The Challenges with Amendment Delivery in Fractured Porous Rocks: Using DFM Simulations to Forecast Remediation Efficacy

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Battelle Chlorinated Conference
Technical Impracticability: Challenges and Considerations for Evaluation of Fractured Rock Sites
Session A3, Abstract #541
Denver, Colorado, June 4, 2024

MORWICK G360 Groundwater Research Institute
University of Guelph

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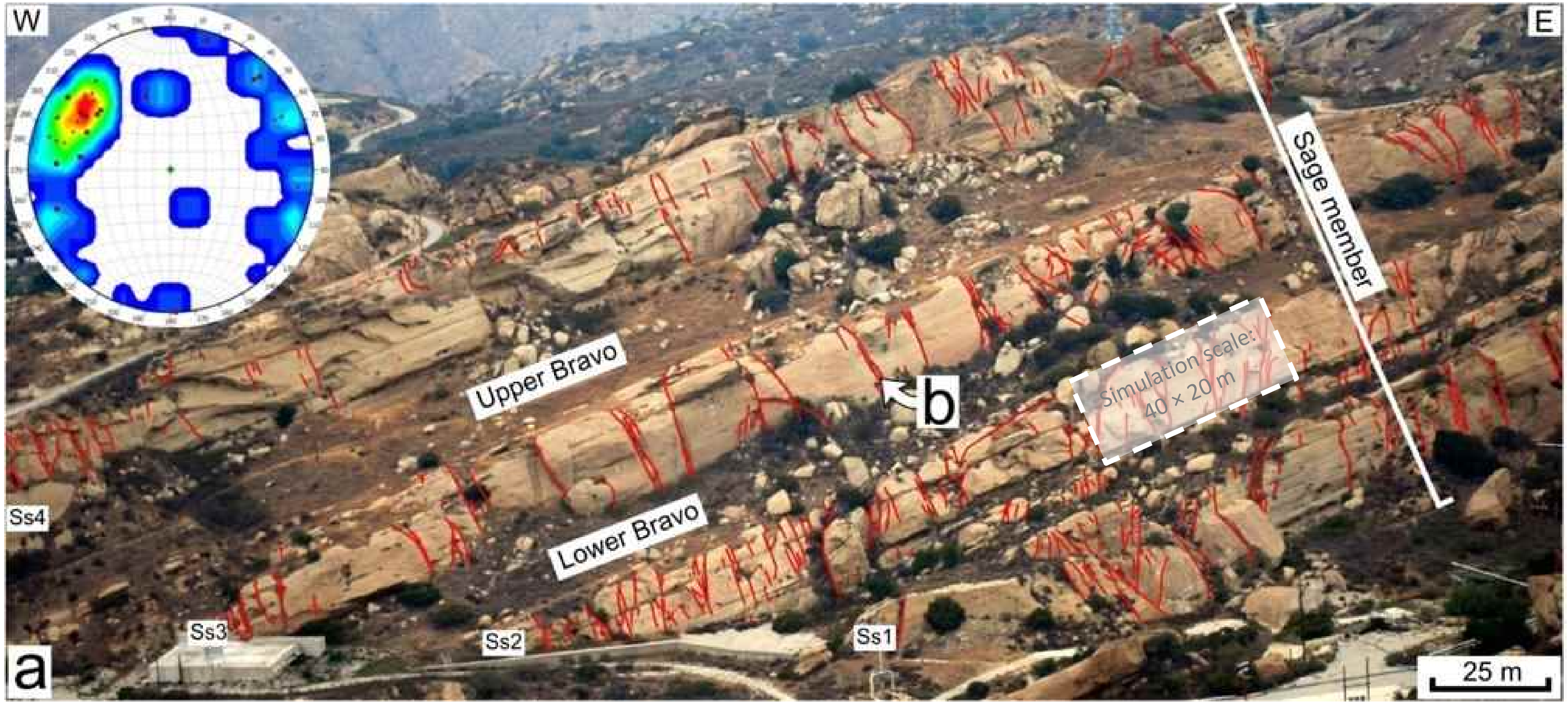
Acknowledgements & Agenda

Funding was provided by
The Boeing Company and
Canadian National Science and Engineering Research Council
grant IRCPJ 363783-18 held by Dr. B. Parker

1. Problem statement
   - *TCE Mass is stored in the rock matrix*
   - *"2-step" amendment delivery*
2. Methods
   - *Composing Simulations*
   - *TCE Loading*
   - *Amendment Loading*
3. Results
   - *Amendment Efficacy*

Addressing trichloroethene (TCE) contamination and Enhanced In Situ Biodegradation (EISB) in fractured sandstone & shale



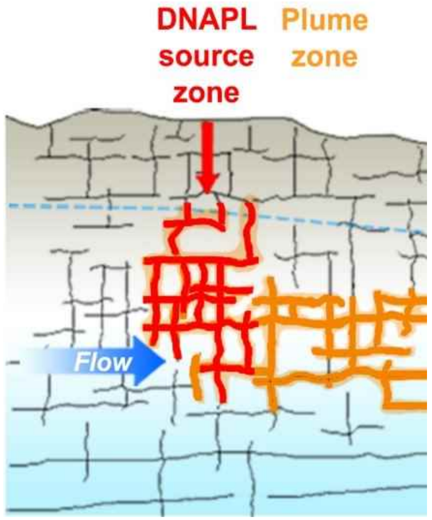
Cilona, Aydin, Likerman, Parker & Cherry. J. Structural Geology (2016)

Complex network of
- bedding planes,
- joints
- faults

Marine turbidite sequence of
- sandstones
- shales

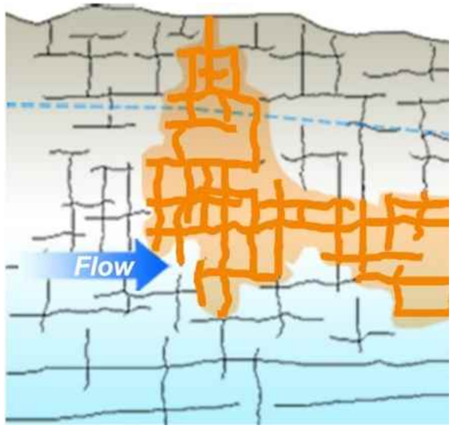
Amendment injection has a very different timescale than contamination in fractured porous rock

1.
DNAPL Loading
Multi-phase
Advection & Diffusion



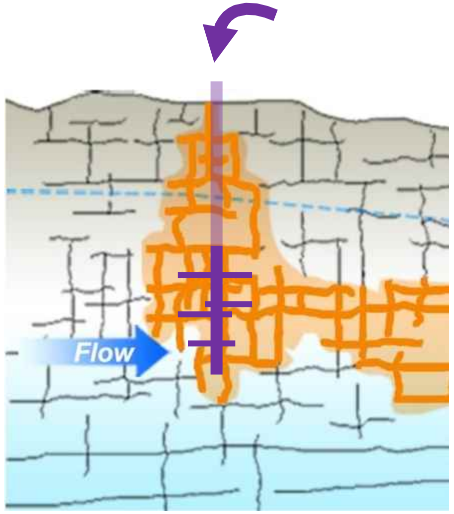
**Days-
Months-
Years**

2.
Plume Aging
Advection & Diffusion



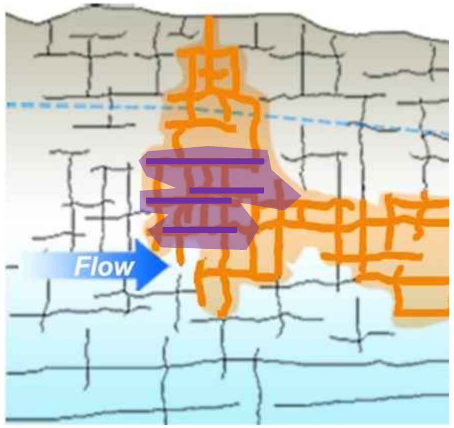
Decades

3.
Amendment Loading
Multi-species
Advection & Diffusion
Strong forced gradients



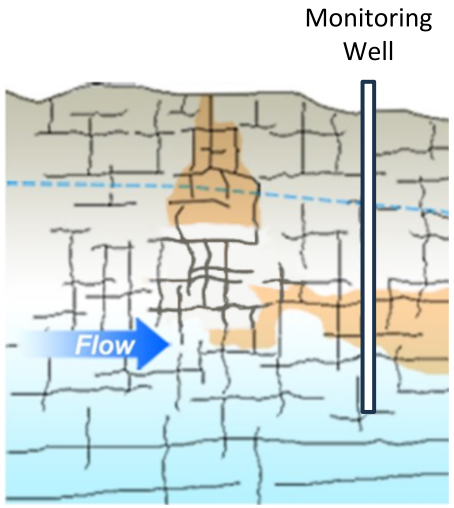
**Minutes-
Hours-
Days**

4.
Amendment Action
Reaction
Advection & Diffusion



**Months-
Years**

5.
Plume Monitoring
Advection & Diffusion



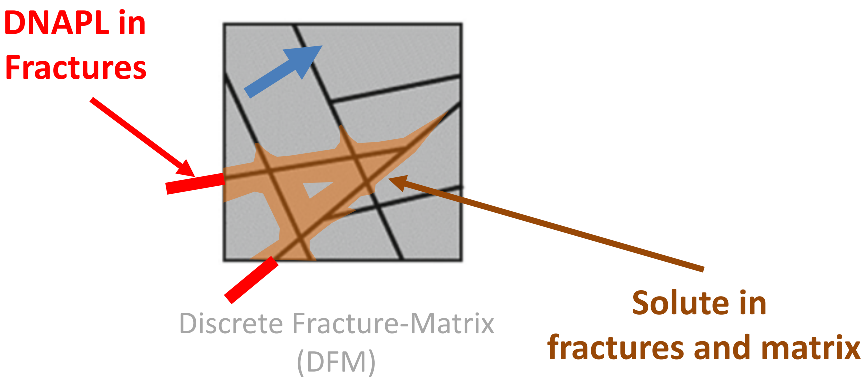
**Years-
Decades-
Centuries**

Critical: DFM geometry & Advection and diffusion physical processes

a)

