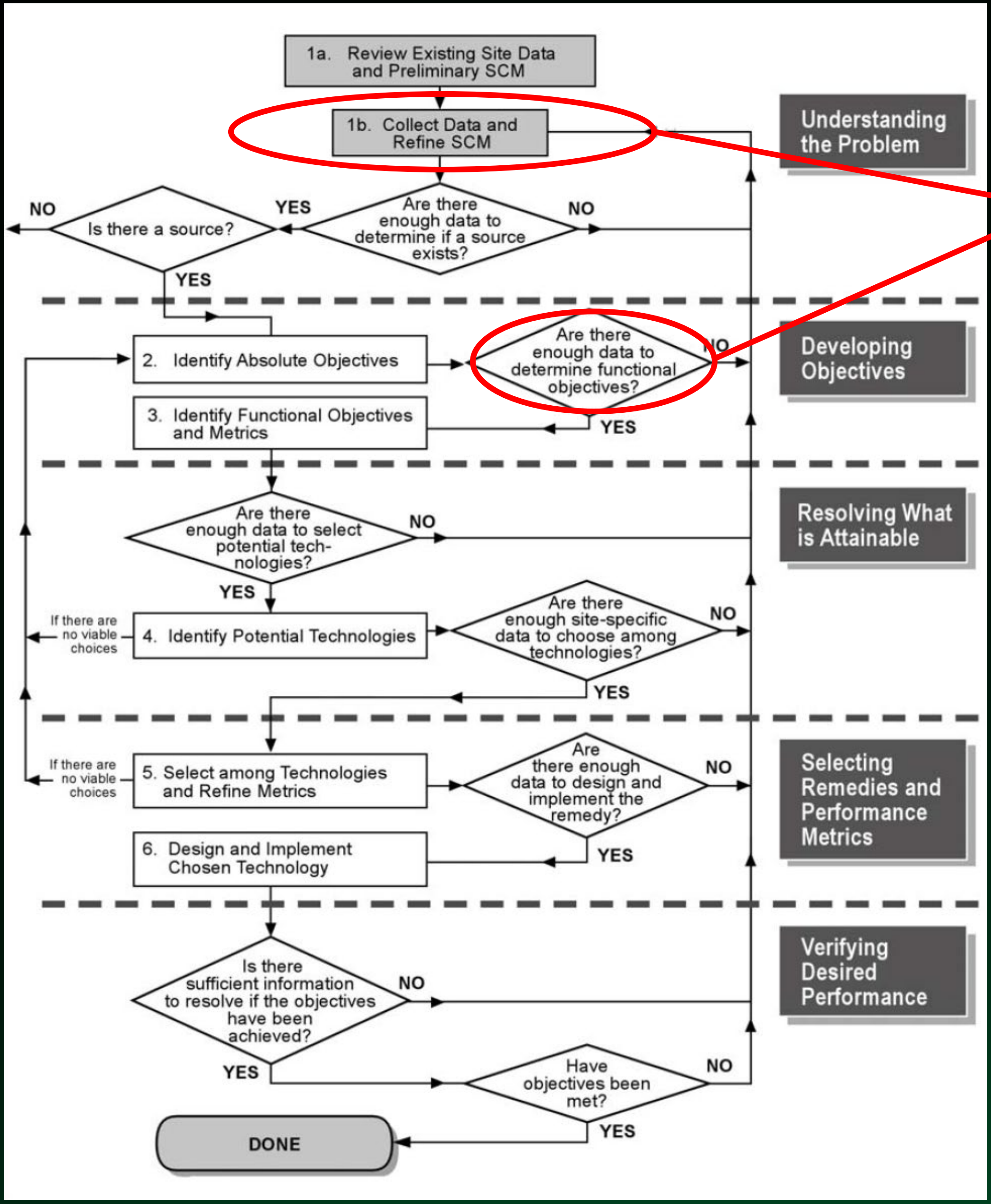
Management Decisions at Sites of Groundwater Contamination



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.)

National Research Council, 2005, https://doi.org/10.17226/11146



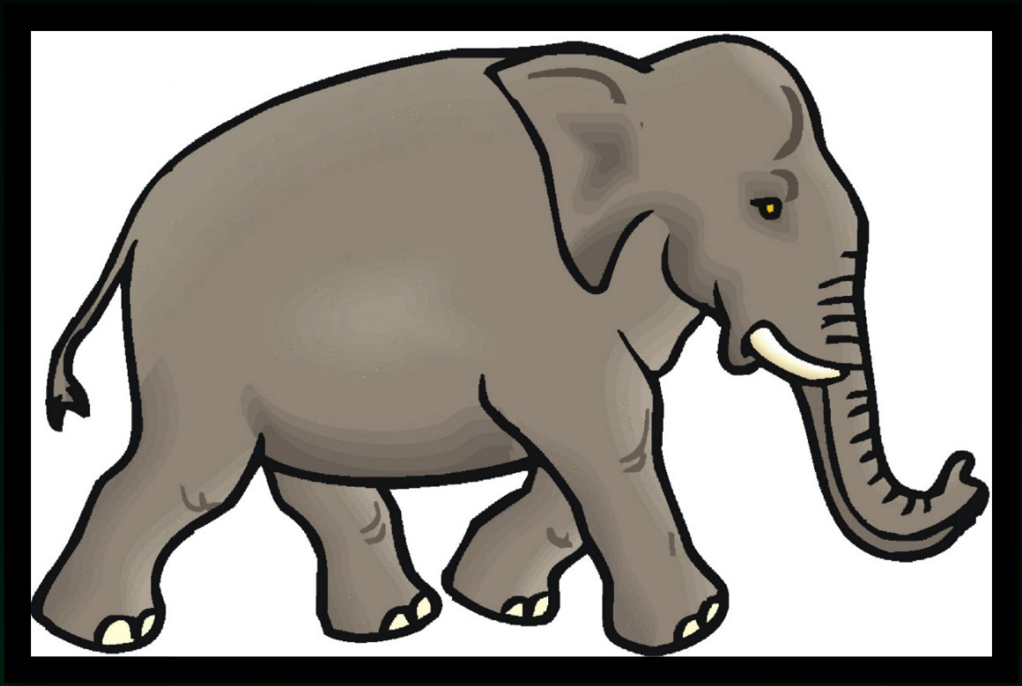
SCM = Site Conceptual Model

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

National Research Council, 2005

Functional objectives are like an elephant . . . they can appear to be large and cumbersome. . .

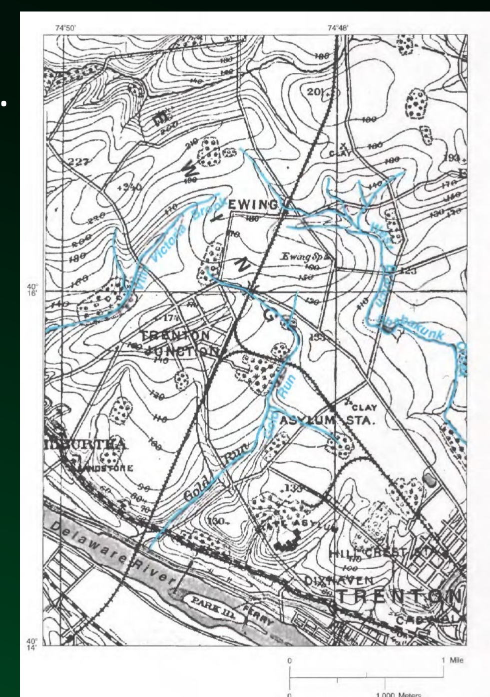


. . . require conceptualizing and synthesizing operational, physical, and biogeochemical processes over multiple spatial and temporal scales. . .

Functional objective: *Mitigating off-site migration*

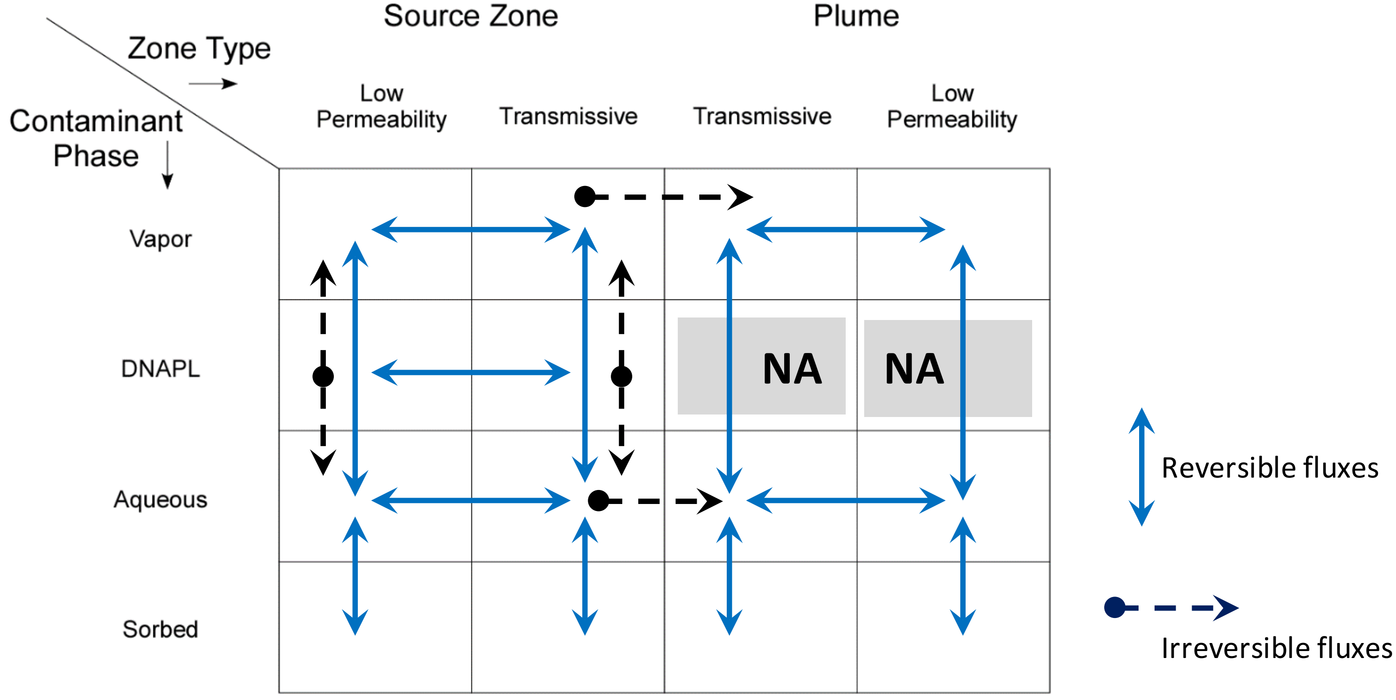
- Source zone characterization. . .source zone architecture and fluxes, chemical phases, solid-phase reactions, biogeochemical process, etc. . . .

