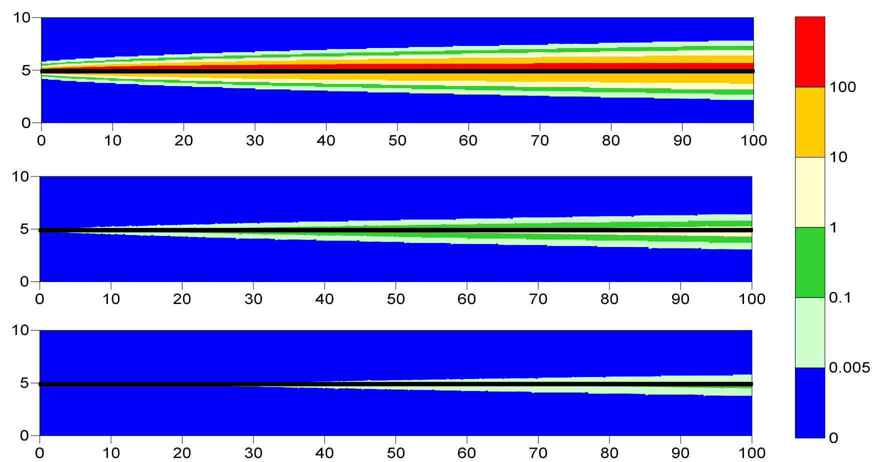
In Situ Remediation (ISR-MT3DMS) for Modeling Back-Diffusion Timeframe

By Grant R. Carey, Ph.D.

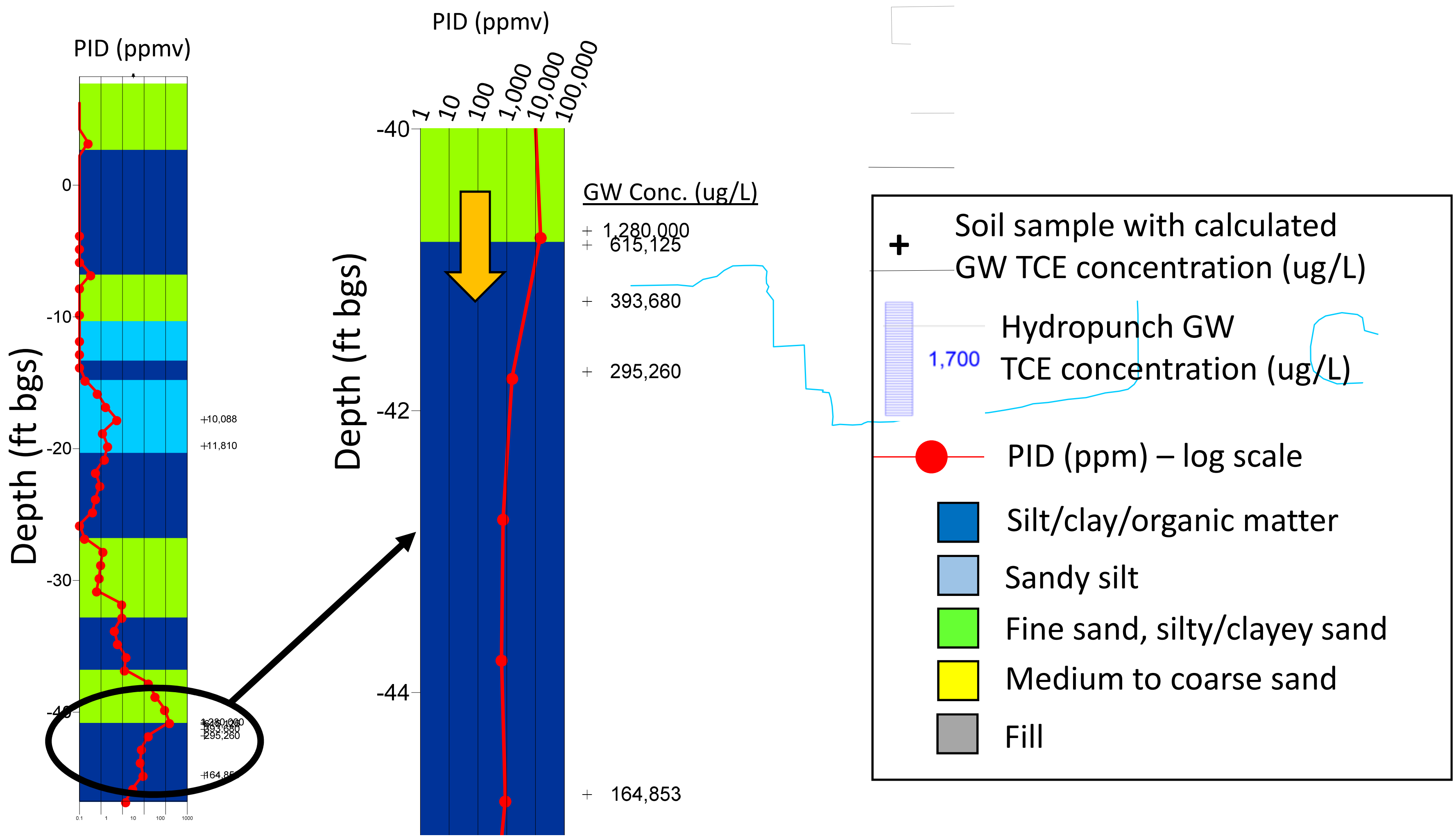
Porewater Solutions, gcarey@porewater.com, www.porewater.com

and Adjunct Professor, Dept. Of Civil Engineering, University of Toronto



Presented at the *Tenth International Conference on Remediation of Chlorinated and Recalcitrant Compounds* (Palm Springs, California | May 22-26, 2016)

Example – TCE Diffusion into Silt / Clay



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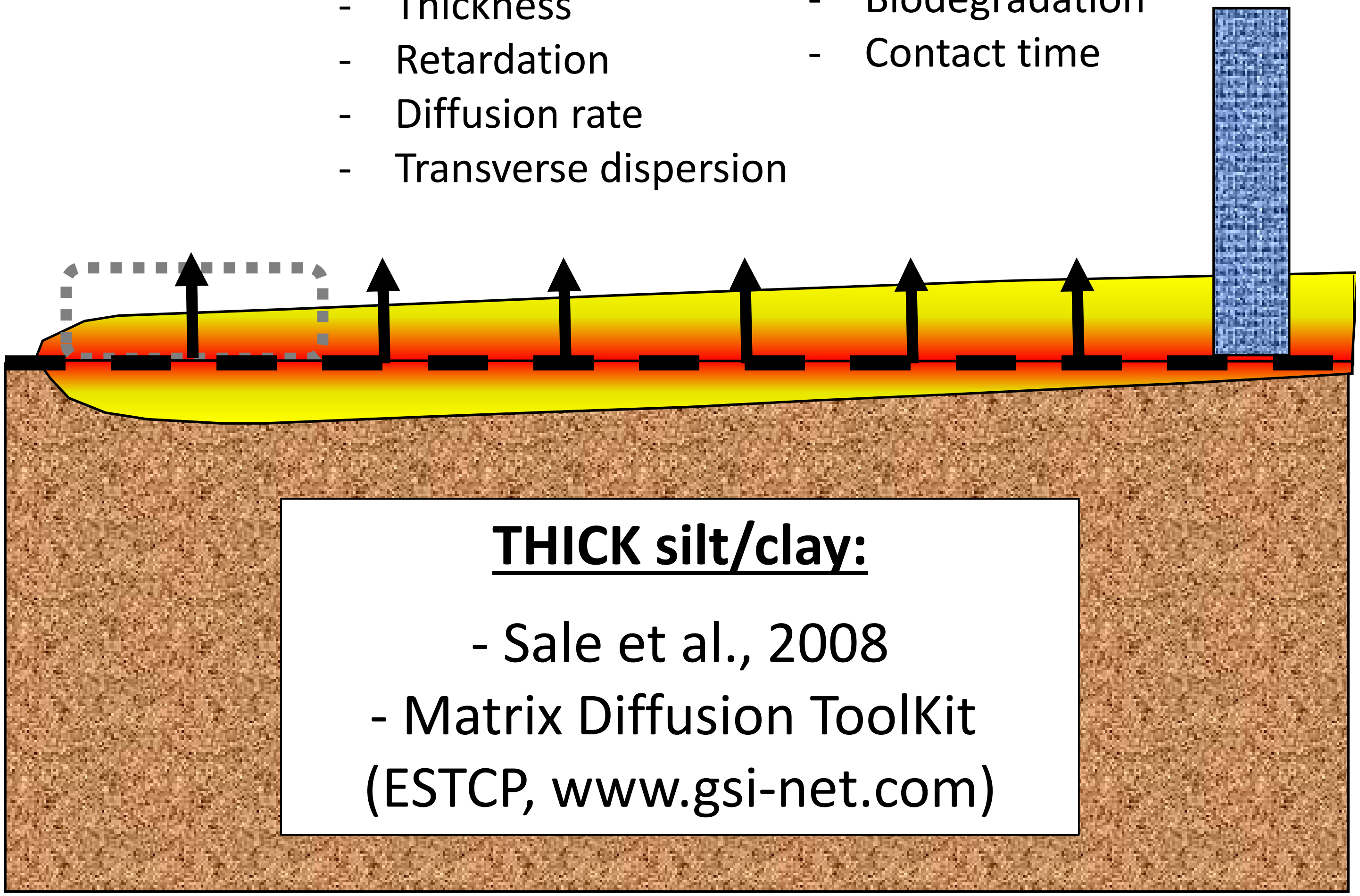
Factors Influencing Remediation Timeframe