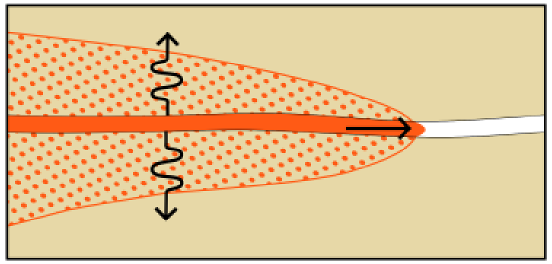
"Real" Fractured Porous Medium

b)

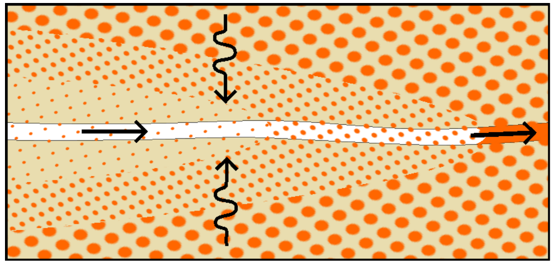


Discrete Fracture-Matrix (DFM)

c) Contaminant: New/advancing



d) Aged/flushing

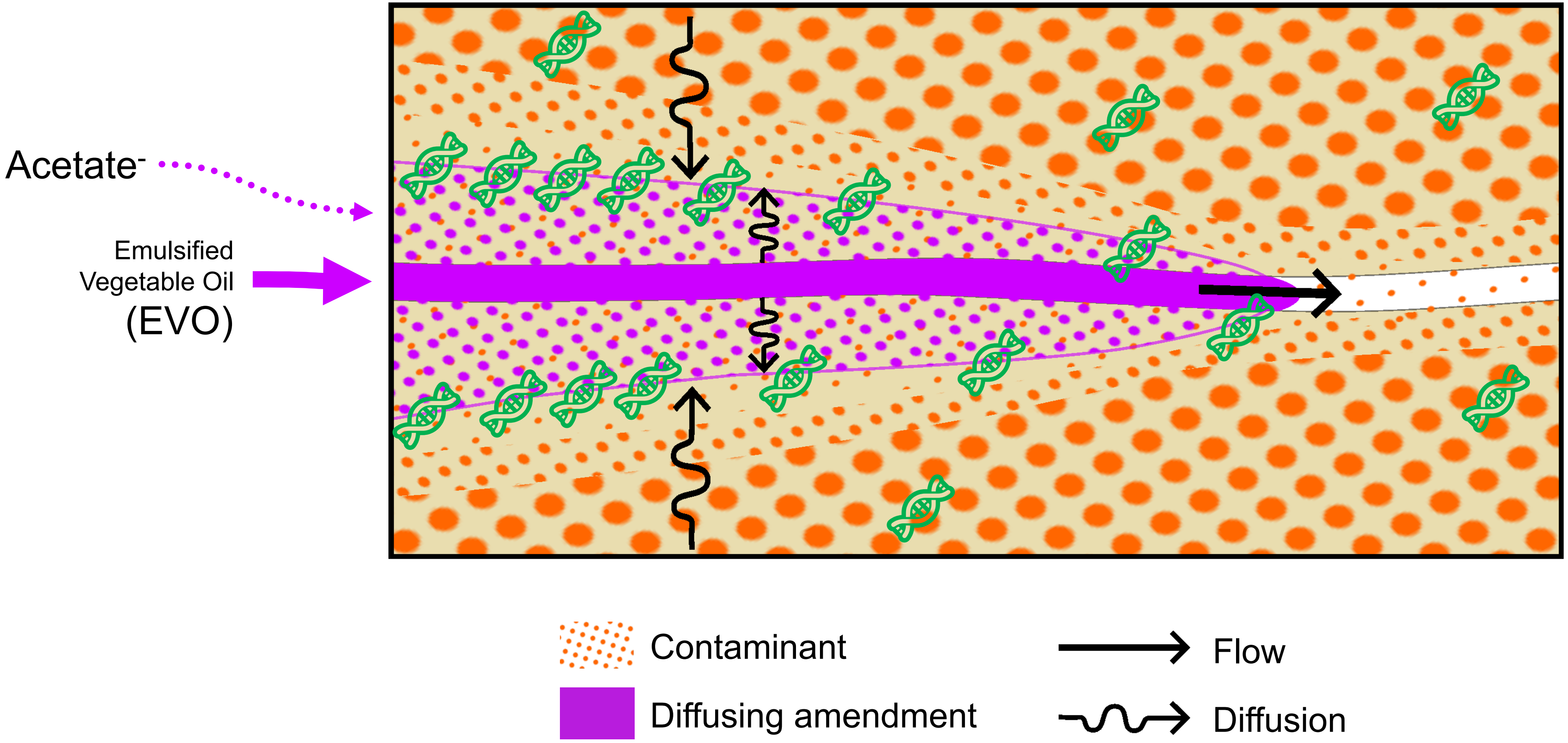


- Explicit representation of
  - Network of fractures
  - Fractures' variable aperture, location, spacing
  - Fracture-matrix interface area
- Physical processes
  - Advection
  - Diffusion
  - Reaction and/or decay

a) & b) Images modified from: Berre et al. (2019)

Delivery is a 2-step Process:
1) Advection through fracture network and
2) Diffusion into the matrix