- 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)

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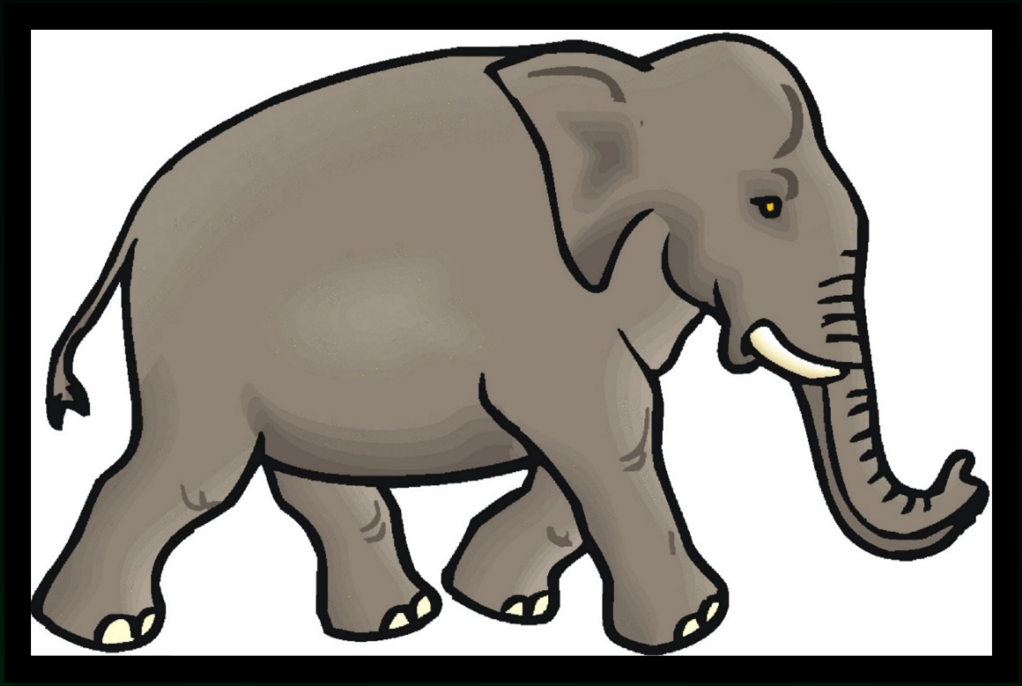
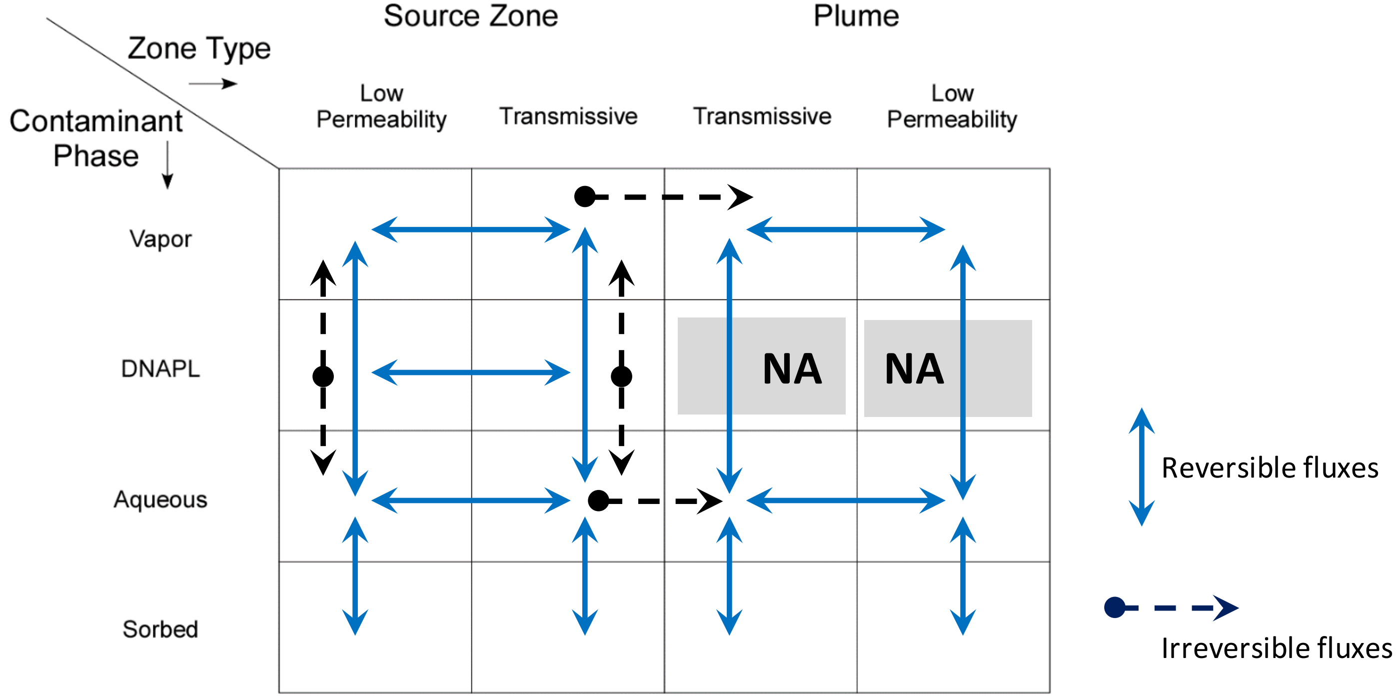


How do you eat an elephant ? . . . One bite at a time. . .

. . . 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

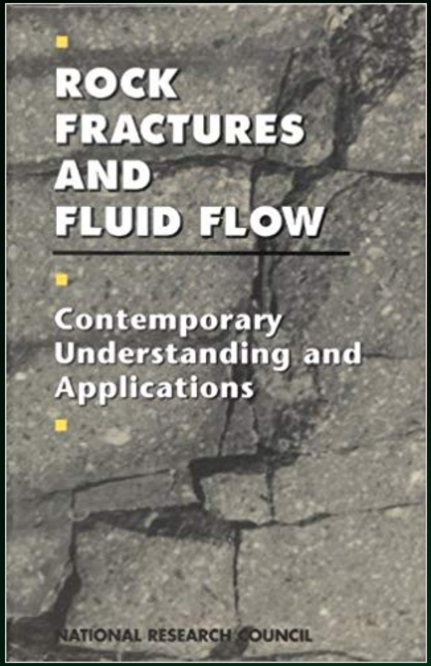


(modified from Sale et al., 2008; Sale and Newell, 2011; ITRC 2011)

An Example of Applying Functional Objectives

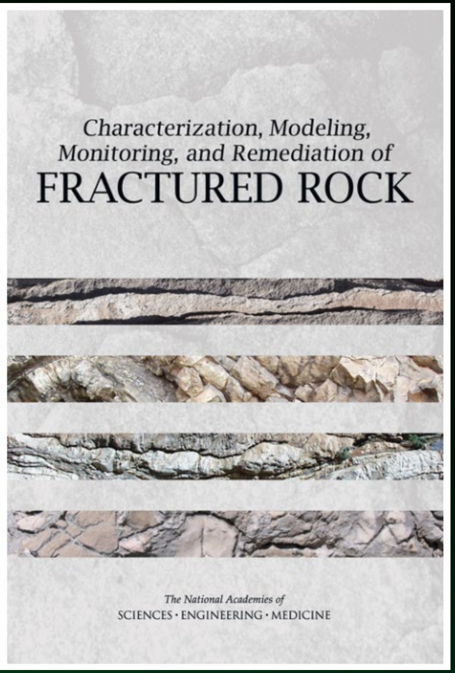
- ❑ Mitigating off-site contaminant migration in fractured rock

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



National Research Council. 1996. https://doi.org/10.17226/2309.

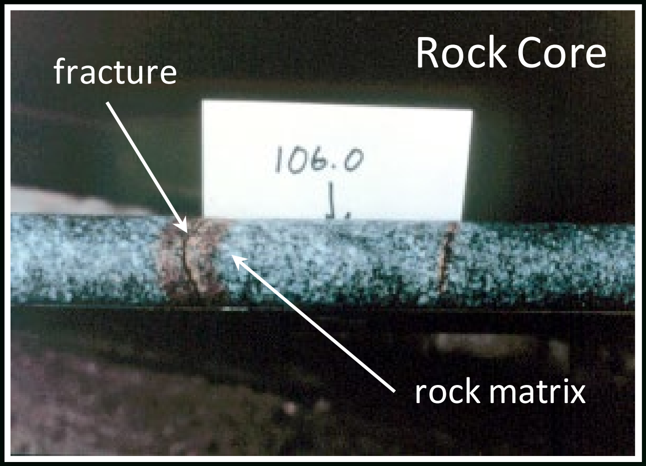
National Research Council. 2013. https://doi.org/10.17226/14668.



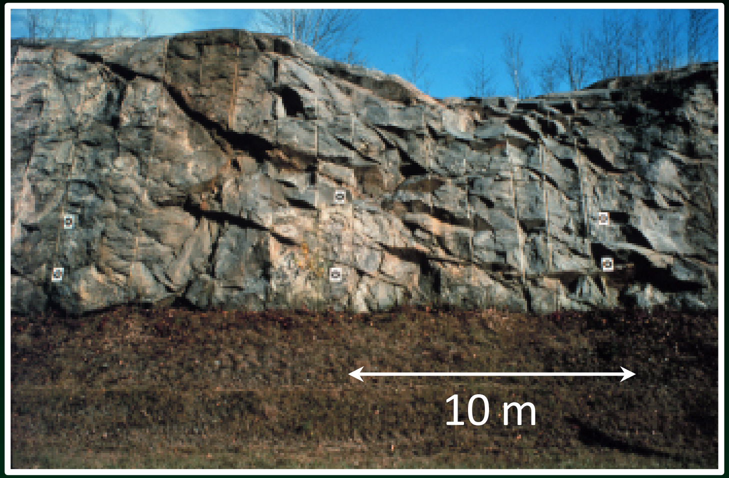
National Academies of Sciences, Engineering, and Medicine. 2015. https://doi.org/10.17226/21742.