Influencing factors:

- Velocity
- Thickness
- Retardation
- Diffusion rate
- Transverse dispersion
- Length of clay lens
- Biodegradation
- Contact time



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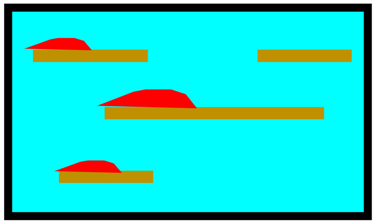
Modeling Challenges

- Analytical solutions not available for:
  - Thin silt/clay lenses
  - Enhanced degradation rates



- Numerical models
  - Small grid spacing, time steps
  - Prohibitive for 3-D models
- **ISR-MT3DMS: local domain approach**

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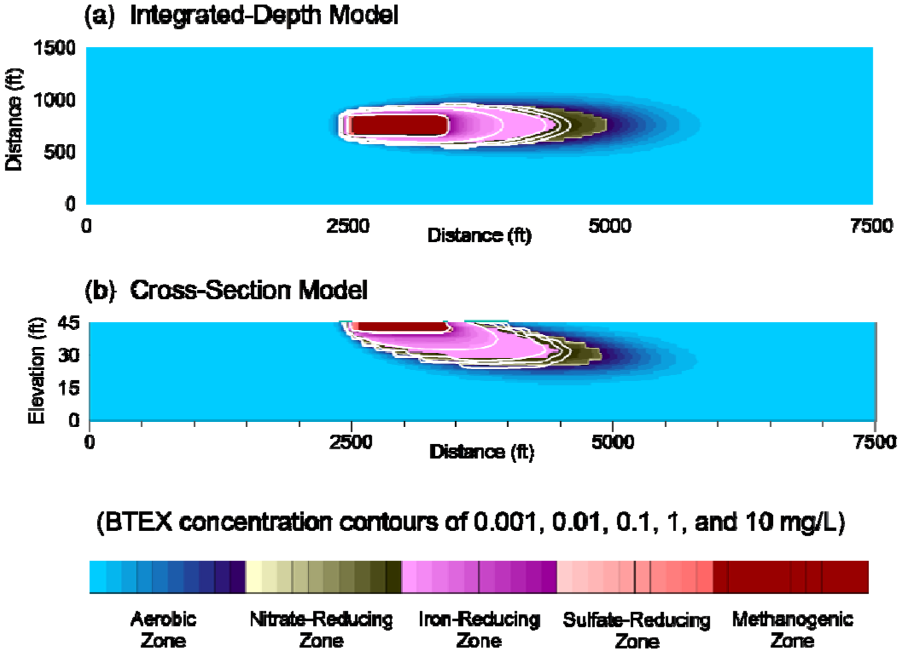
In-Situ Remediation (ISR-MT3DMS)

MT3DMS v5.3

BioRedox RCT package



- Reactions: **solvents, hydrocarbons, metals**
- **Unique visualization methods**
- Mineral precipitation/dissolution
- Rate stimulation/inhibition

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Carey, Van Geel, and Murphy (1999)

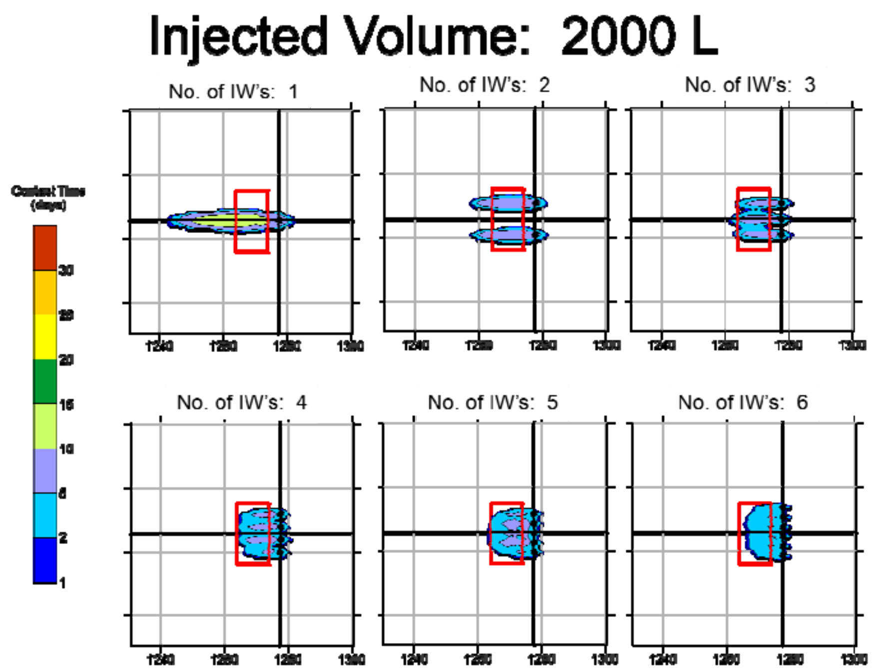
In-Situ Remediation (ISR-MT3DMS)

MT3DMS v5.3

BioRedox RCT package

Contact Time Calculator

Optimization Metric



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In-Situ Remediation (ISR-MT3DMS)

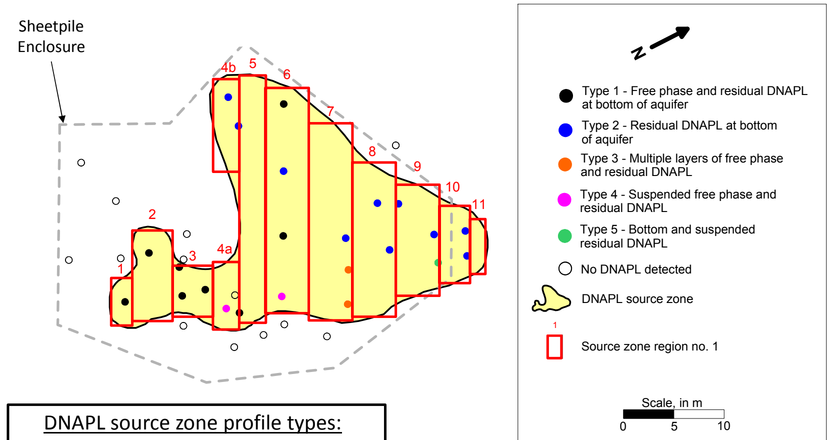
MT3DMS v5.3

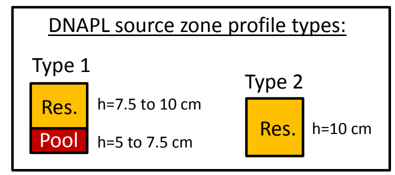
BioRedox RCT package

Contact Time Calculator

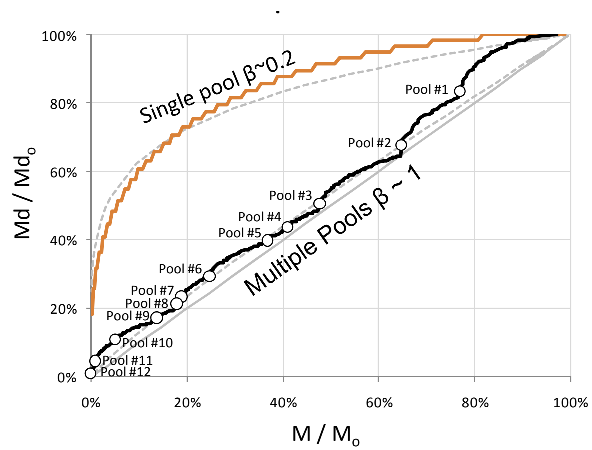
NAPL Depletion Model

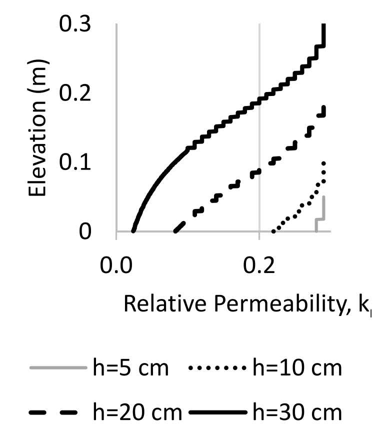
FREE (www.porewater.com)