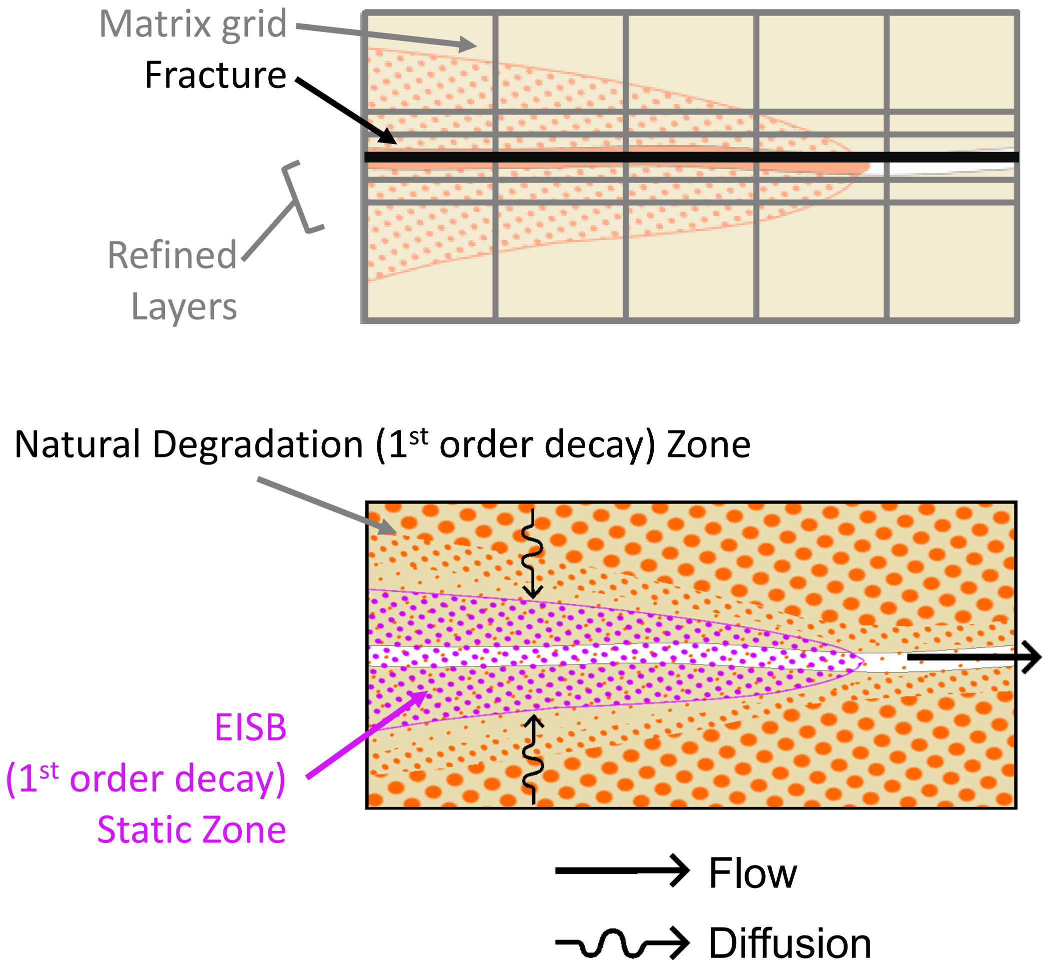
Contaminant + Amendment + Microbes



2. Methods

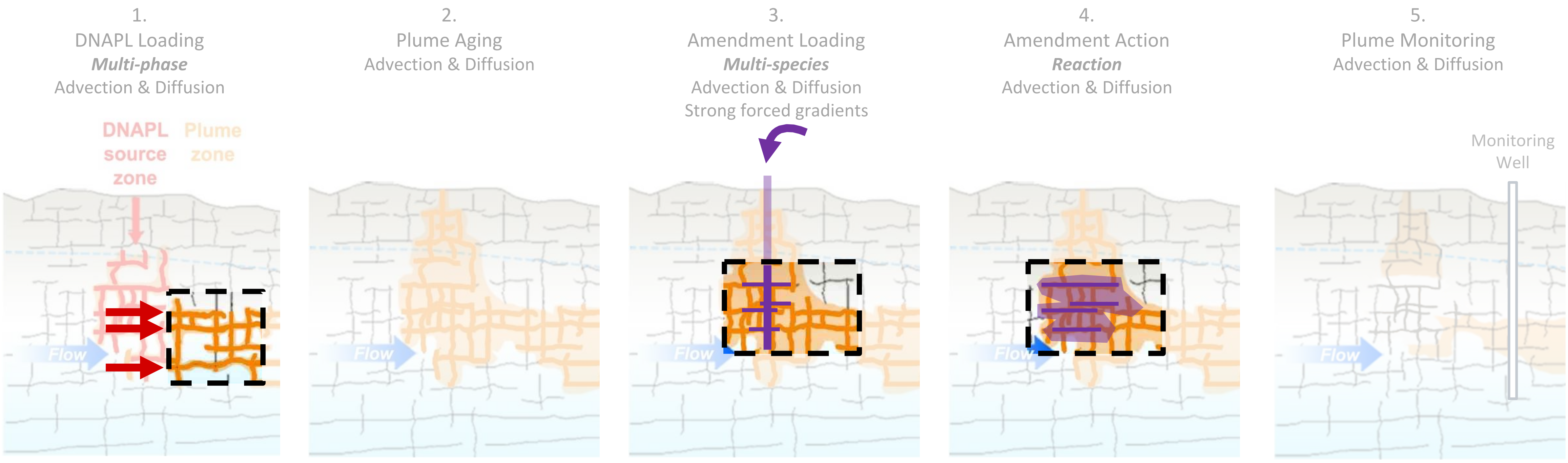
- *Composing simulations*
- *TCE loading*
- *Amendment loading*

Discrete fracture-matrix (DFM) model: Hydrogeosphere by Aquanty Inc.



- Physical processes (one solute, here)
  - Advection
  - Diffusion
  - "First order" decay
- Explicit representation of
  - Network of fractures
  - Fractures' variable aperture, location, spacing
  - Fracture-matrix interface area
- Discretization of the rock matrix away from fractures
- Tractable 3D simulation for
  - 10s of meters domain and 100s of fractures

Simulation domain is centered on the amendment injection zone



TCE solute arrives at solubility, C_0=1100 mg/L
(No DNAPL simulated.)

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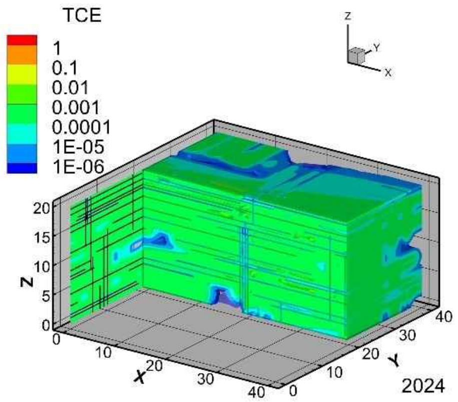
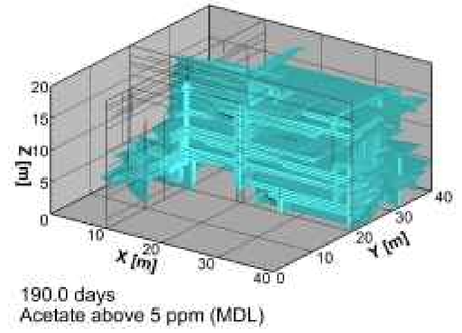
EISB simulations are the combination of 1-4 distinct simulation runs

1: TCE Loading and ageing



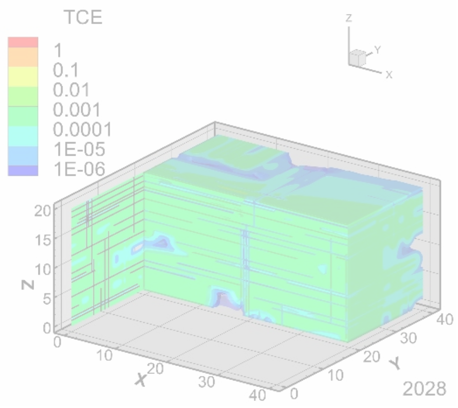
2: Amendment Loading



Amendment reach and diffusion distance is taken 6 months from injection for acetate.

Natural Degradation

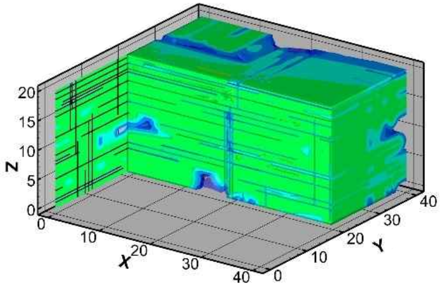
1 (continued): Natural degradation only for comparison to EISB



Aged plume concentrations are the initial conditions for enhanced degradation

EISB

3: EISB active continuously

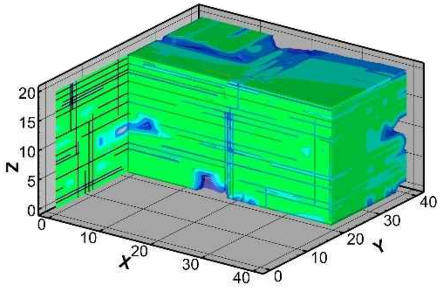


Diffusion halo informs spatial zones of enhanced degradation

4: EISB active temporarily, then natural degradation

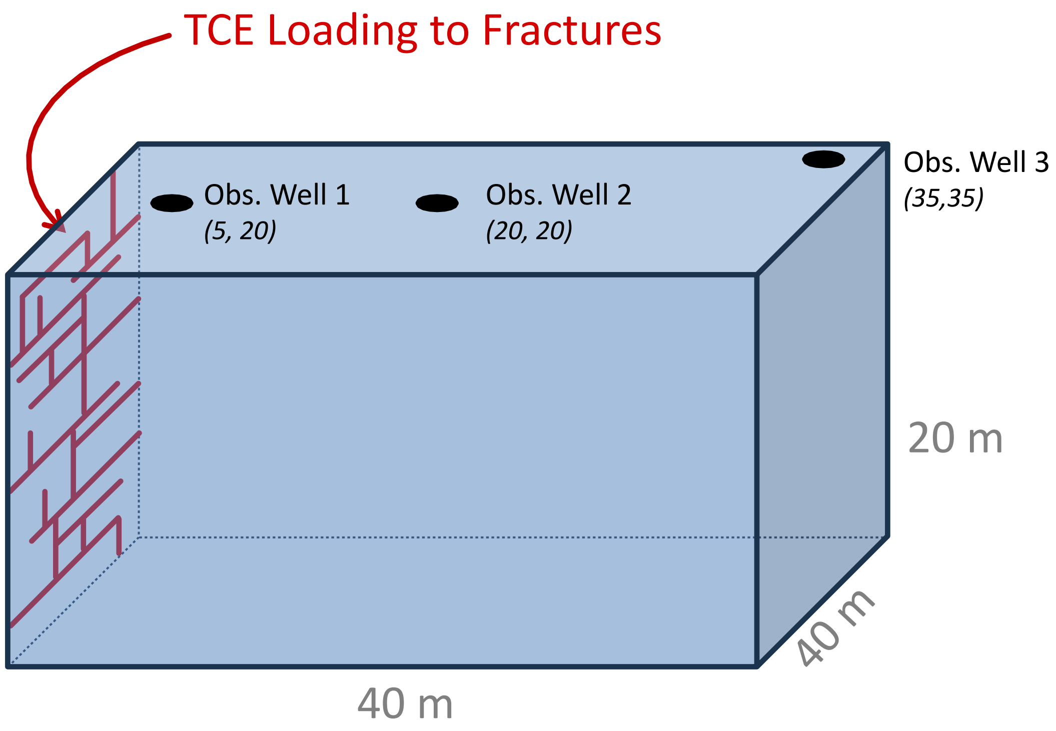
Natural Degradation

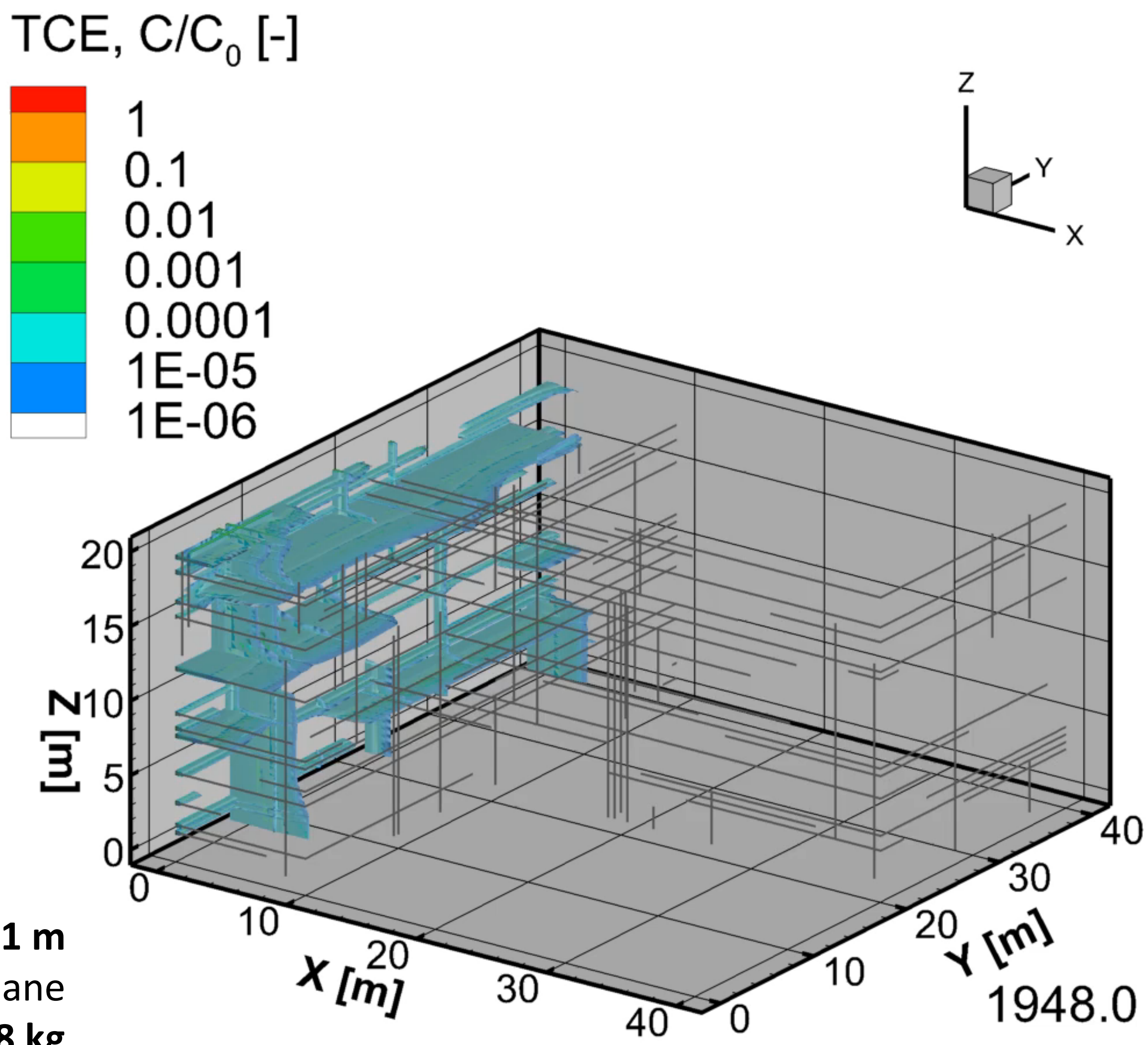
Natural degradation takes over when EISB is no longer effective