An Example of Applying Functional Objectives

- ❑ Mitigating off-site contaminant migration in fractured rock



Hierarchy of void space

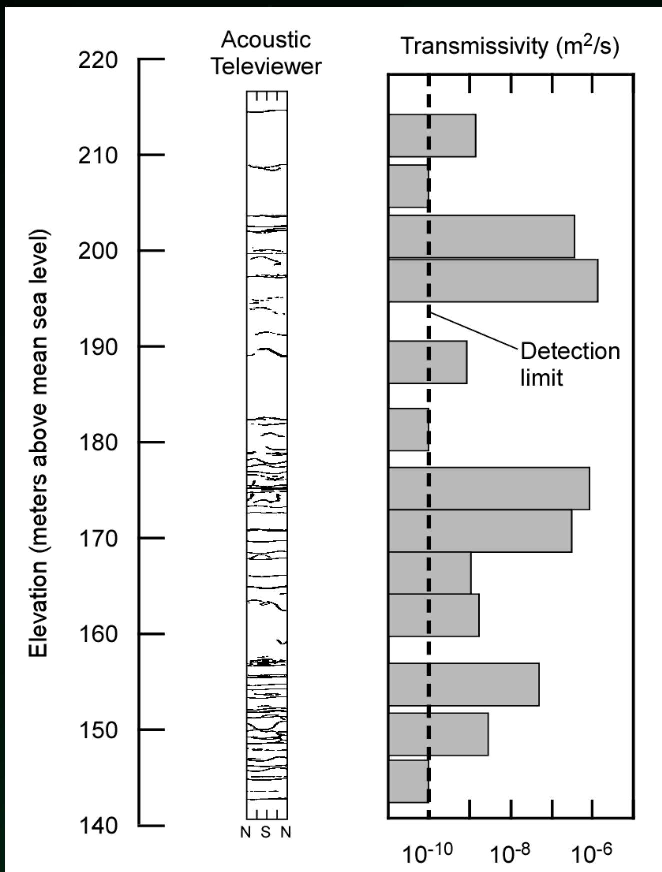


Fault Zone

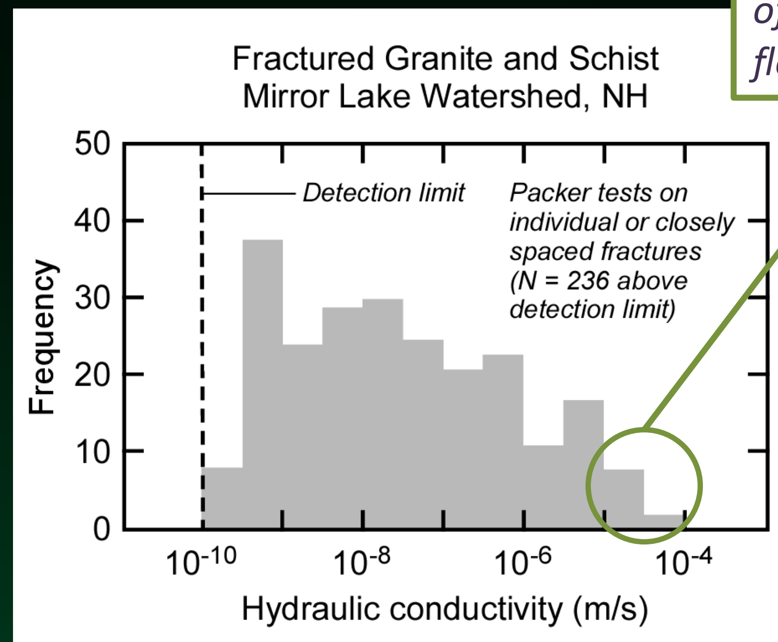
Fractures control groundwater flow. . .
. . but, there are a lot of fractures. . .
. . .over dimensions of centimeters to kilometers. . .

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

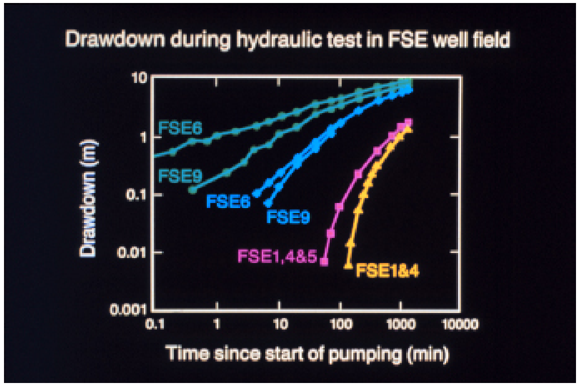
Critical Process and Scales:

- 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

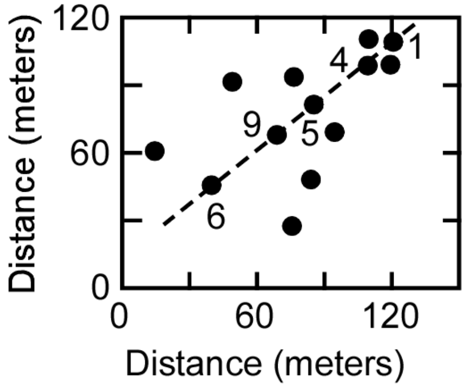
Advances over 25+ years

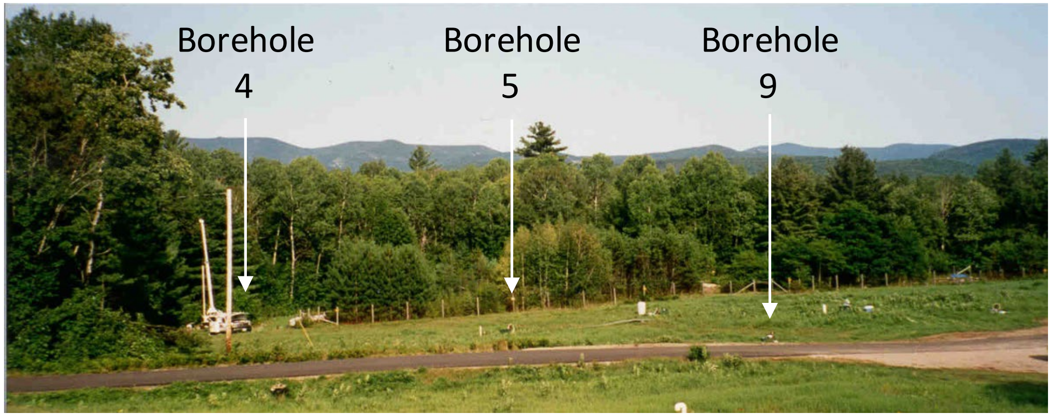
- Local and regional tectonic and lithologic controls on fracturing
- Surface and borehole geophysical methods
- Multilevel monitoring equipment
- Design and interpretation of hydraulic and tracer tests
- Modeling groundwater flow and parameter estimation methods



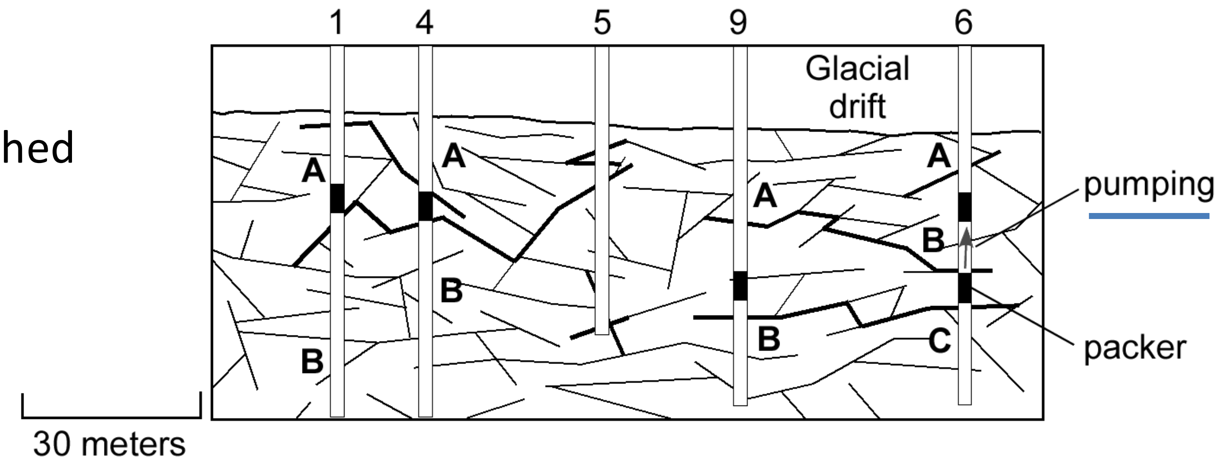
Identifying Transmissive Fractures and Their Connectivity