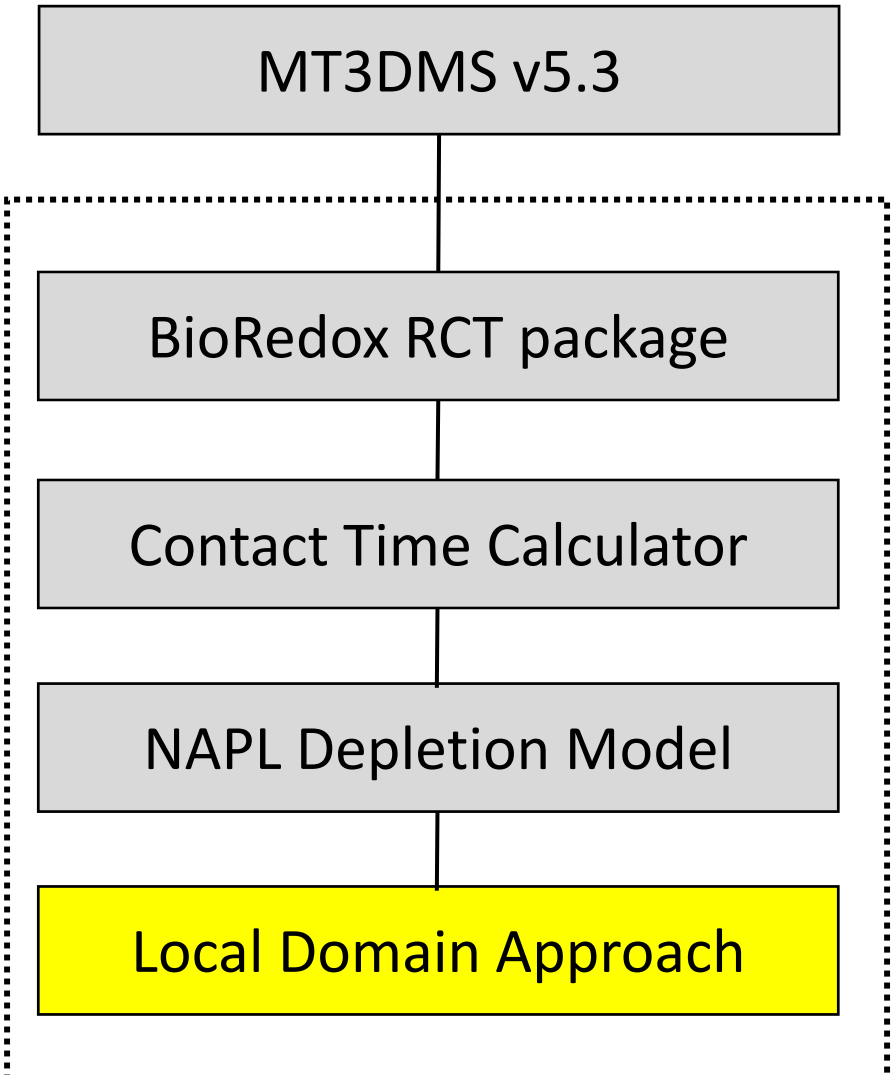
Parker et al., 2003
Parker et al., 2004
Chapman and Parker, 2005
Stewart, 2002





Carey, McBean, and Feenstra (2014a,b; 2016a,b,c)

In-Situ Remediation (ISR-MT3DMS)



Collaborative research:

Physical and numerical models

UNIVERSITY OF TORONTO

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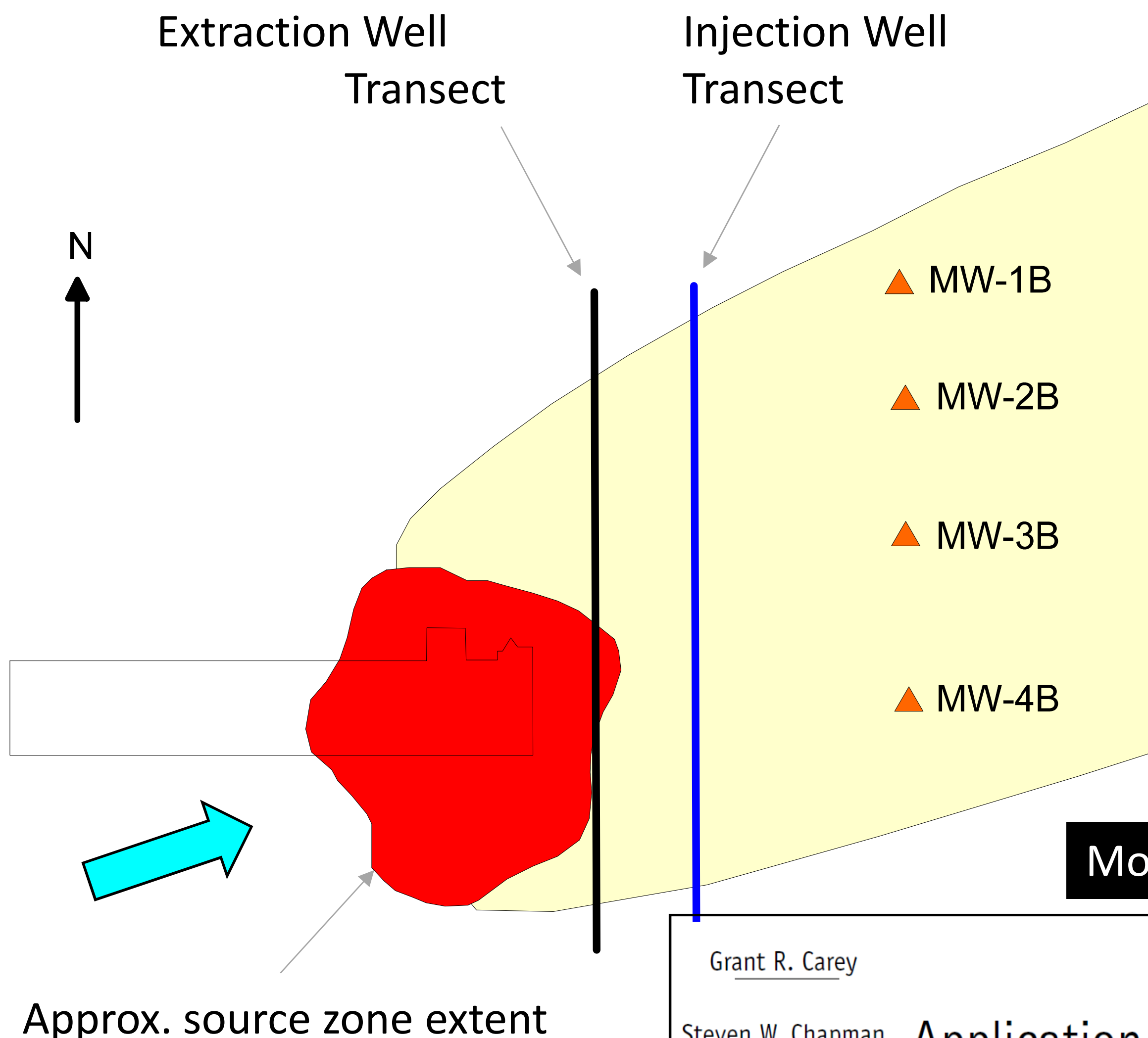
Case Study – Florida Site