Active duration for acetate is 1 year.

Conceptually, DNAPL exists just upgradient of the domain, then enters at solubility concentration, C_0, in fractures





Porous Medium (PM) Refinement at 0.05 & 0.1 m
adjacent to each fracture plane
$\text{Mass}_{TCE,1949}$ = 308 kg

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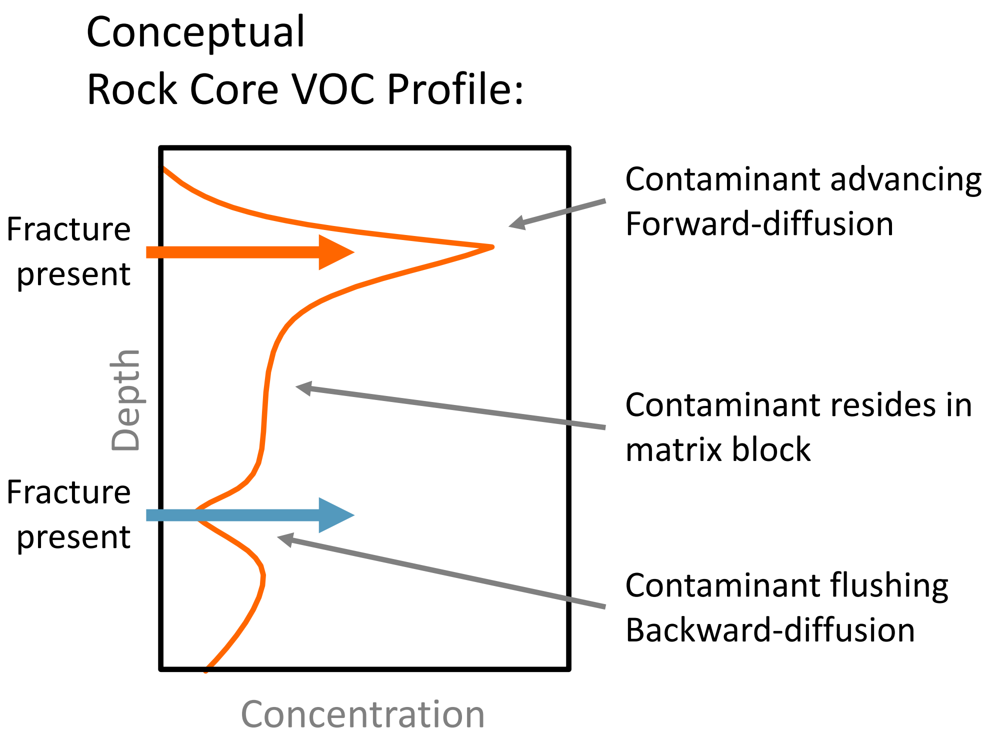
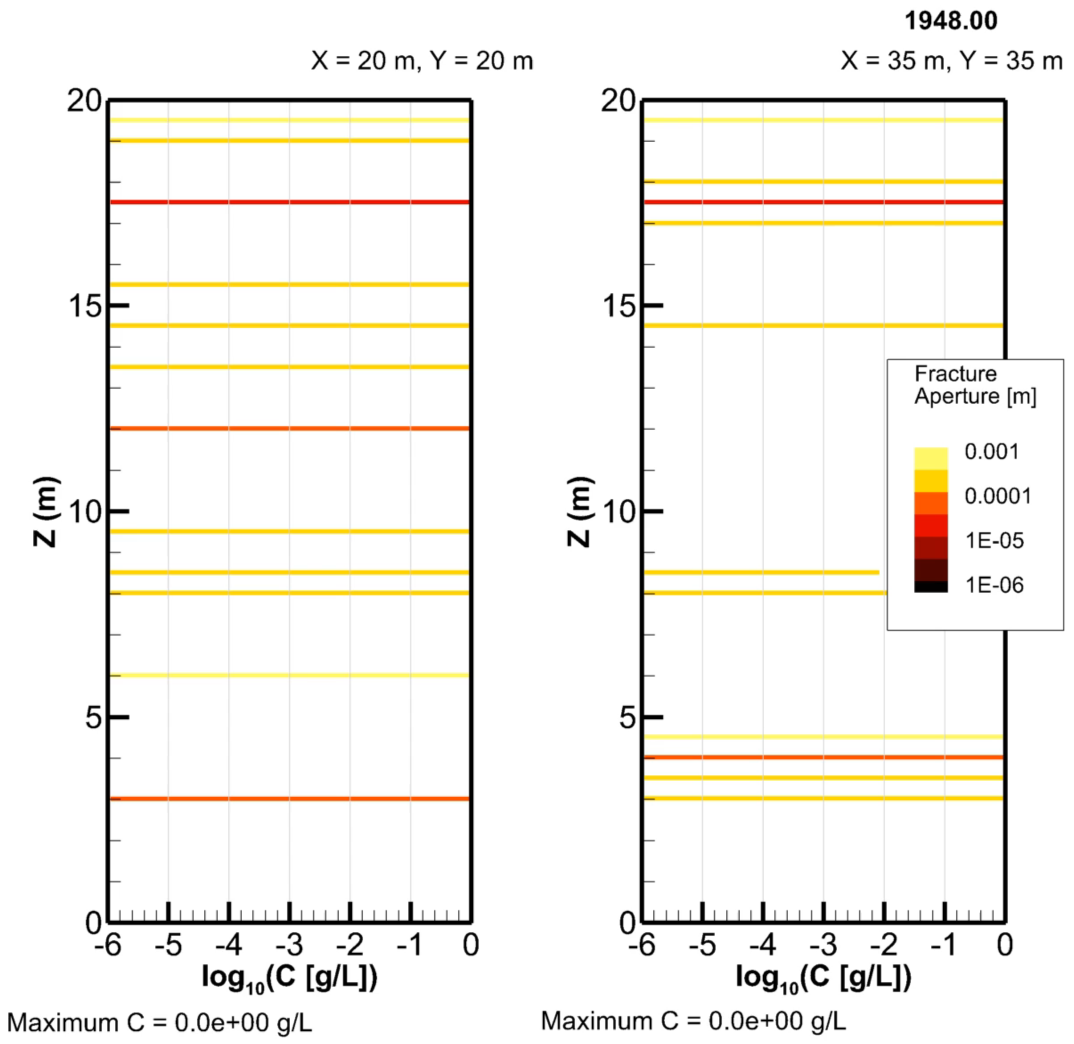
Simulations show the expected forward- and backward-diffusion effects