FSE Well Field
Plan View



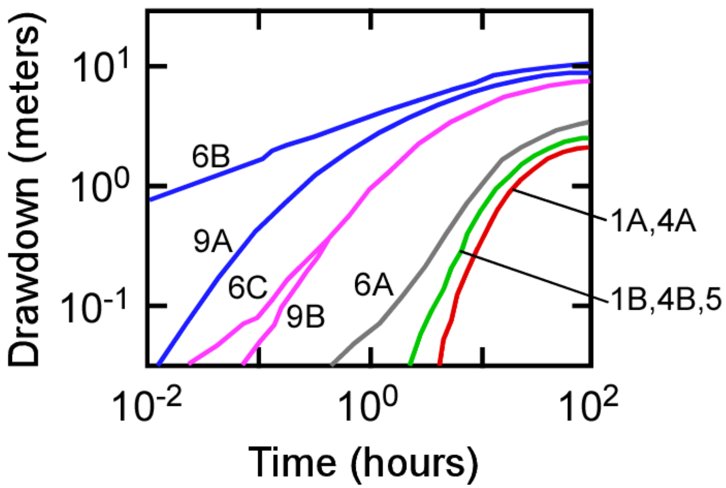


FSE Well Field Cross Section



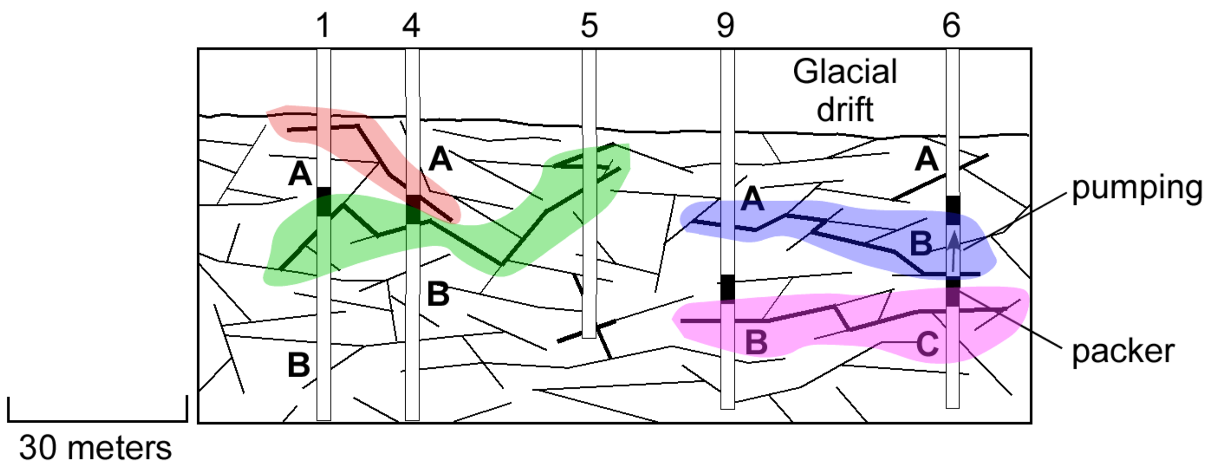
Granite and Schist,
Mirror Lake Watershed
New Hampshire

Identifying Transmissive Fractures and Their Connectivity



Clustering of drawdown records from different monitoring intervals during hydraulic tests provides evidence of transmissive fractures & fracture connectivity. . .

FSE Well Field Cross Section



An Example of Applying Functional Objectives

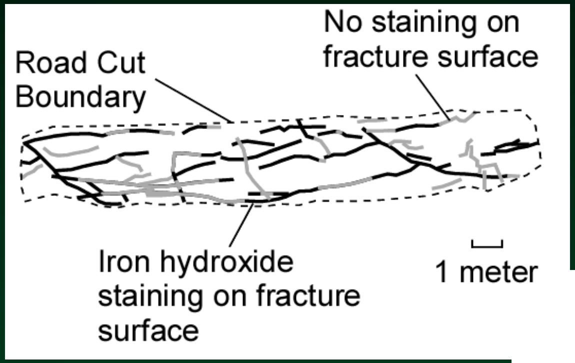
- Mitigating off-site contaminant migration in fractured rock
  - Identify the most transmissive fractures & their connectivity

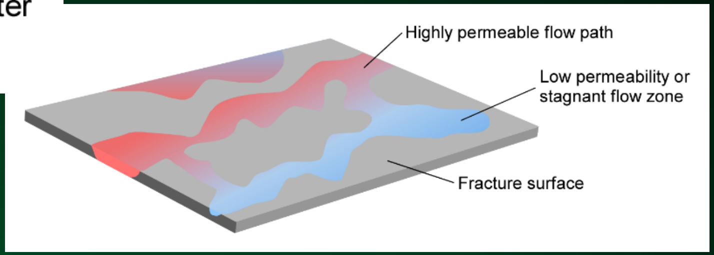
    . . .identify pathways of contaminated groundwater , but extent of contamination requires further analyses. . .

  - Accounting for source zone inputs and attenuation processes

    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. . .

Road Cut

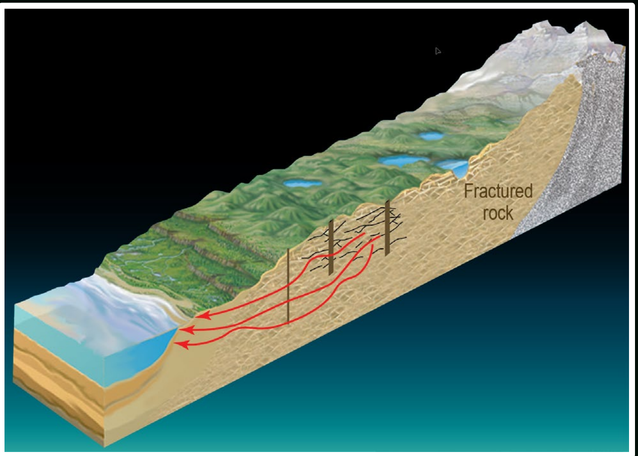


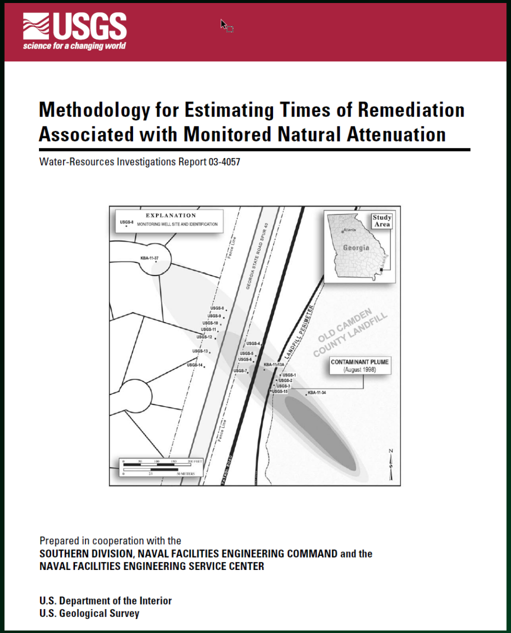


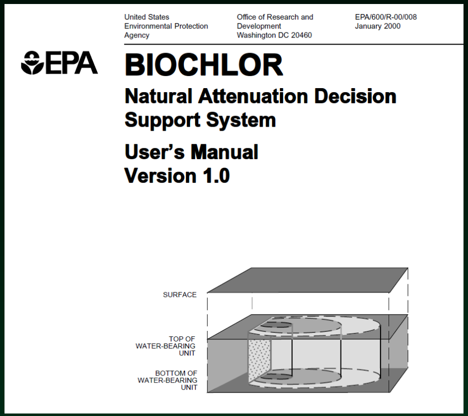
An Example of Applying Functional Objectives

- Mitigating off-site contaminant migration in fractured rock
  - Accounting for source zone inputs and attenuation processes

. . .alternatively -> conceptualize biogeochemical processes along <u>representative flow paths</u> and identify conditions that bound process responses. . .

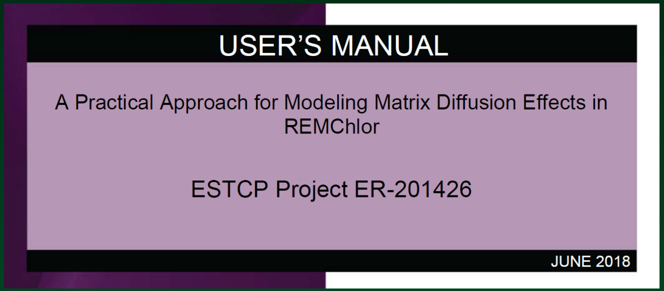


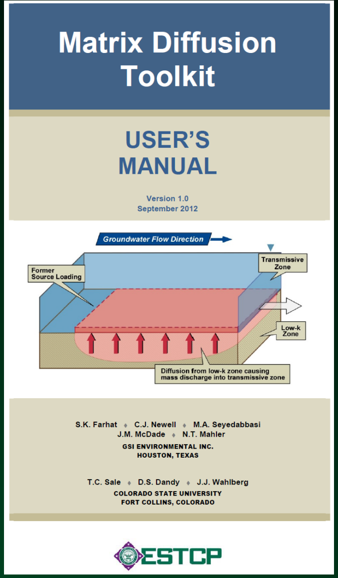




Natural Attenuation Software

REMChlor

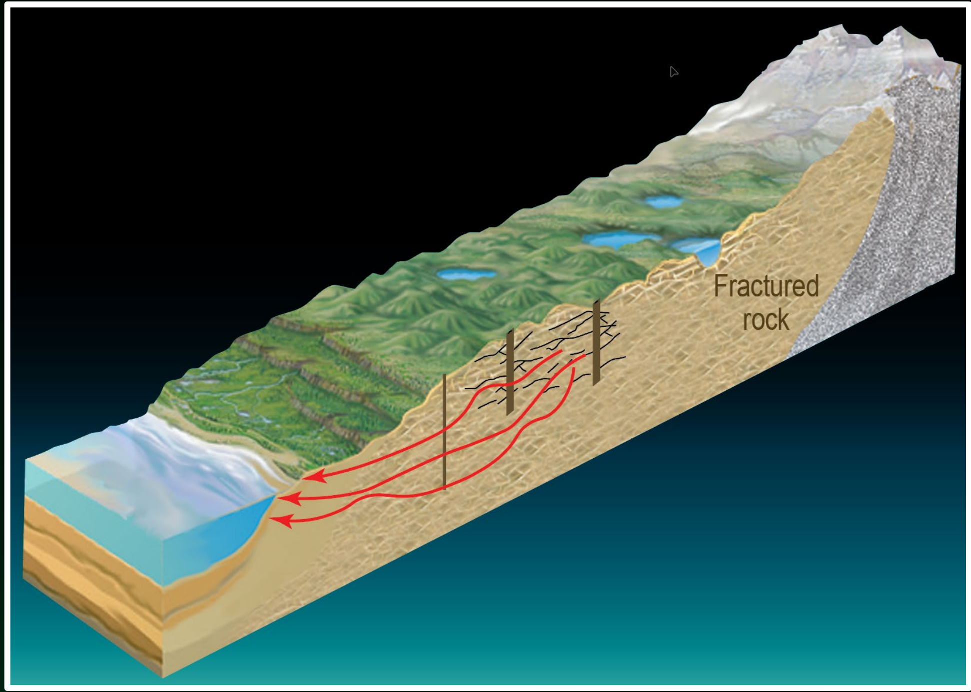




An Example of Applying Functional Objectives

❑ Mitigating off-site contaminant migration in fractured rock

Conceptual Site Model:



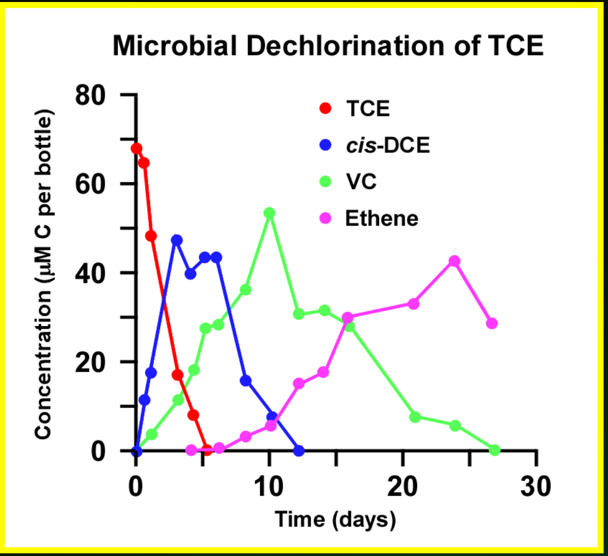
- <u>Critical process:</u> Chemical advection by most transmissive fractures
- <u>Bounding process outcomes:</u>
  - Source zone and attenuation processes along representative groundwater flow paths
  - Account for uncertainty in groundwater flow paths

An Example of Applying Functional Objectives

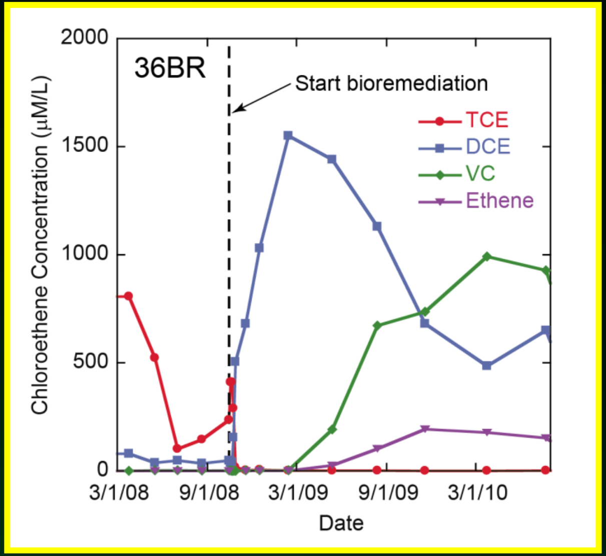
- ❑ Reduce/eliminate source zone contaminant mass

Evaluating efficacy of source zone remediation in fractured rock

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



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



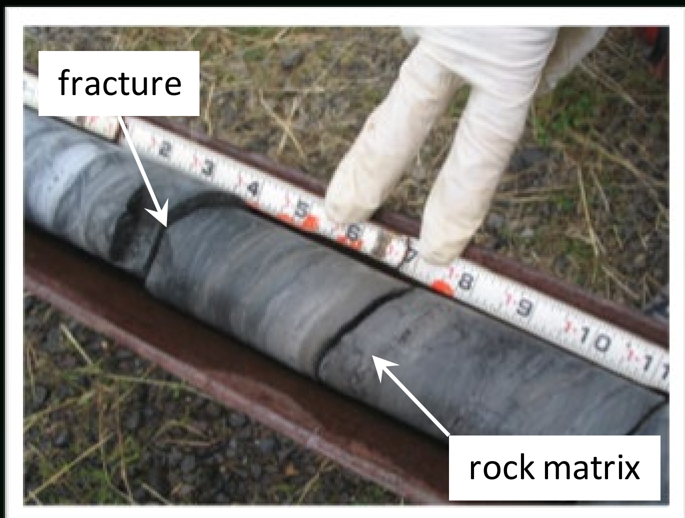
in situ biostimulation and bioaugmentation
Shapiro et al., Groundwater, 2018

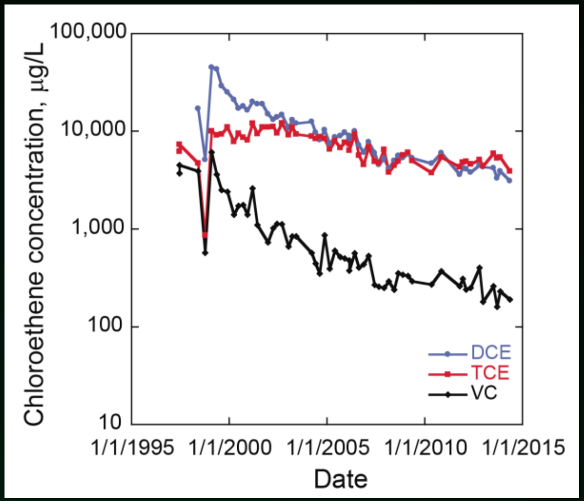
Decisions. . . how long and how much ?. . .next steps ?. . .additional treatments or continued hydraulic containment ?

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

"challenges". . . may limit our capacity to characterize processes at a given scale. . .

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

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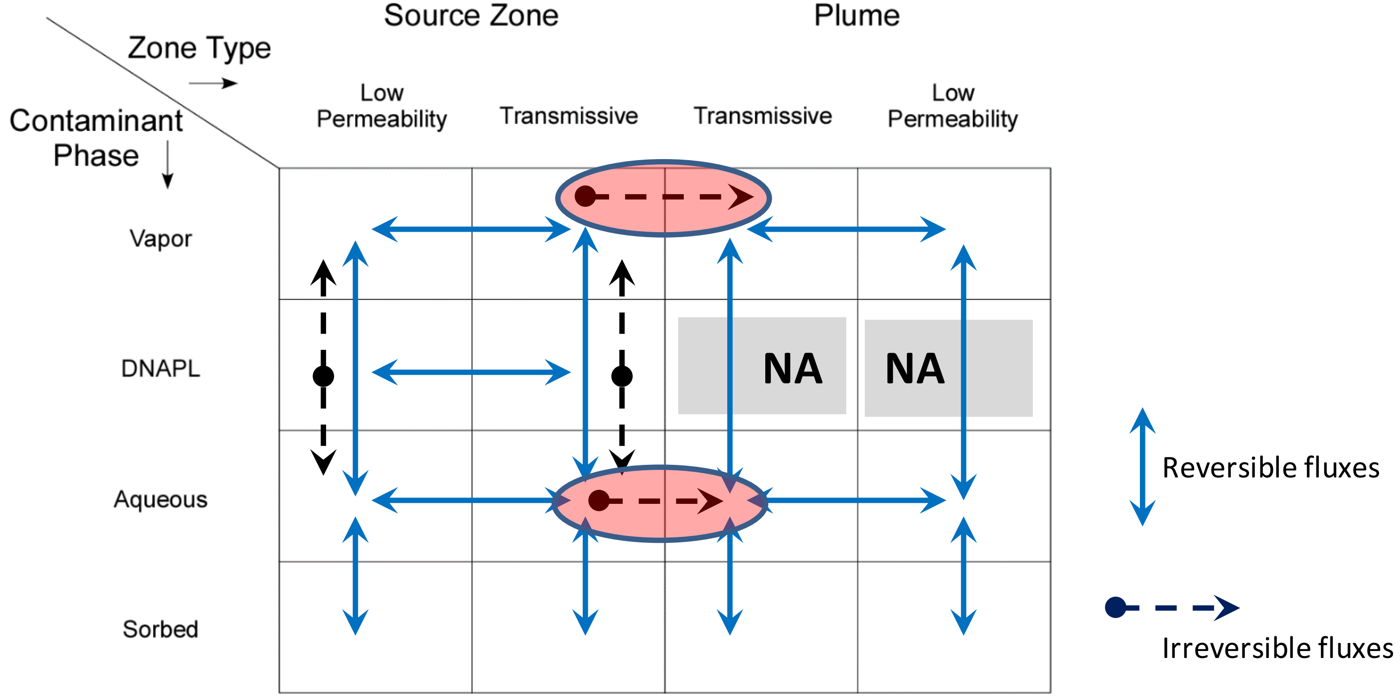
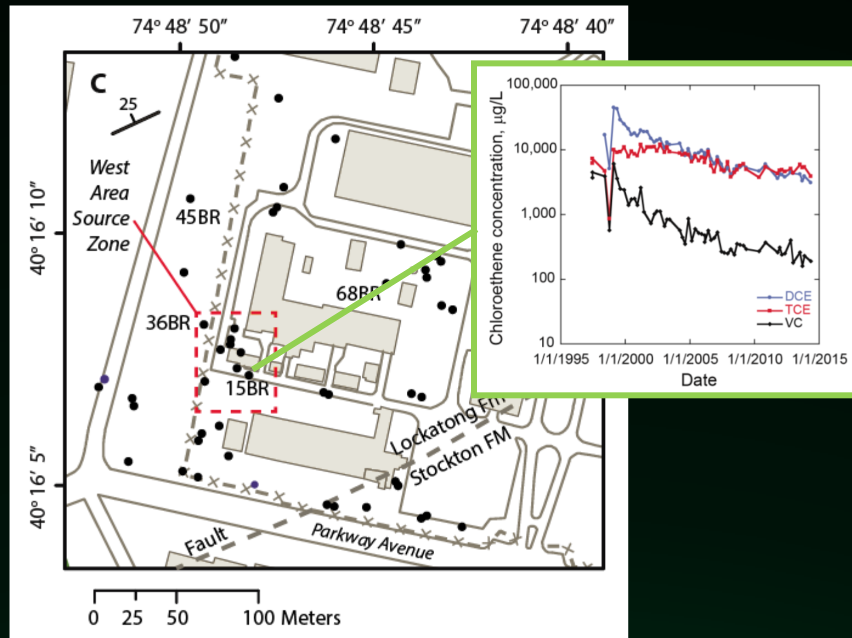


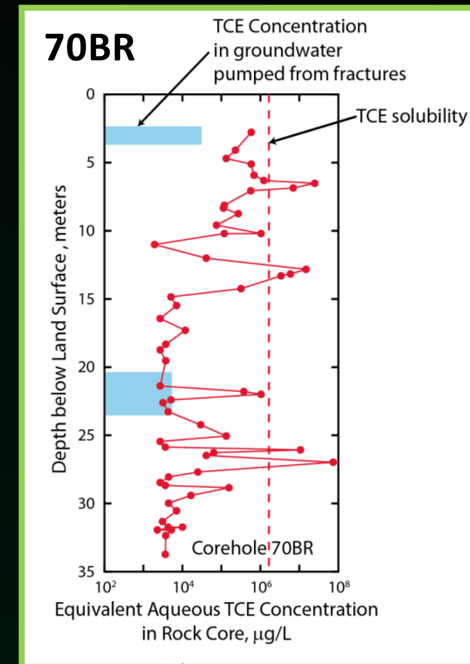
(modified from Sale et al., 2008; Sale and Newell, 2011; ITRC 2011)