Site Characteristics

- Beach sand aquifer
- Continuous, thin clay layer across site
- Other discontinuous, thin silt/clay layers
- Multiple, thin suspended DNAPL layers in source zone

Modified from Parker et al., 2008

REMEDIATION Autumn 2015

Grant R. Carey
Steven W. Chapman
Beth L. Parker
Rick McGregor

Application of an Adapted Version of MT3DMS for Modeling Back-Diffusion Remediation Timeframes

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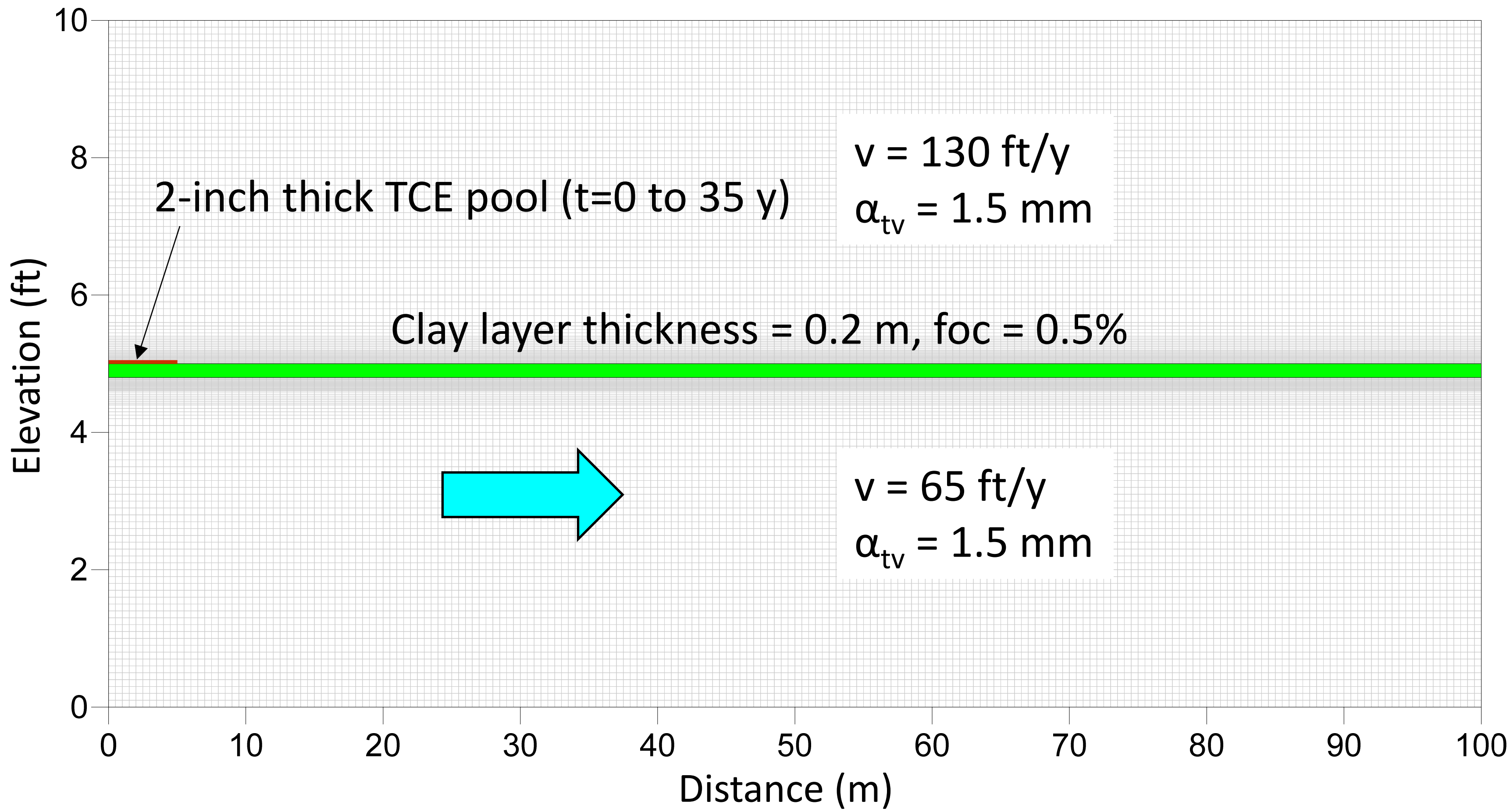
2-D Model Grid

200 columns, 158 rows (layers)
Minimum grid spacing: Δz = 1.25 cm, Δx = 0.5 m
Run-time = 45 minutes for 85-y simulation (Δt = 0.24 d)



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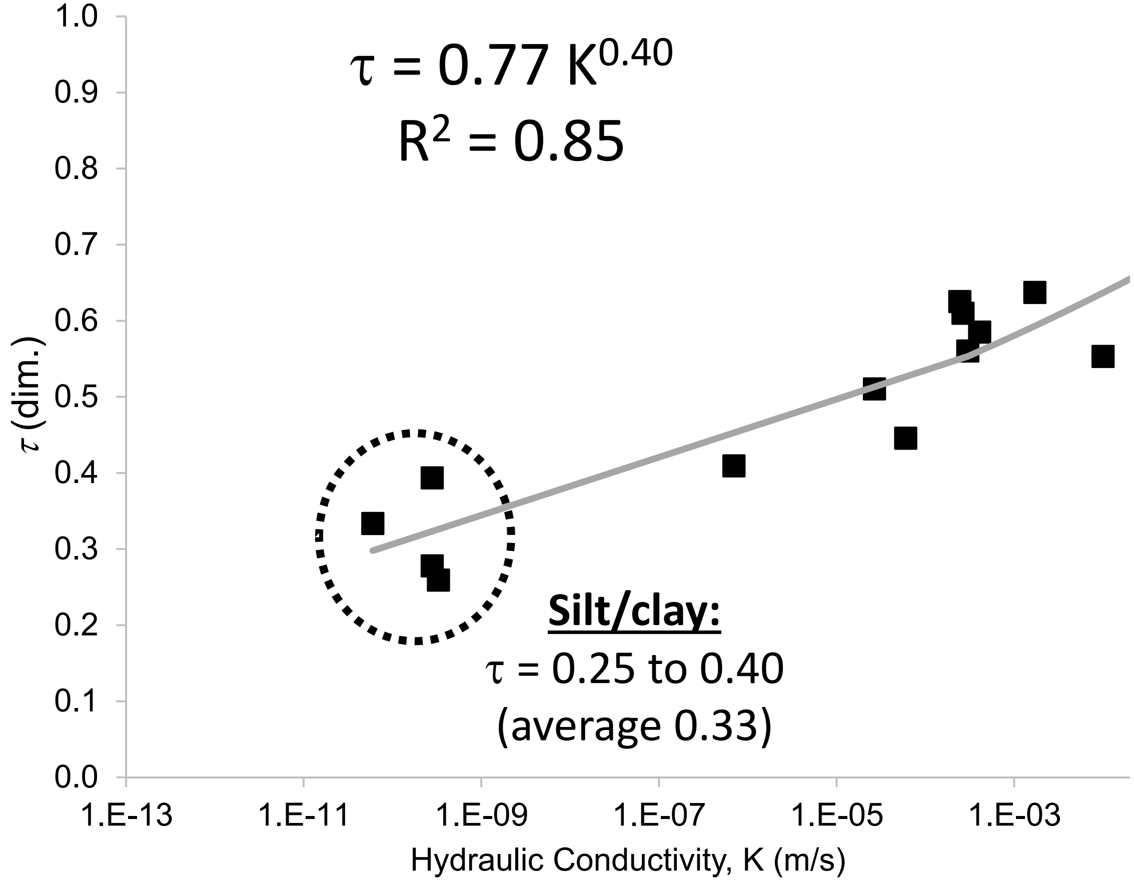
Carey et al. (2015) – Modified from Parker et al. (2008)

Tortuosity Coefficient

τ proportional to θ_e (not θ_t)