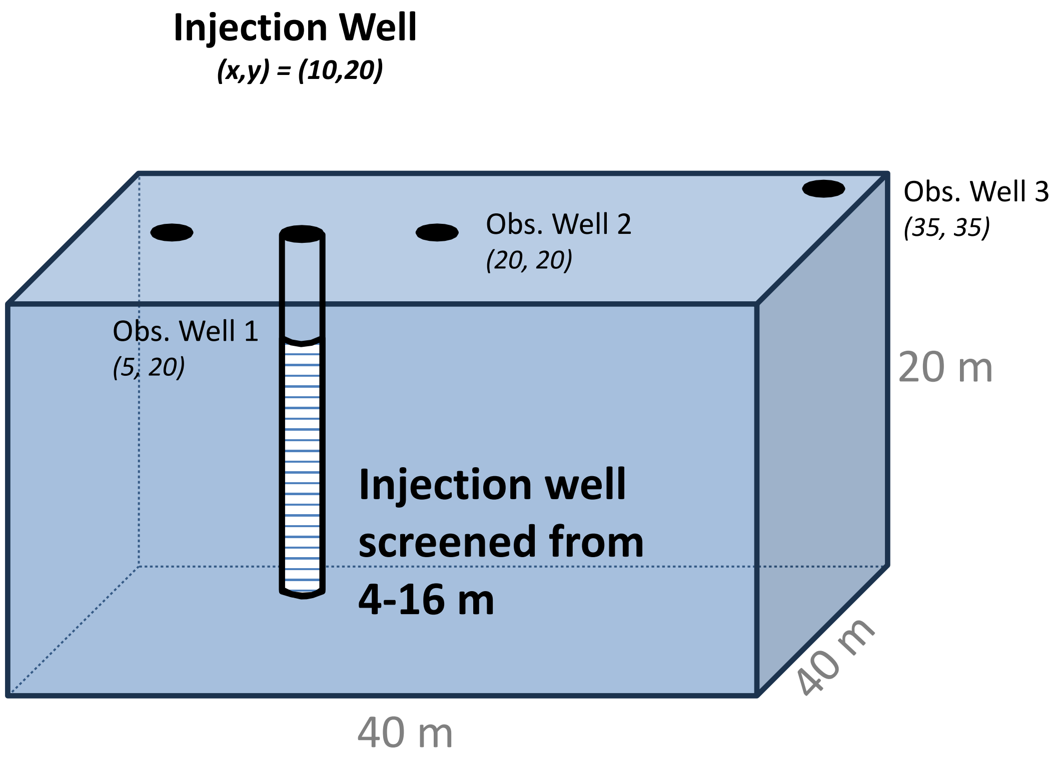


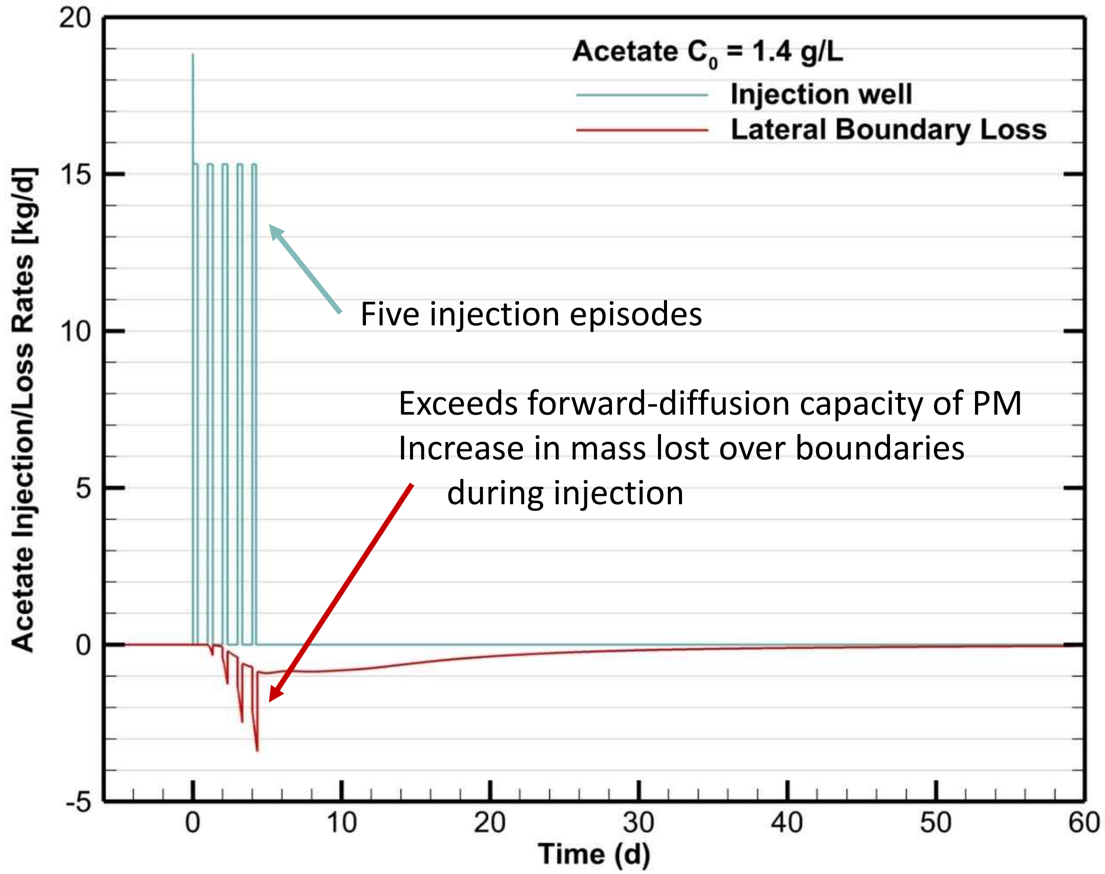


TCE loading results summary

- Loading at solubility concentration (1 year)
- Advection, diffusion, natural degradation, & flushing (70 years)
- TCE mass diffuses deep into matrix blocks, away from fractures
- Matches (stylistically) to field data

Amendment injection is a *forced gradient* condition – different from natural gradients acting on the plume

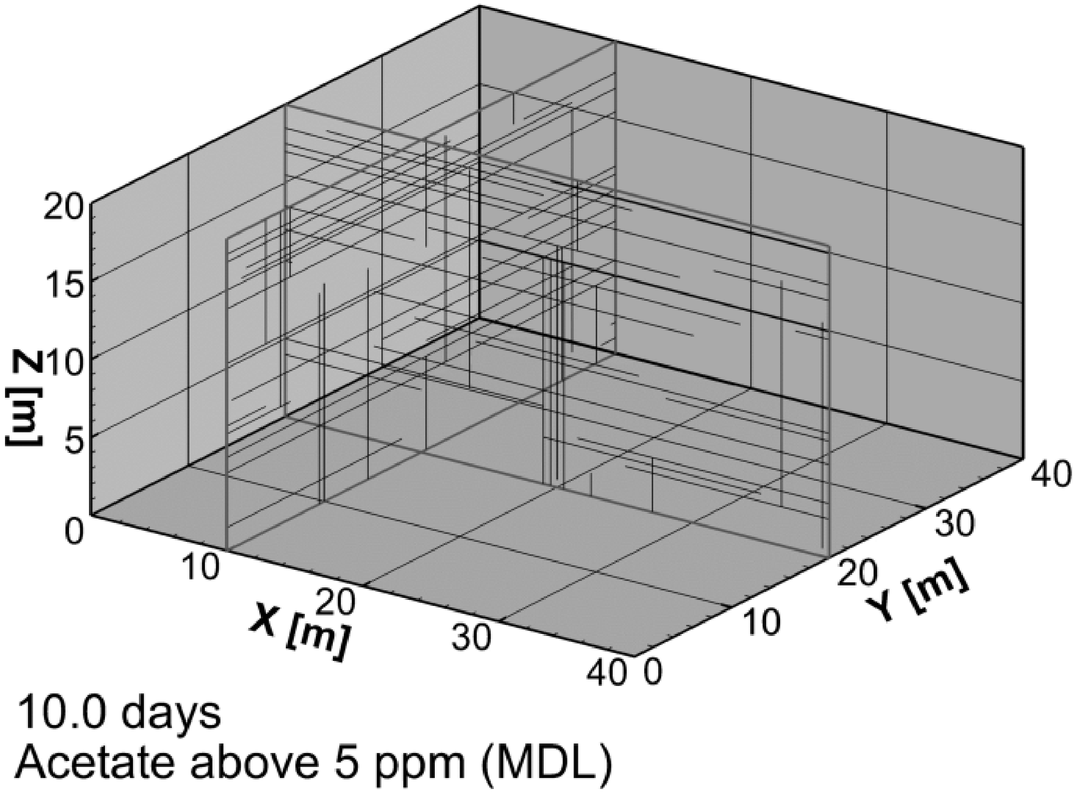


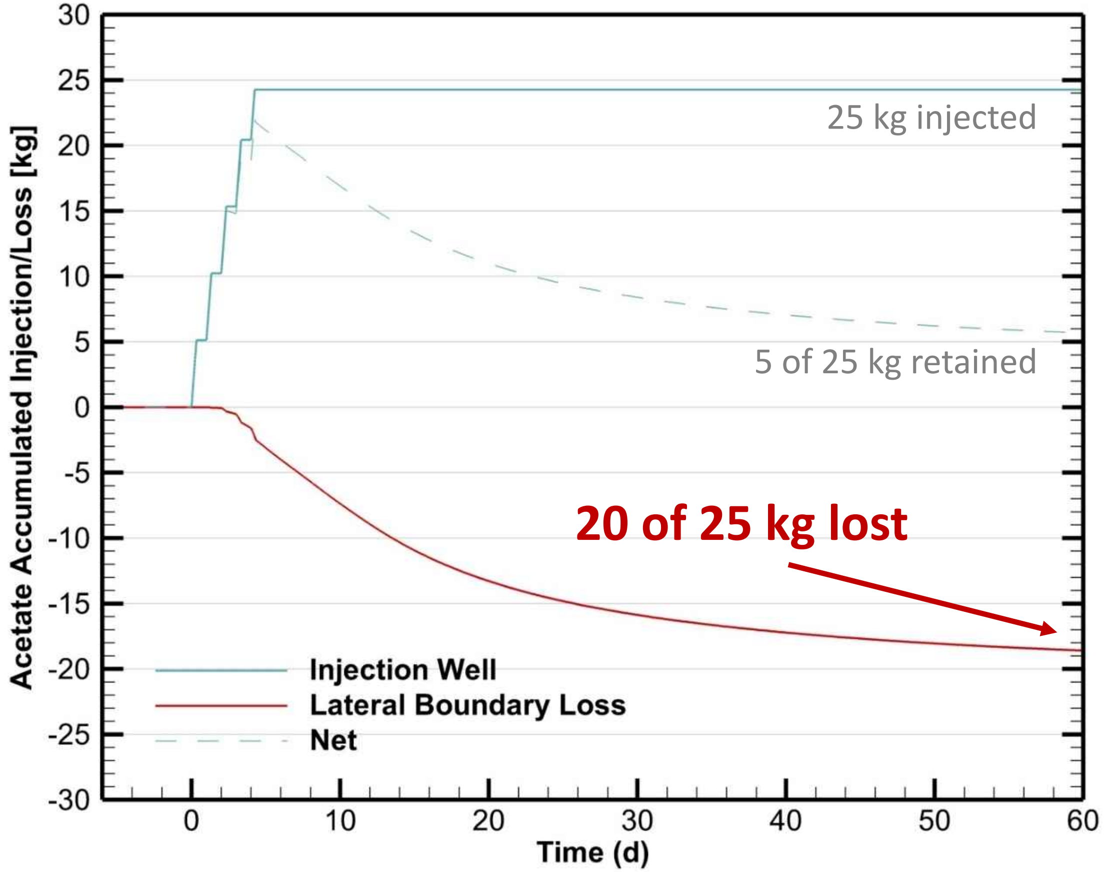


80% of injected acetate mass is lost over domain boundaries

Emulsified Vegetable Oil (EVO) as Acetate

Amendment Reach in PM*:	15%
Amendment Reach in Fractures**:	40%





* $\text{Volume}_{PM} = 40\times40\times20 = 32{,}000\ m^3$

** $\text{Volume}_{fracture} = \sim6\ m^3$

Injection results summary

- Episodic injection
- Most of amendment fluid exited domain
- Allowed 6 months of diffusion into the rock matrix
  Defined spatial “halo” for EISB