TCE Contamination in a Fractured Mudstone

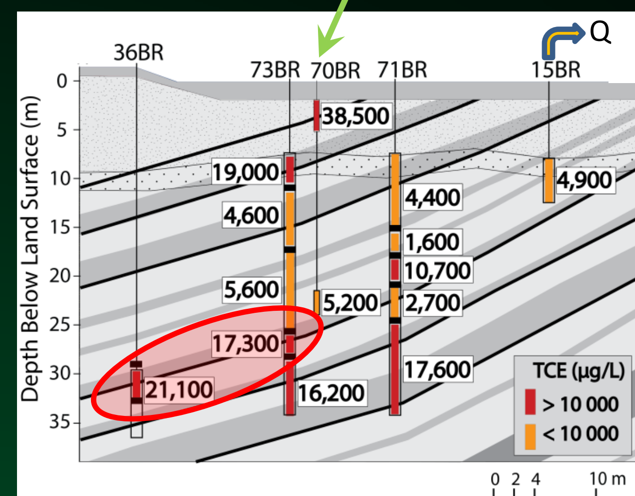
Former Naval Air Warfare Center, West Trenton, NJ



TCE in rock matrix



- 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



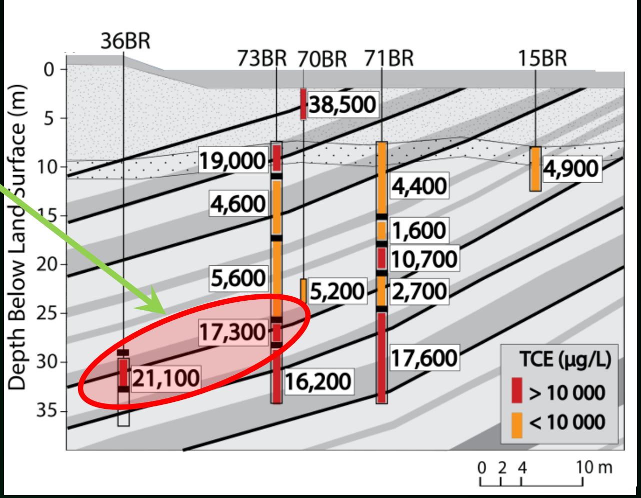
TCE in fractures

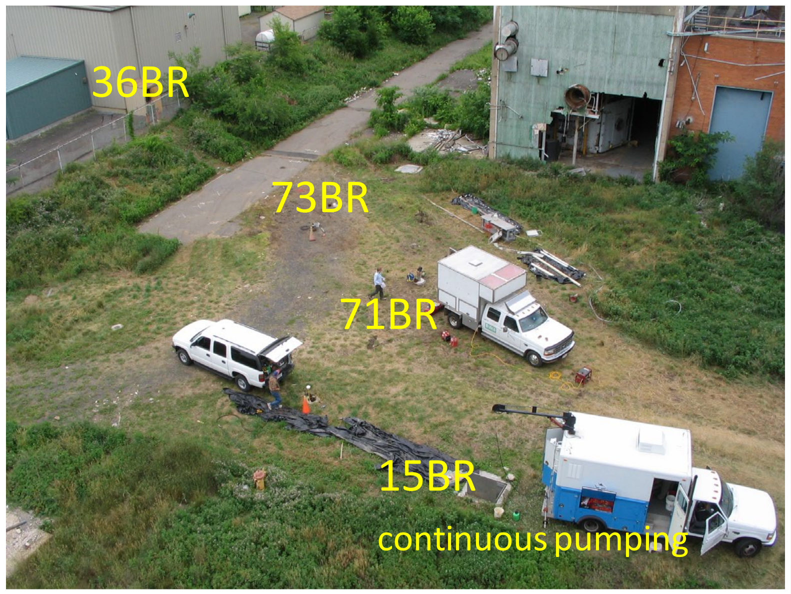
Pilot Study: Biostimulation and Bioaugmentation

Accelerate reductive dechlorination

TCE ⟶ *cis*-DCE ⟶ VC ⟶ Ethene

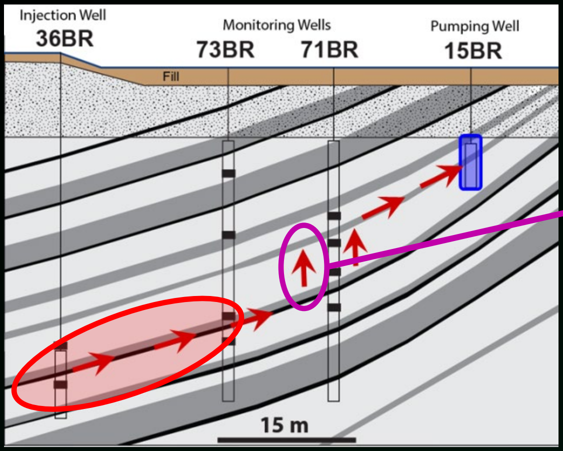
Amendment distribution





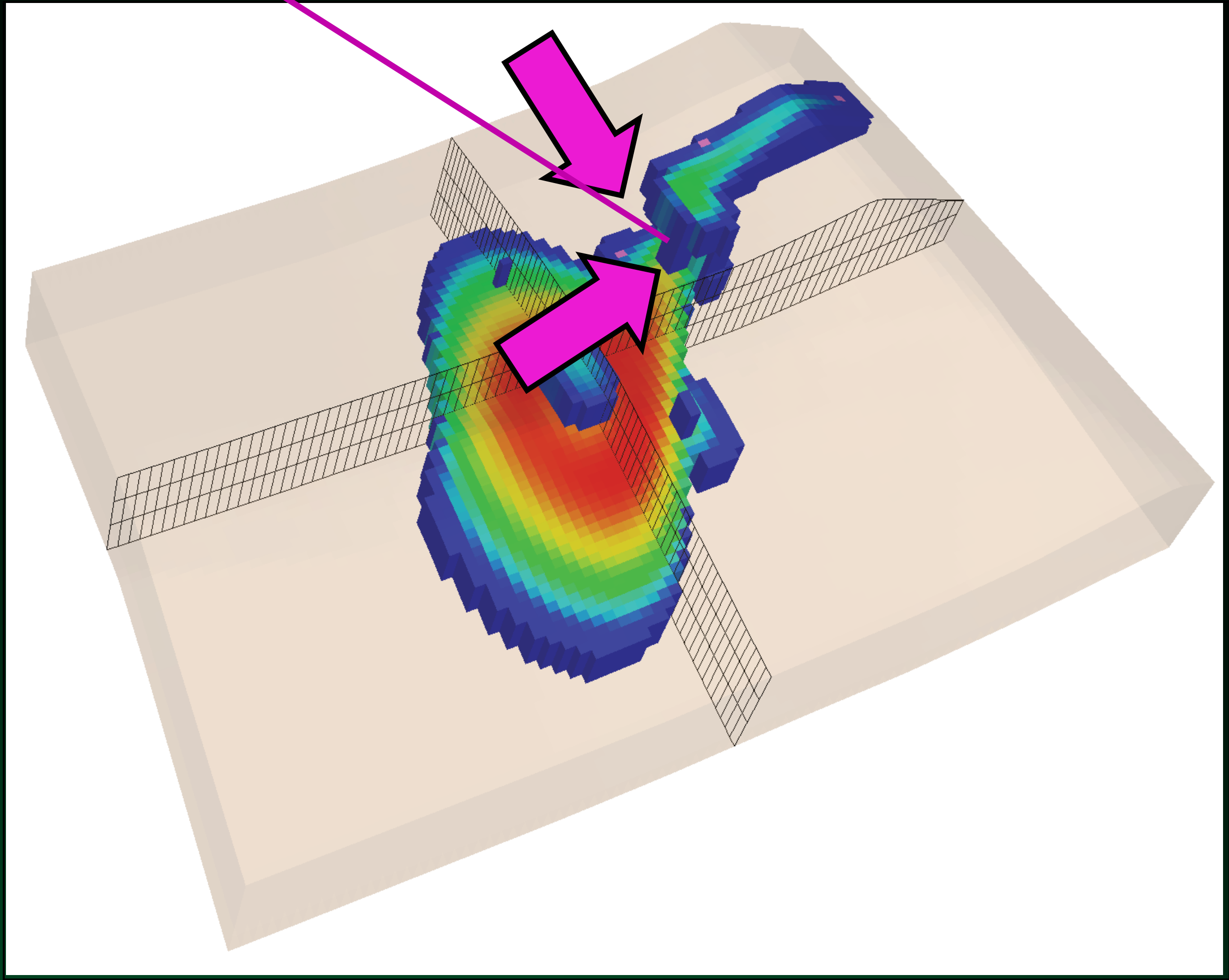
Inject electron donor (emulsified soybean oil) & microbial consortium known to degrade TCE

Characterizing the Groundwater Flow Regime



Characterizing groundwater fluxes to identify chemical fluxes

Cross-bed fractures



Groundwater flux through cross-bed fractures:

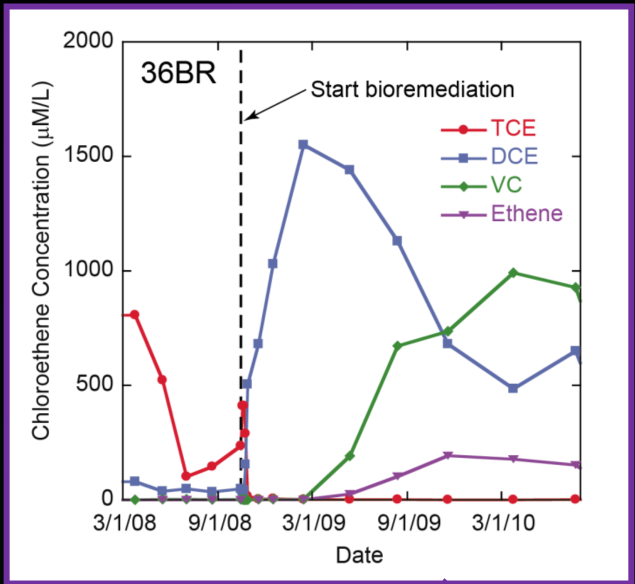
4% From Lower-K zone

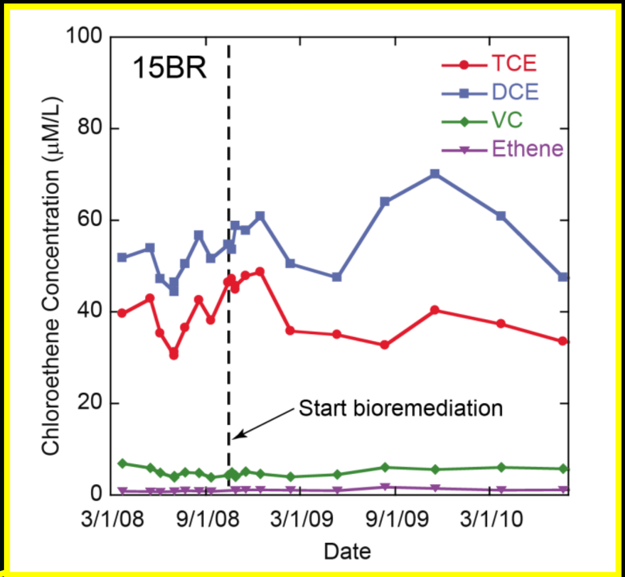
96% From along strike

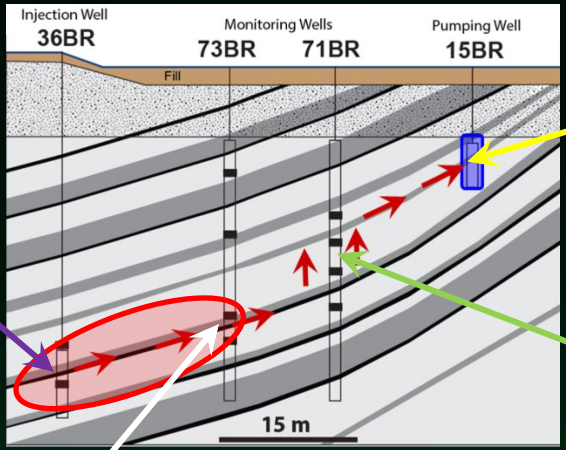
→ amendment concentrations diluted at up-dip monitoring wells

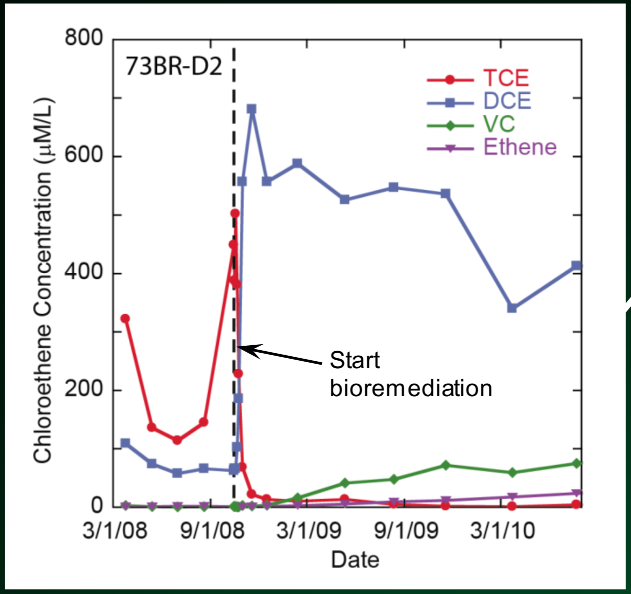
→ long residence time in treatment zone (low-permeability)

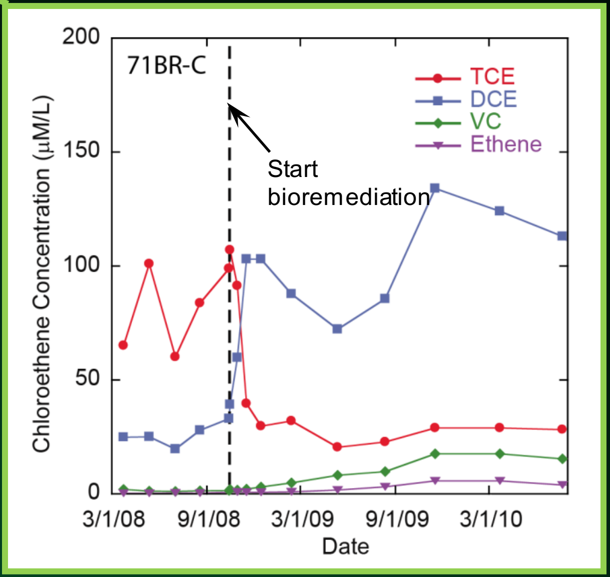
Biostimulation & Bioaugmentation: Results