Carey, McBean, and Feenstra (2016d)
Accepted for publication in Ground Water

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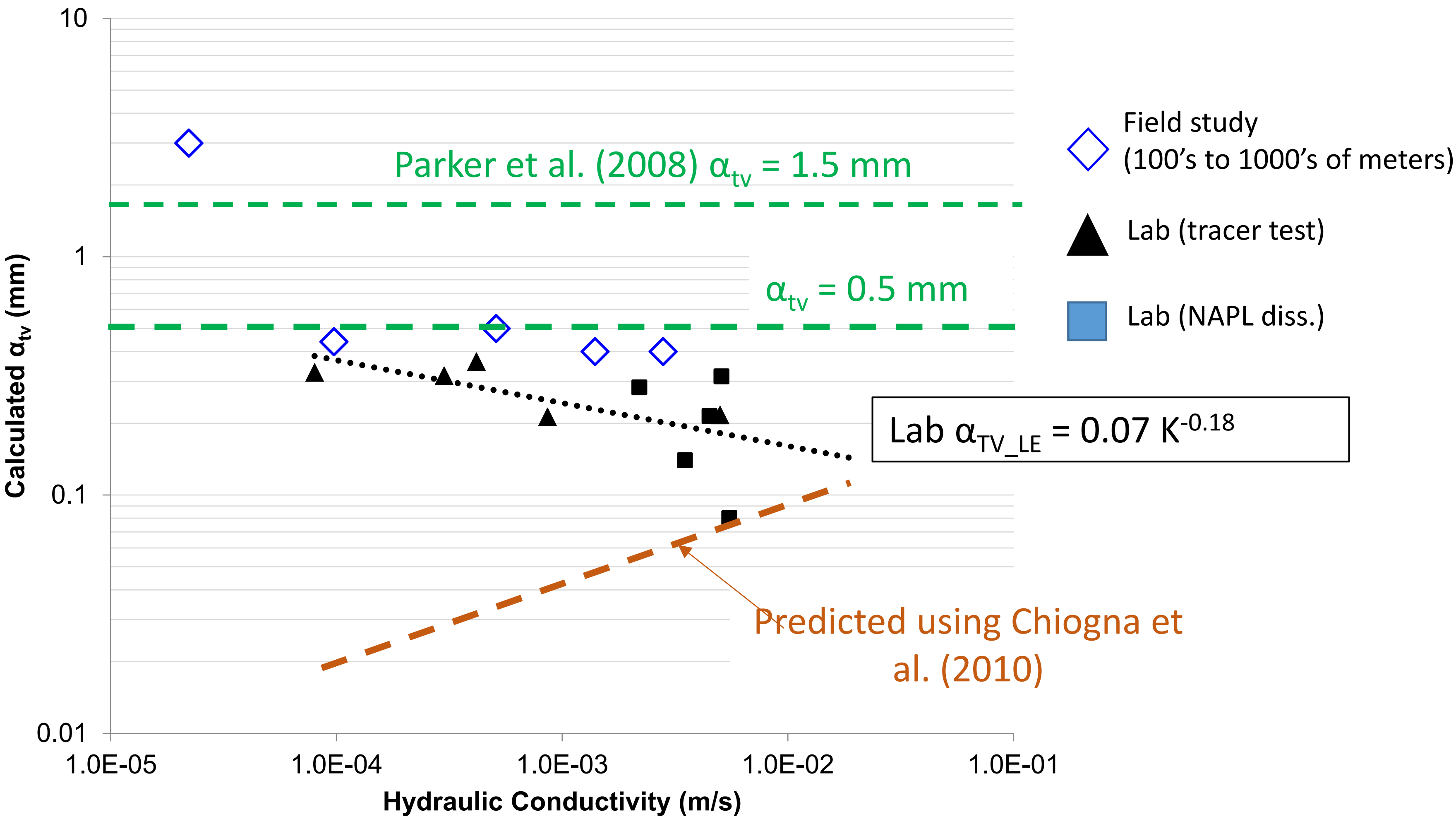
Transverse Dispersivity vs. K



Note – results not shown for glass bead studies.
LE = Local equilibrium.

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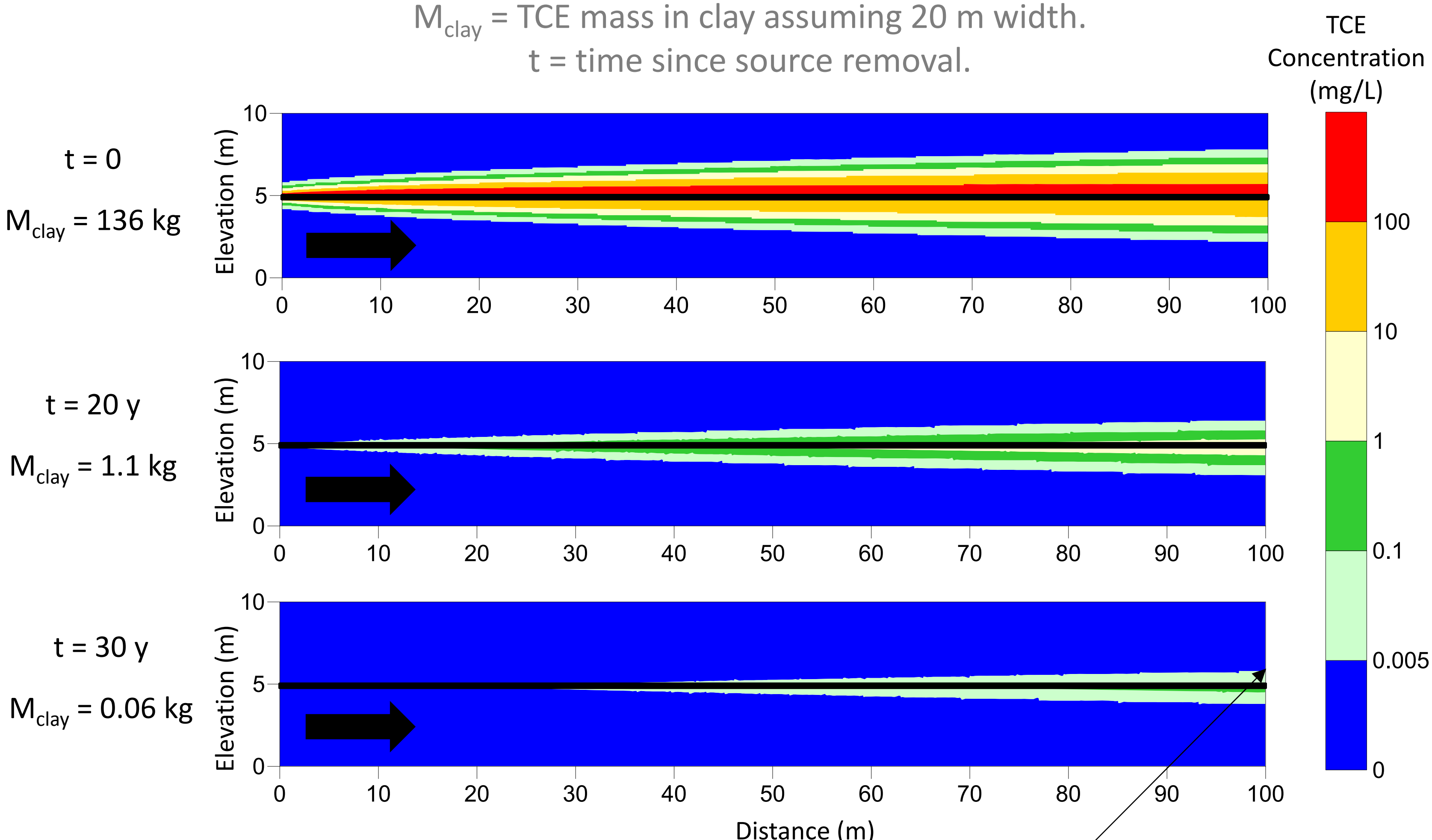
Carey, McBean, and Feenstra (2016e)

Simulated TCE After Source Removal

M_{clay} = TCE mass in clay assuming 20 m width.
t = time since source removal.