Come see the poster:

The Challenges with Amendment Delivery in Fractured Rock: Using Discrete Fracture Matrix Simulation to Quantify Reach

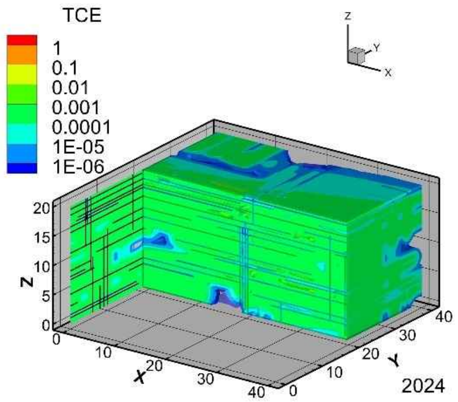
Session A3, Abstract #236, ***Poster #15***

June 3, 2024, 4:30-6:30 pm

3. Results

– *Amendment Efficacy*

Recall: Two cases of TCE degradation rates



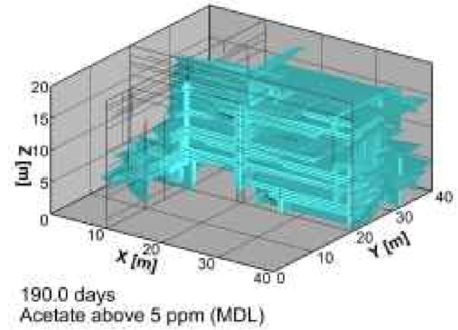
“Natural”
$t_{1/2}$= 27 years

Only Natural Degradation

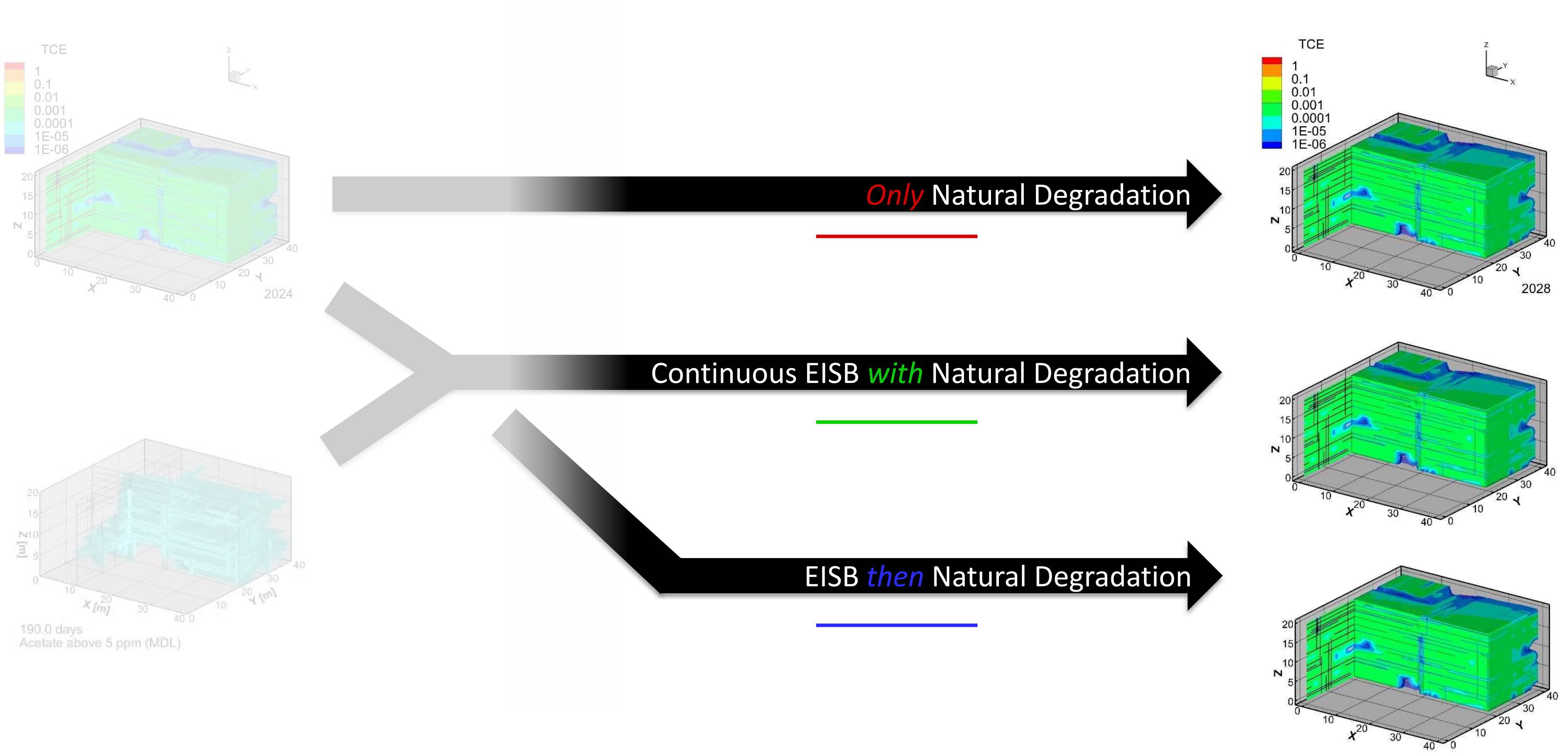
Continuous EISB with Natural Degradation

Emulsified vegetable oil “EVO” EISB rate
$t_{1/2}$= 3 years
…Limited to “halo” spatial zone