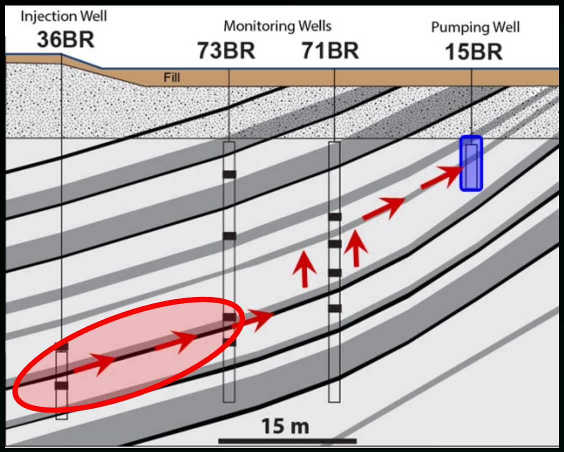






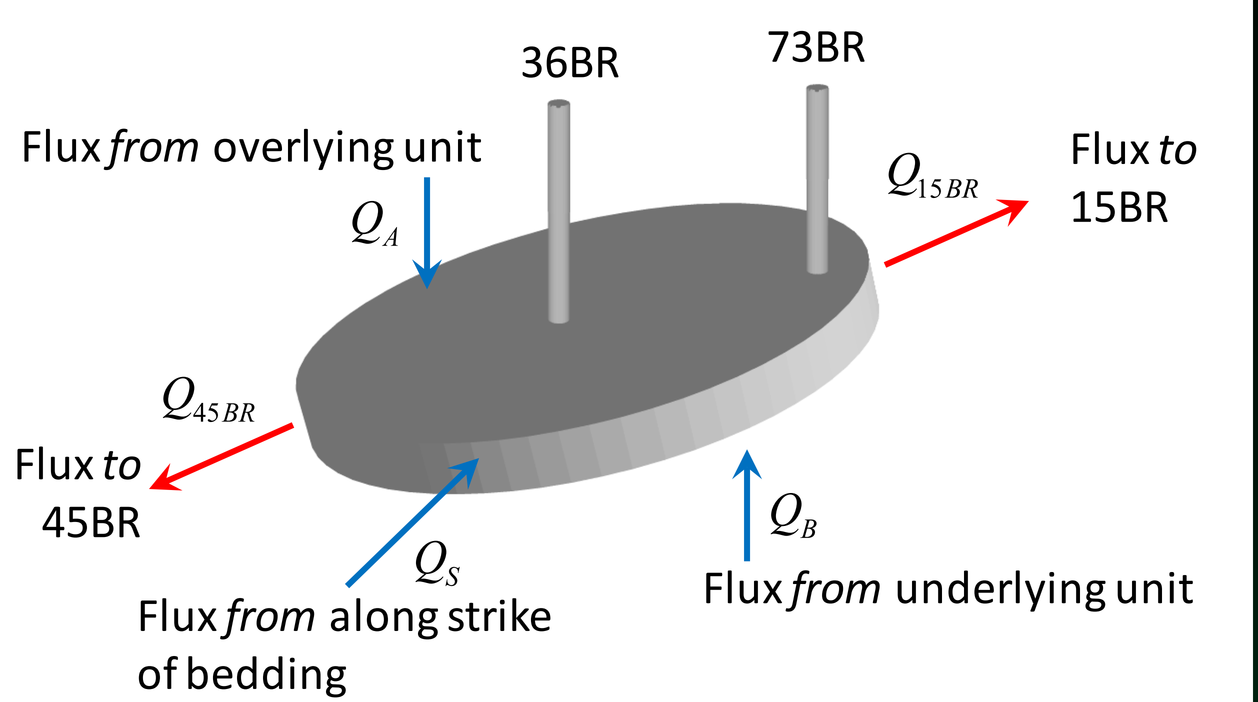


Monitoring and Evaluating the Bioremediation

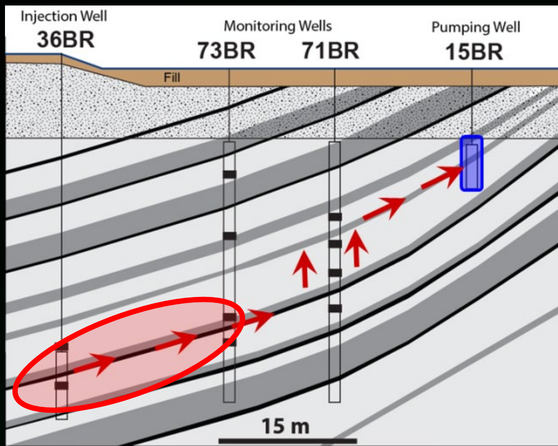


Amendments injected into lower permeability strata have long residence time

$$Q_A + Q_B + Q_S - Q_{15BR} - Q_{45BR} = 0$$



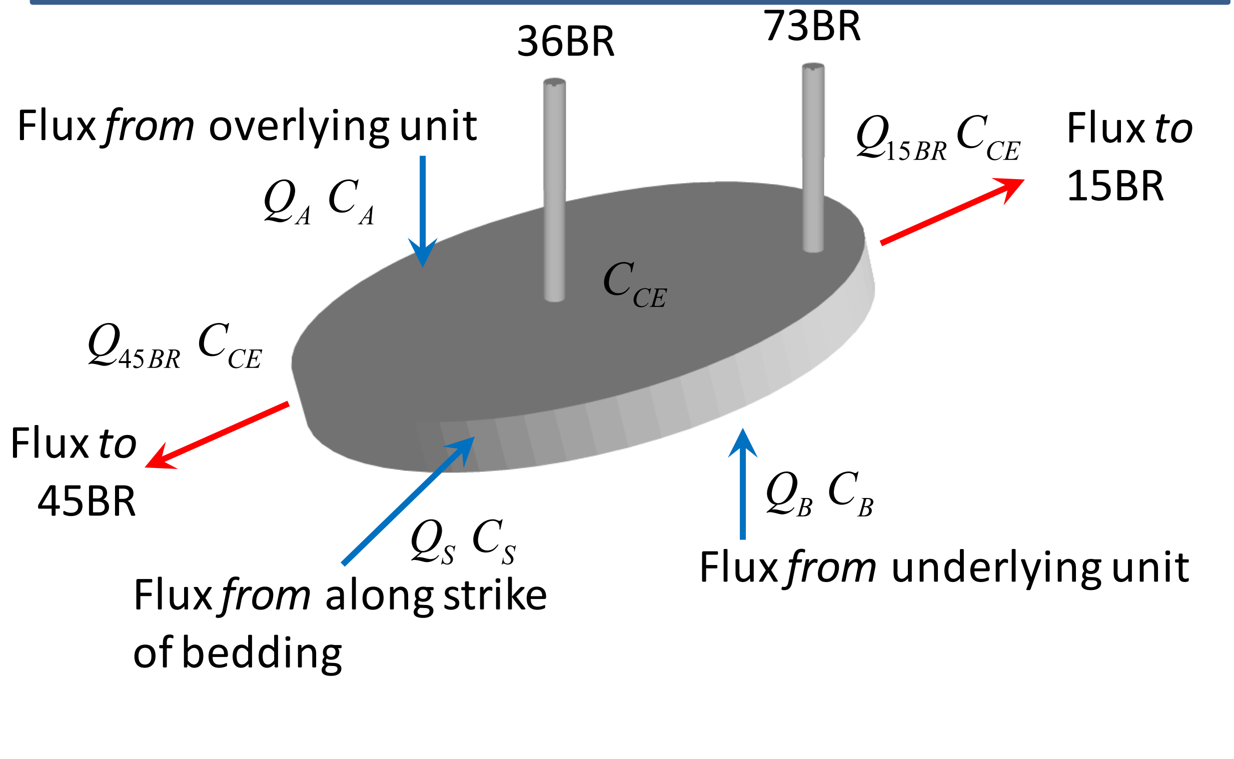
Monitoring and Evaluating the Bioremediation



CE = Chloroethenes

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

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



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

Chloroethene Mobilization Rate

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

CE mobilized from rock matrix, desorption, dissolution of NAPL TCE

	CE Mobilization Rate $V_F F_{CE}$ (kg TCE/yr)
Before start of remediation	4.2 - 7.3
After start of remediation	34.0 - 44.6

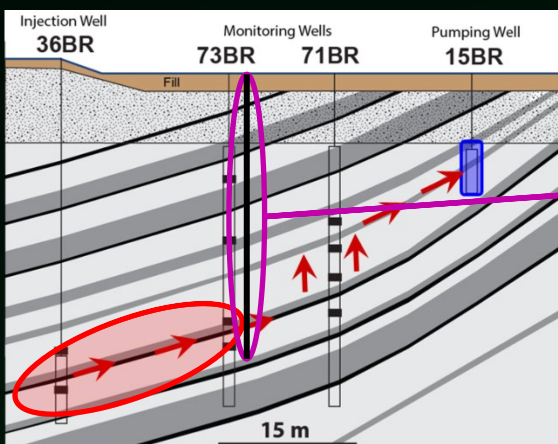
Biostimulation and bioaugmentation increase CE mobilization rate out of treatment zone by 5X – 10X

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

Tiedeman *et al.*, *Groundwater*, 2018
*https://doi.org/*10.1111/gwat.12585

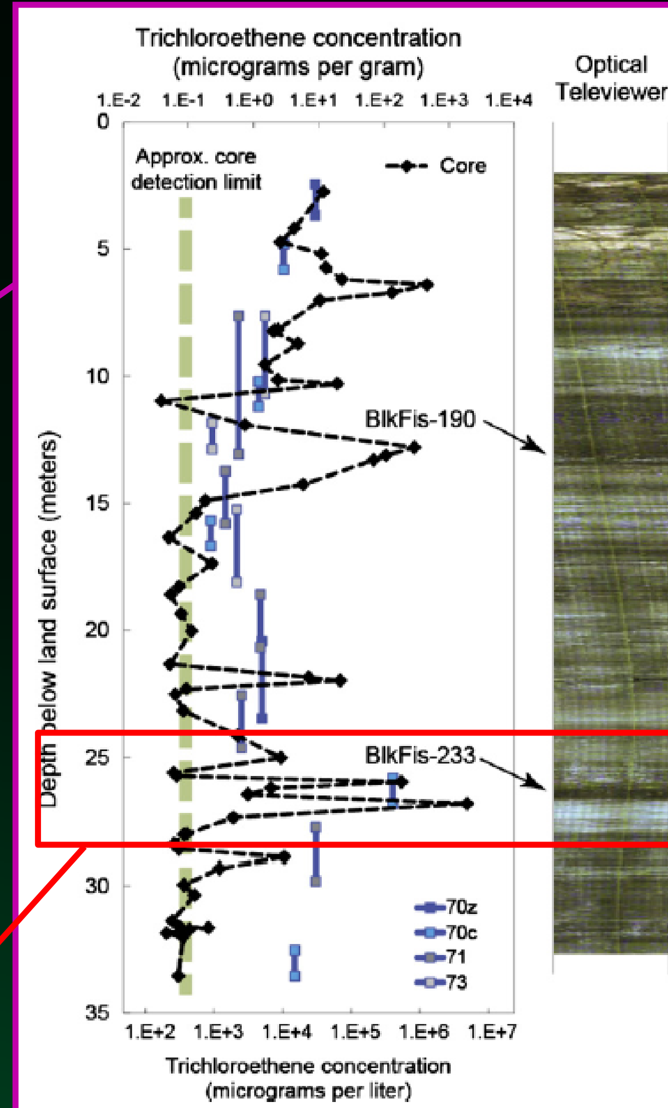
Significance of the Chloroethene Mobilization Rate

	CE Mobilization Rate $V_F F_{CE}$ (kg TCE/yr)
Before start of remediation	4.2 - 7.3
After start of remediation	34.0 - 44.6



Rock core collected from 70BR and analyzed for CE

70BR



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

~1000 kg TCE

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

An Example of Applying Functional Objectives

- ❑ Reduce/eliminate source zone contaminant mass

Evaluating efficacy of source zone remediation in fractured rock

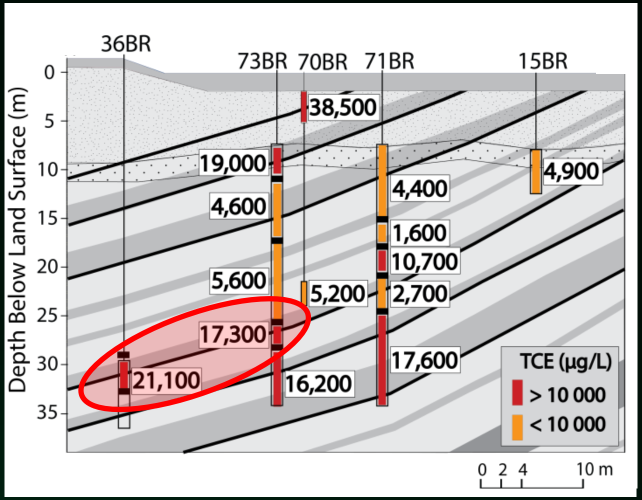
Conceptual Site Model:

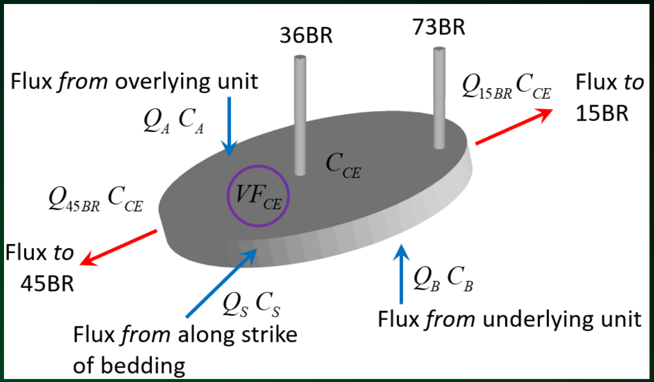
- <u>Critical process:</u>

  Chemical fluxes into and out of treatment zone

  Chloroethene mobilization from rock matrix

  Chloroethene mass in rock matrix



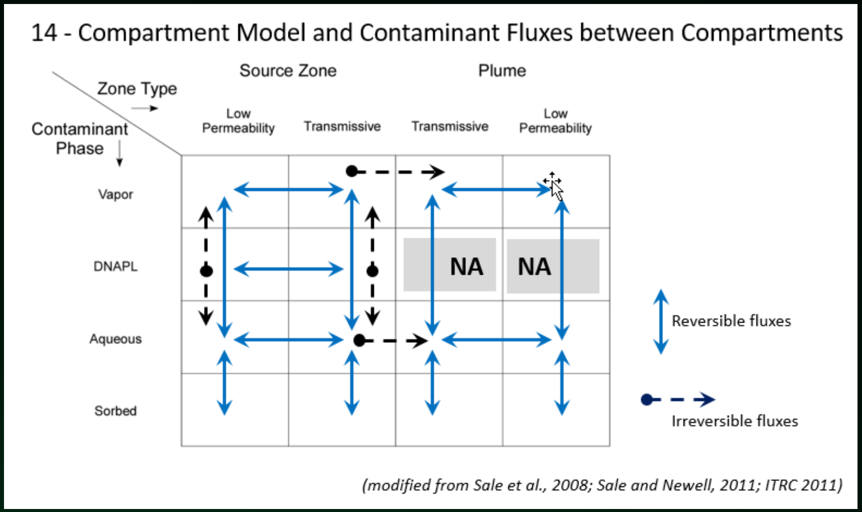


Recognizing Critical Processes and Scales in Conceptual Site Models for Decision Support at Sites of Groundwater Contamination

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. . .