30 years after source removal:
99.96% mass depletion in clay, avg. C_{well} = 12 to 126 ug/L

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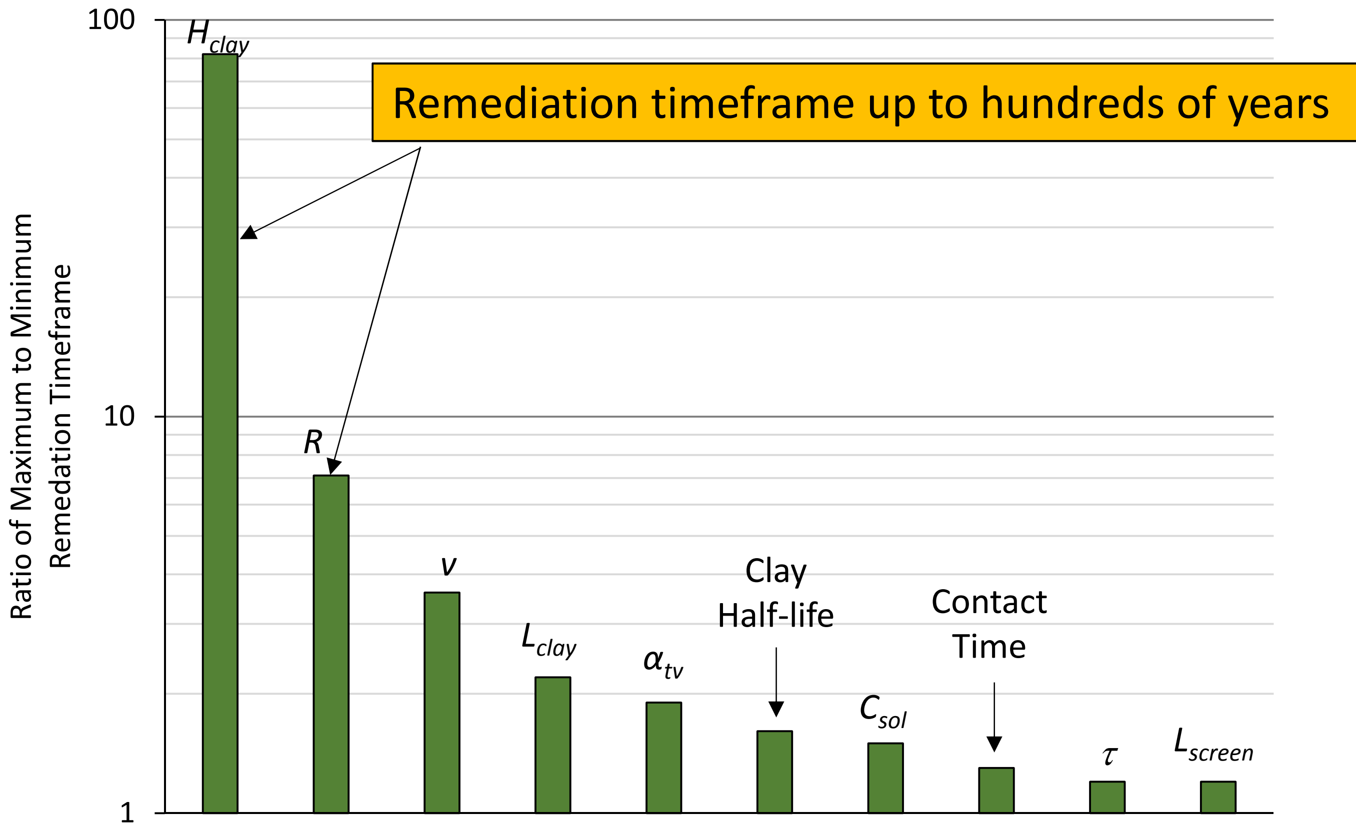
Carey et al. (2015)

Remediation Timeframe Sensitivity Analysis



H_{clay} = silt/clay layer thickness

R = retardation coefficient

v = groundwater velocity

L_{clay} = silt/clay layer length

α_{TV} = transverse dispersivity

Half-life → biodegradation

C_{sol} = solubility

Contact time – between NAPL and silt/clay

τ = tortuosity coefficient

L_{screen} = well screen length

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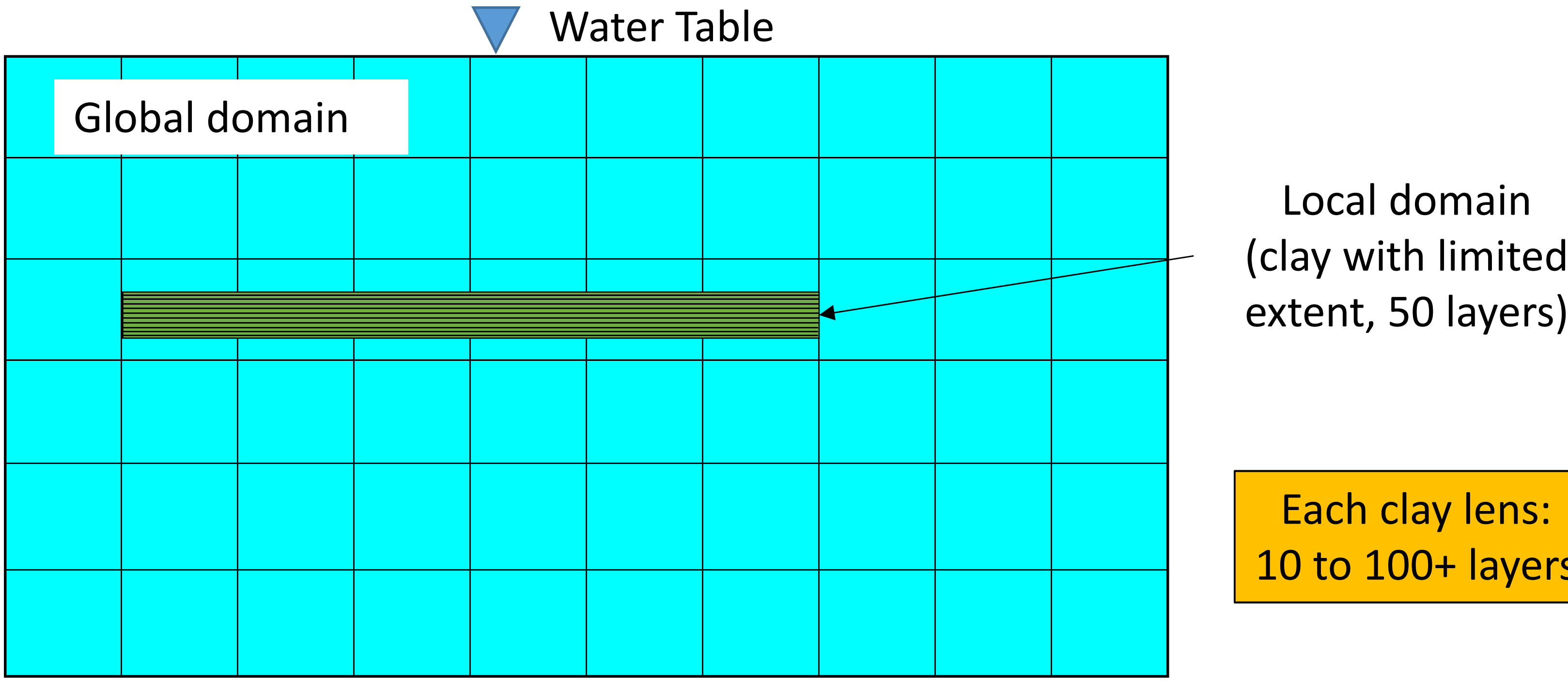
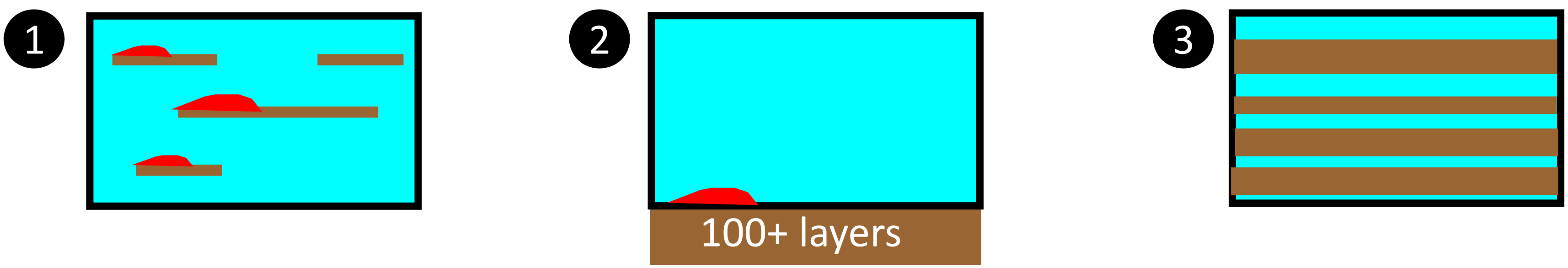
Carey et al. (2015)