EISB then Natural Degradation



Recall: Three cases for efficacy comparison



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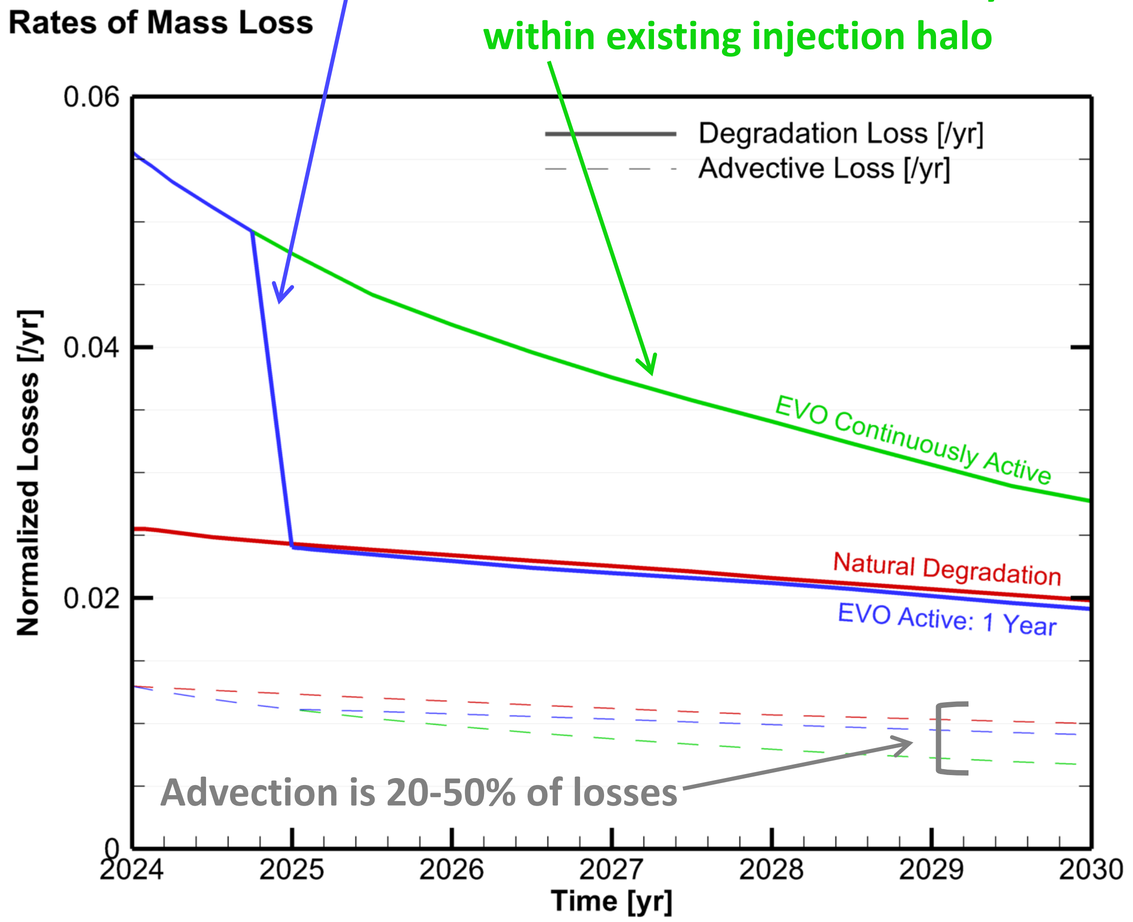
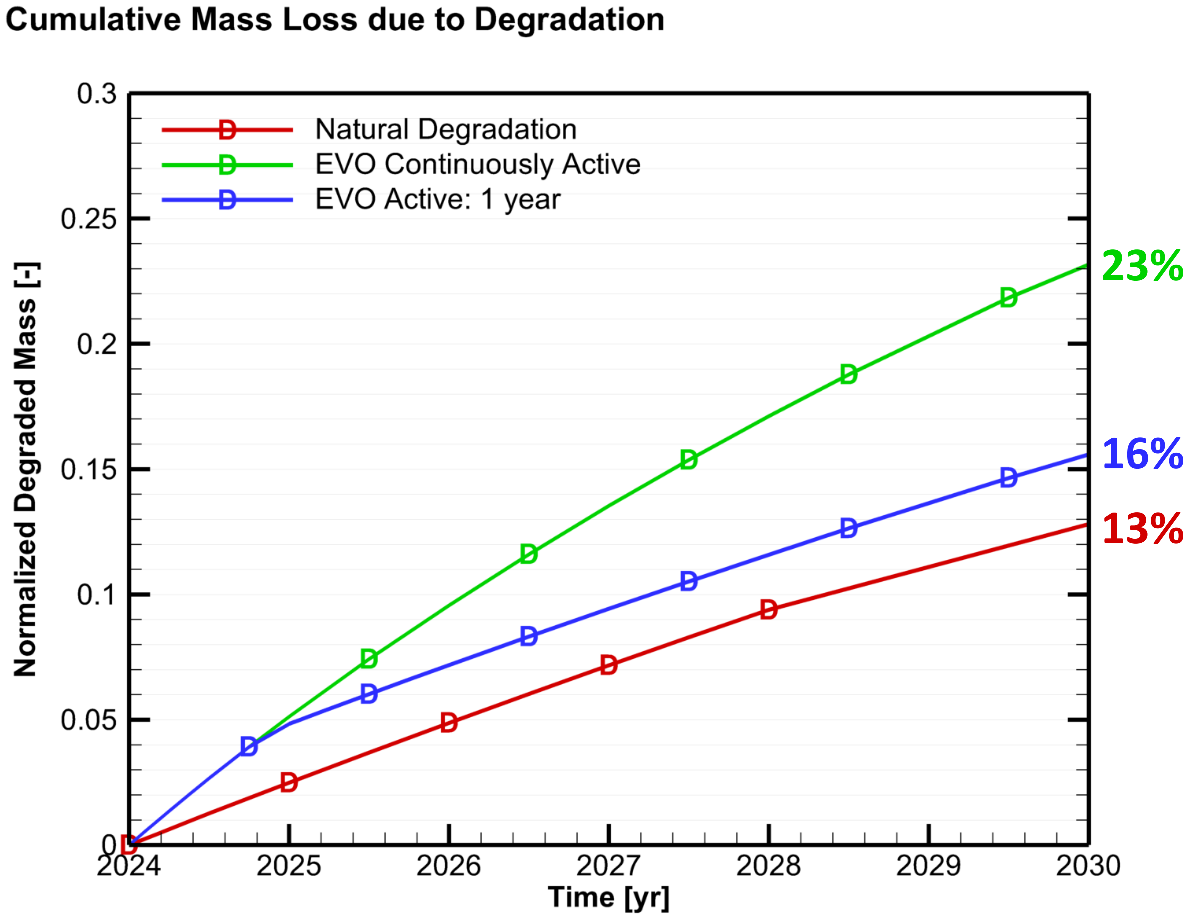
Short-term effectiveness shows 10% increased mass degraded over natural rates

EVO (acetate) "consumed"

Natural Degradation resumes

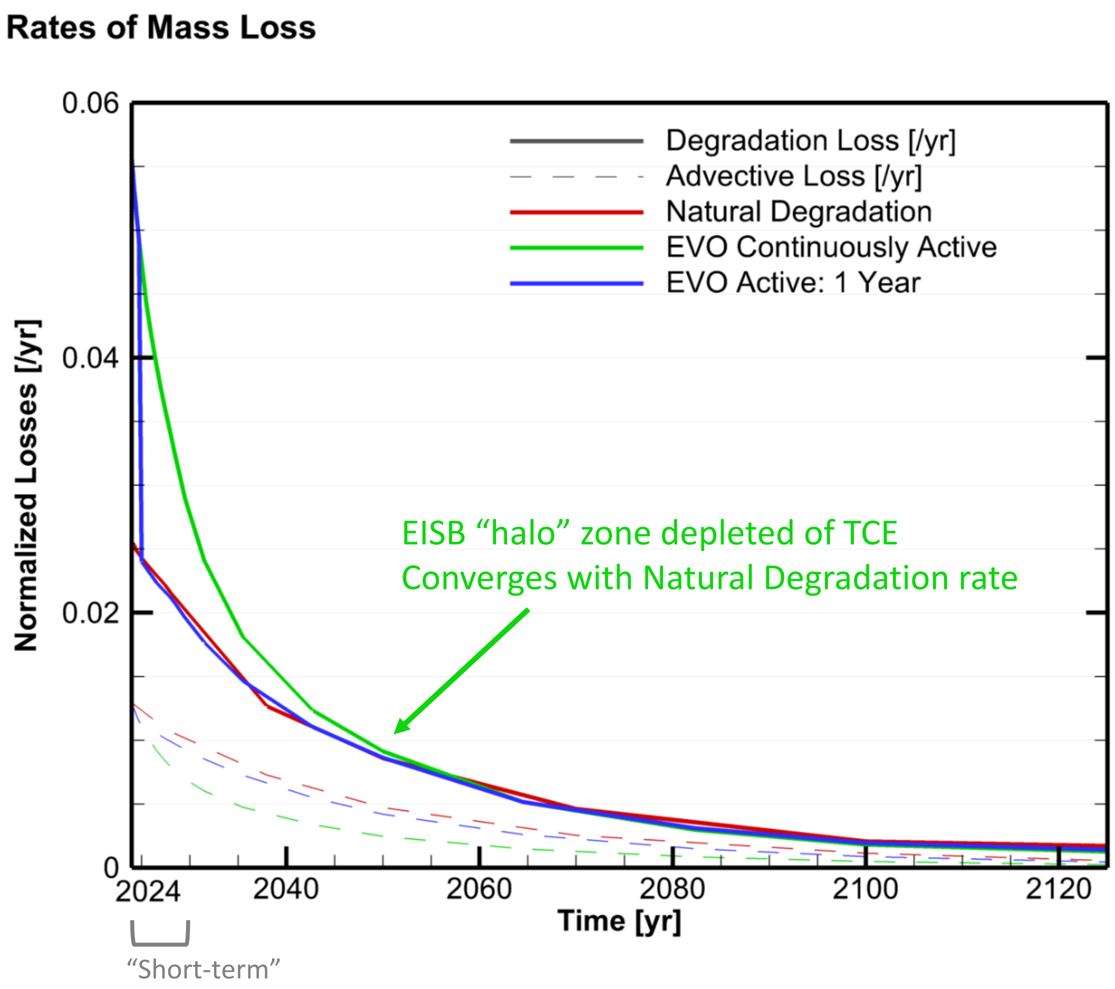
Continued amendment activity within existing injection halo