Local Domain Approach



Each clay lens:
10 to 100+ layers



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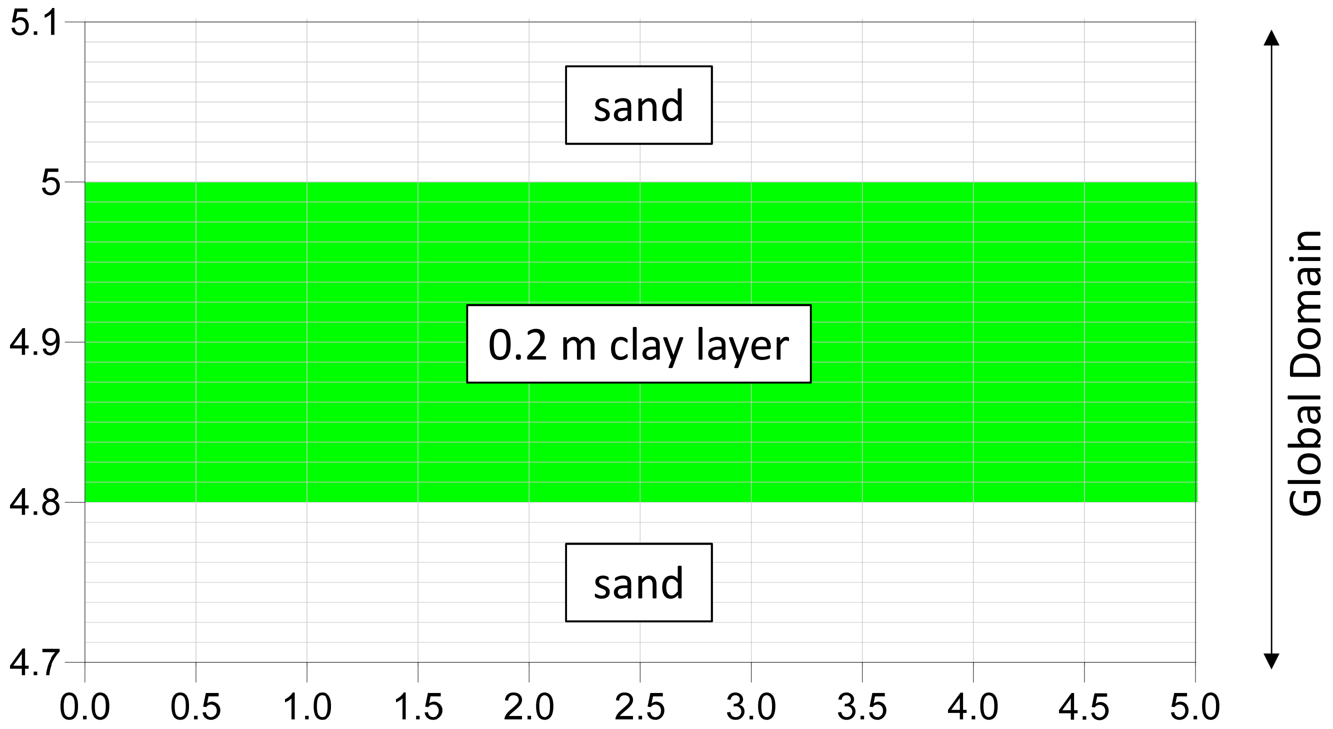
Local Domain Approach

1. Global domain section (example)



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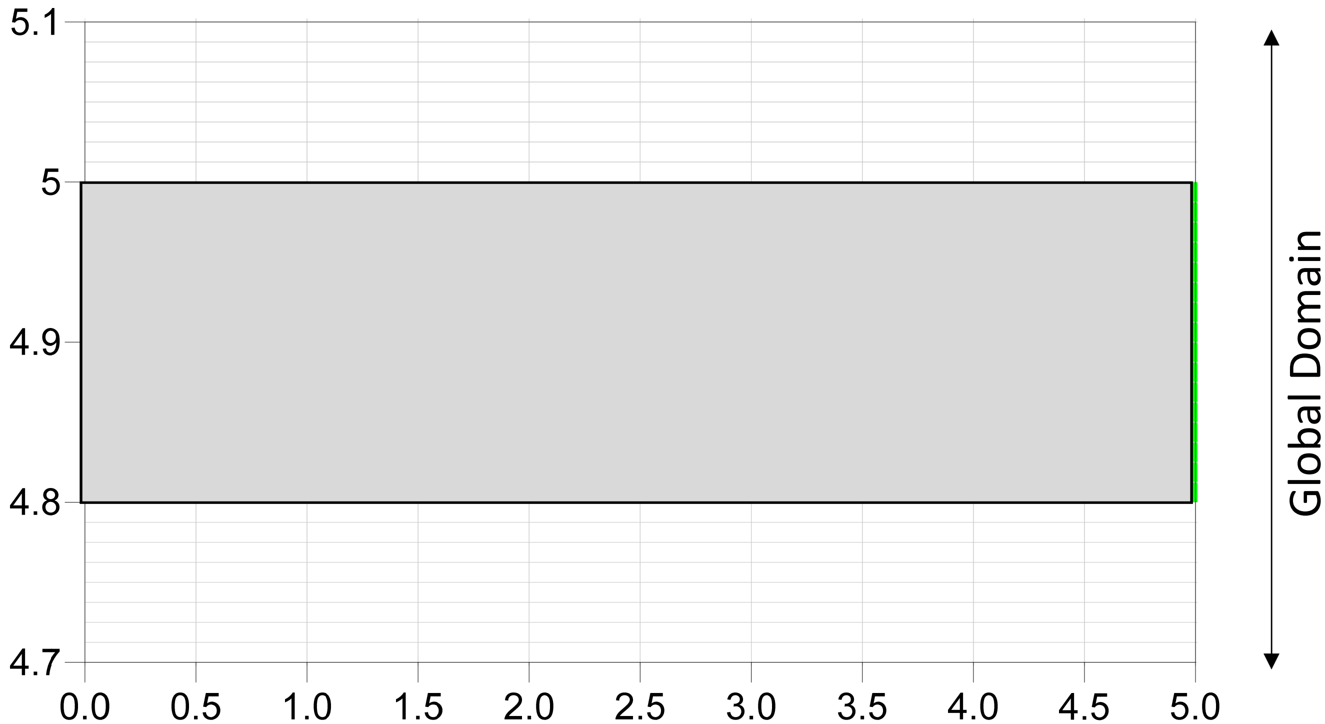
Local Domain Approach