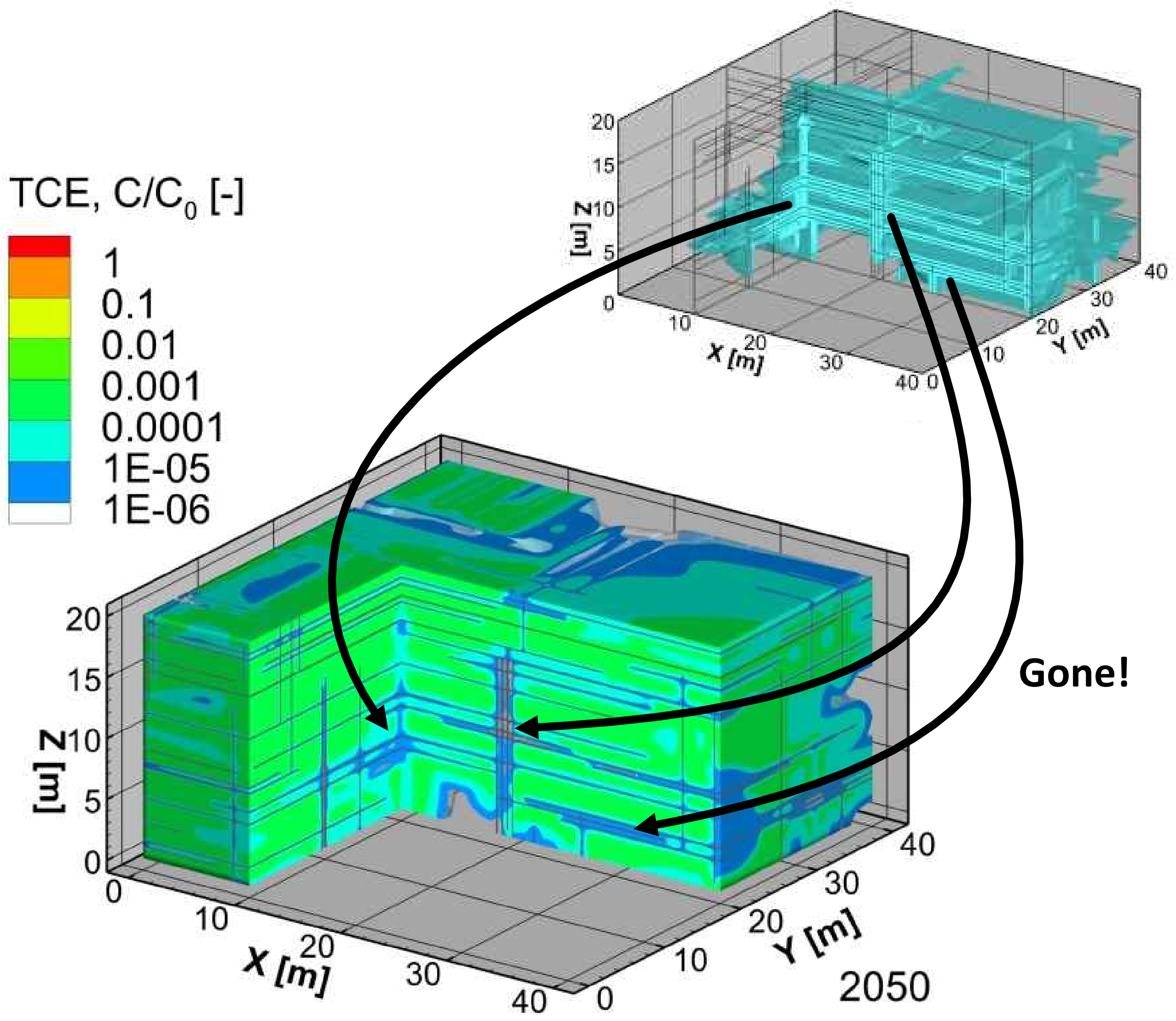




Degradation returns to natural rate in the long-term

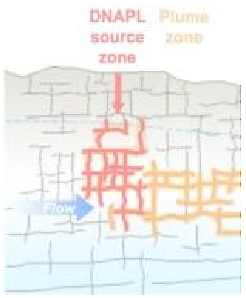
TCE depleted by orders-of-magnitude within halo



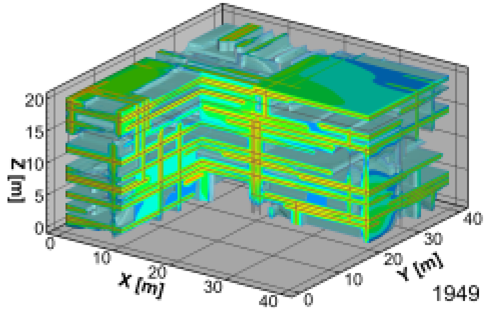


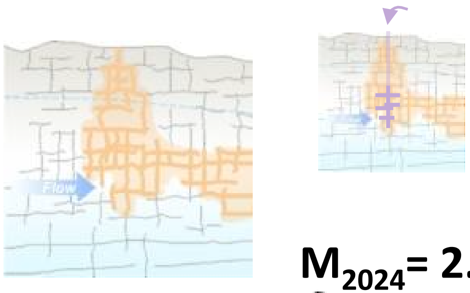
Was it worth it?

“Continuous EVO Treatment” case

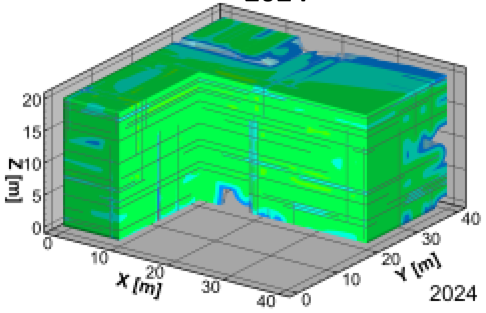


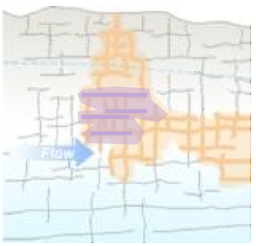
M_{1949}=308 kg



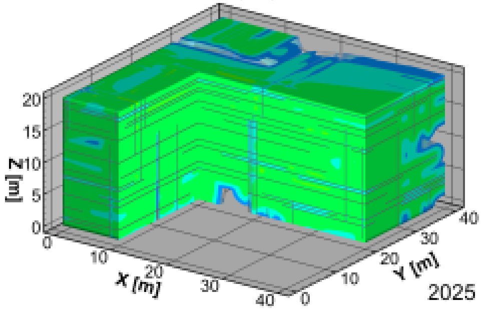


M_{2024}= 2.5 kg

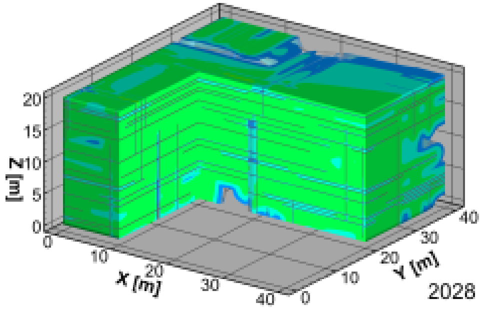


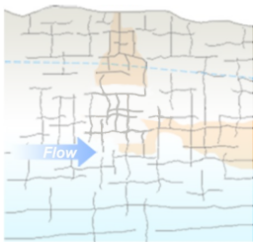


M_{2025}= 2.35 kg

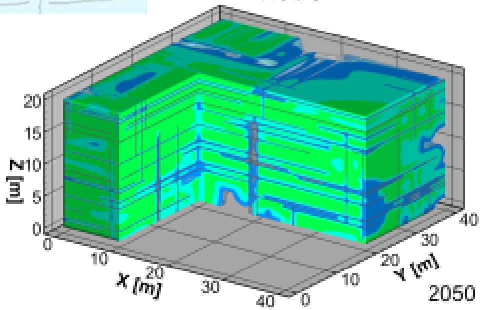


M_{2028}= 2.0 kg



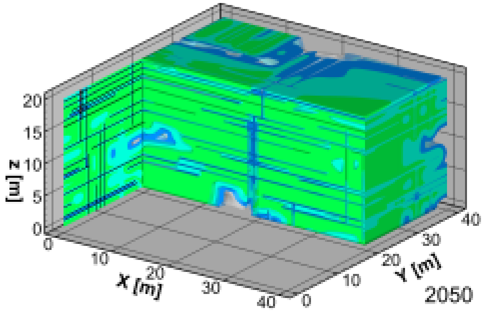


M_{2050}= 0.8 kg

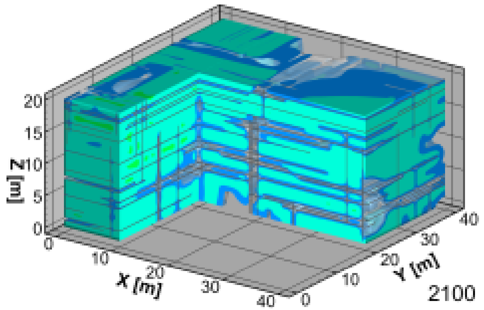


Natural Attenuation:

M_{2050}= 1.1 kg

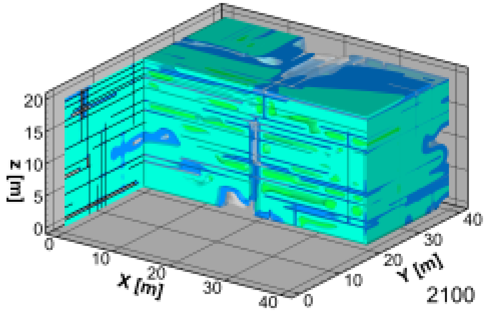


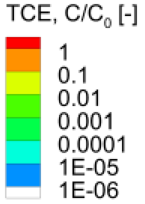
M_{2100}= 0.2 kg



Natural Attenuation:

M_{2100}= 0.3 kg





Conclusions/Summary

1. Modeling approach tied to conceptual model and field data
2. Discrete fracture matrix (DFM) transport modeling tools are useful!

- Modeling platform to *interrogate the feasibility* of EISB
  - What improvement does engineered remediation give?
  - Can we design and implement *anything* to reach the mass in the rock matrix?

- Hard to deliver amendments to matrix (where amendment is needed)

- Knowing natural degradation rates might be *most* important

Thank you!

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Funding was provided by
The Boeing Company and
Canadian National Science and Engineering Research Council
grant IRCPJ 363783-18 held by Dr. B. Parker.

Extras

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Table of Parameters: General model properties

Sandstone	
Hydraulic Conductivity, K_m (m/s)	4.1×10^{-9}
Tortuosity (-)	0.09
Porosity (-)	0.136
Density (kg/m^3)	2290
f_{oc} (-)	0.000375
$R_{m,\ TCE}$	1.59
$R_{m,\ Lactate}$	1.13
$R_{m,\ Acetate}$	1.01

Fracture Network	
P_{10} (#/m)	0.6
Average BP Length (m)	
Average Joint Length/Height (m)	
Mean aperture, 2b (µm)	190

Model Discretization	
Maximum Element Size (m)	0.5 × 0.5 × 0.5
Refinement about Fractures (m)	0.05, 0.1

Flow Boundary Conditions	
$Head_{x=0}$ (m) $Head_{x=40}$ (m)	550.78 550.60
Other boundaries (y=0,40; z=0,20)	*Linear gradient*
i_x	0.0045

Combined PM + Fracture Network	
Hydraulic Conductivity, K_{bulk} (m/s)	1×10^{-6}

Table of Parameters: Solutes used in loading and amendment injection scenarios

Solute	K_{oc}	D_0 (m^2/d)	$t_{1/2}$ (yr)	C_0 (mg/L)	EISB Effective Duration (yr)	TCE $t_{1/2,\ EISB}$ (yr)
TCE	0.094	8.73E-05	27	1400*	-	-
Lactate	0.021	9.50E-05	0.08	1000	0.08 - 0.17	1
EVO/LCFA/**Acetate**	0.001	1.04E-04	0.5	20000	0.5 - 1	3

*at DNAPL saturation

Effectiveness duration estimates from field studies, tied to implementation in a passive context

Estimates