2. Inactive transport in clay zone, in global domain.



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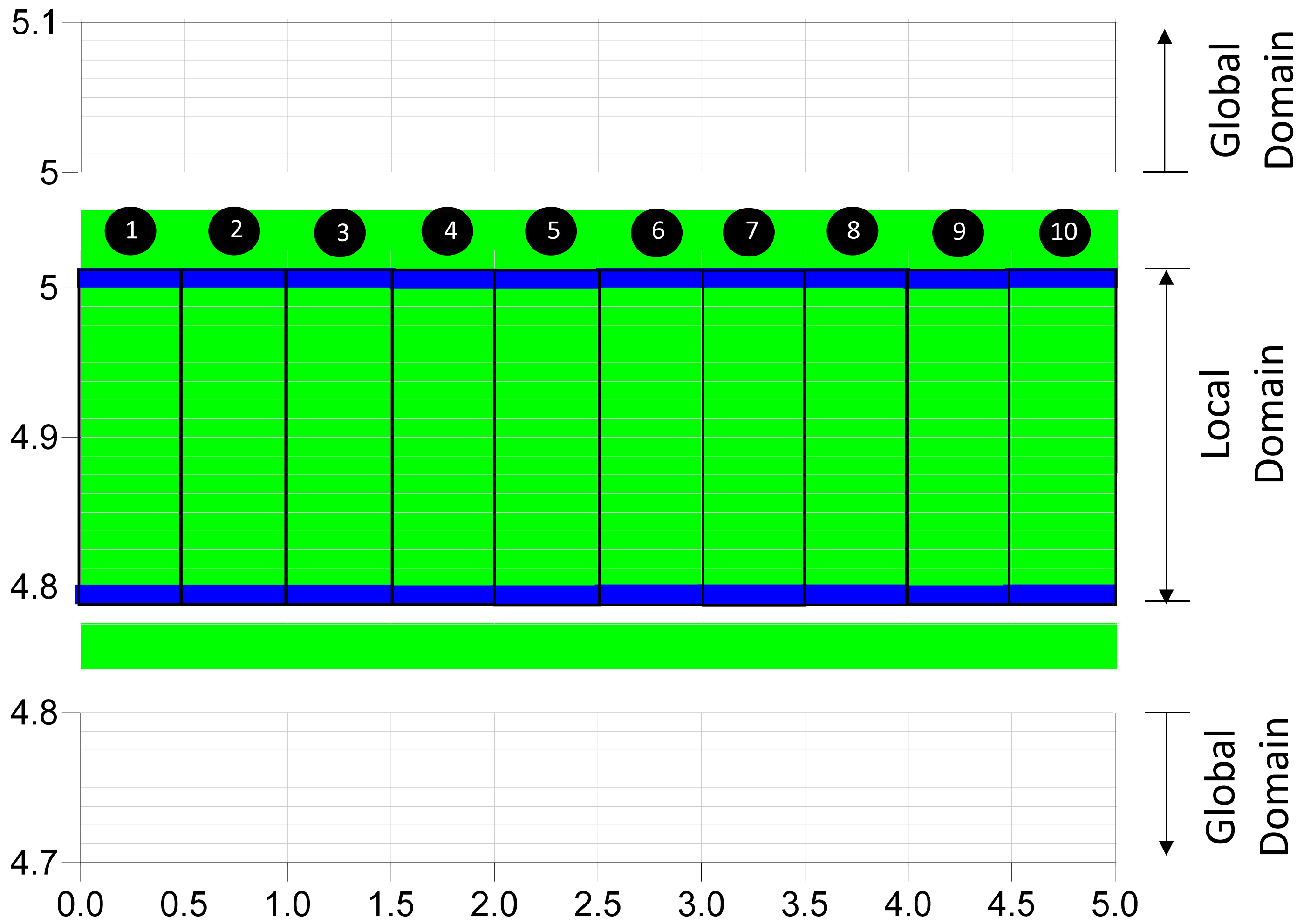
Local Domain Approach

3. Insert 200 local domains (Δx = 0.5 m, Δz = 1.25 cm).



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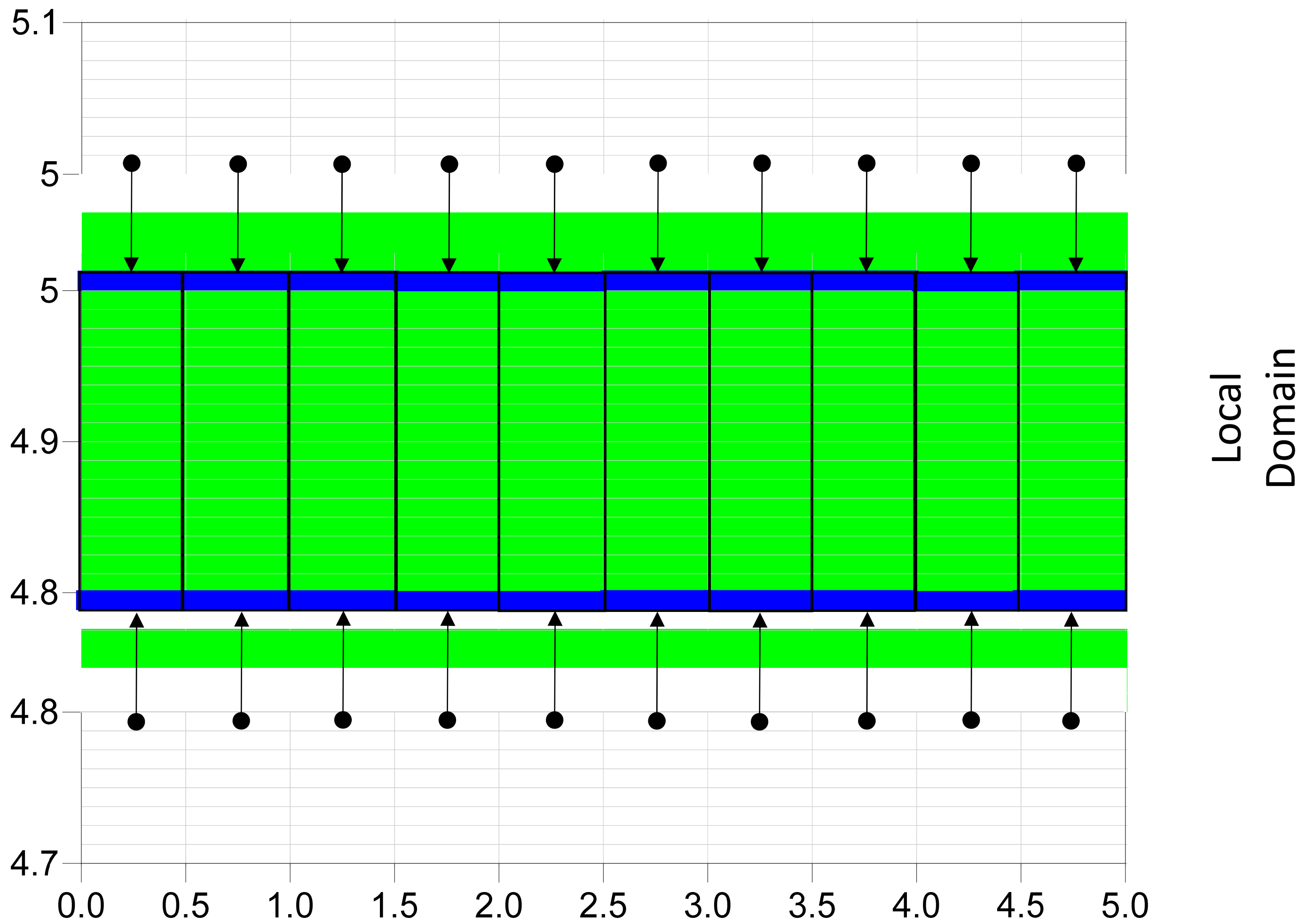
Local Domain Approach

4. Associate global domain conc. with local domain boundaries.



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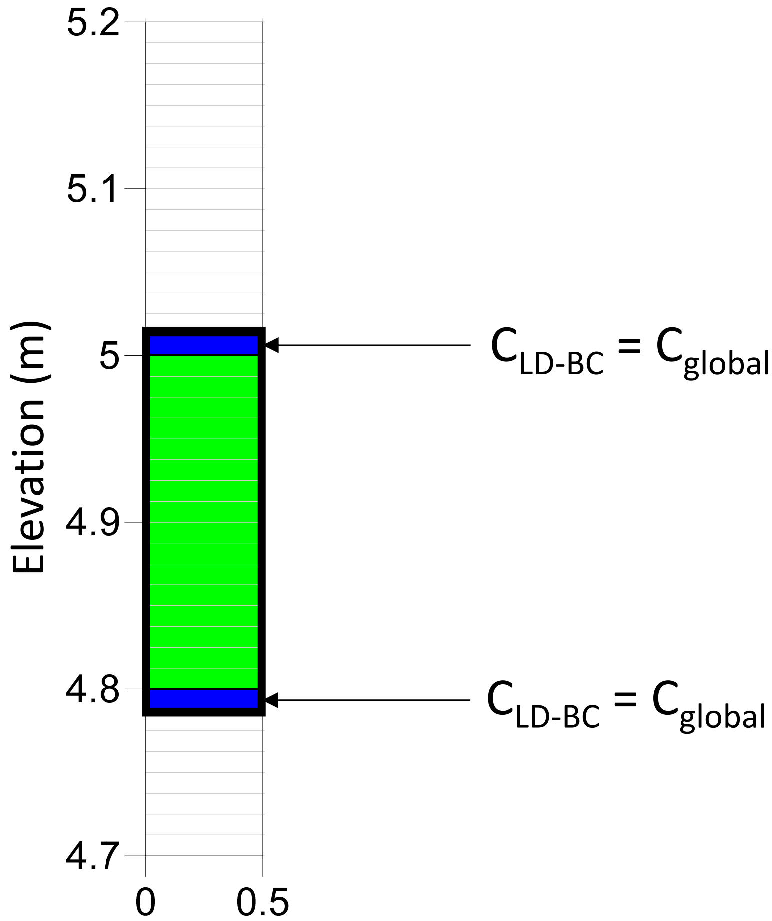
Local Domain Boundary Condition



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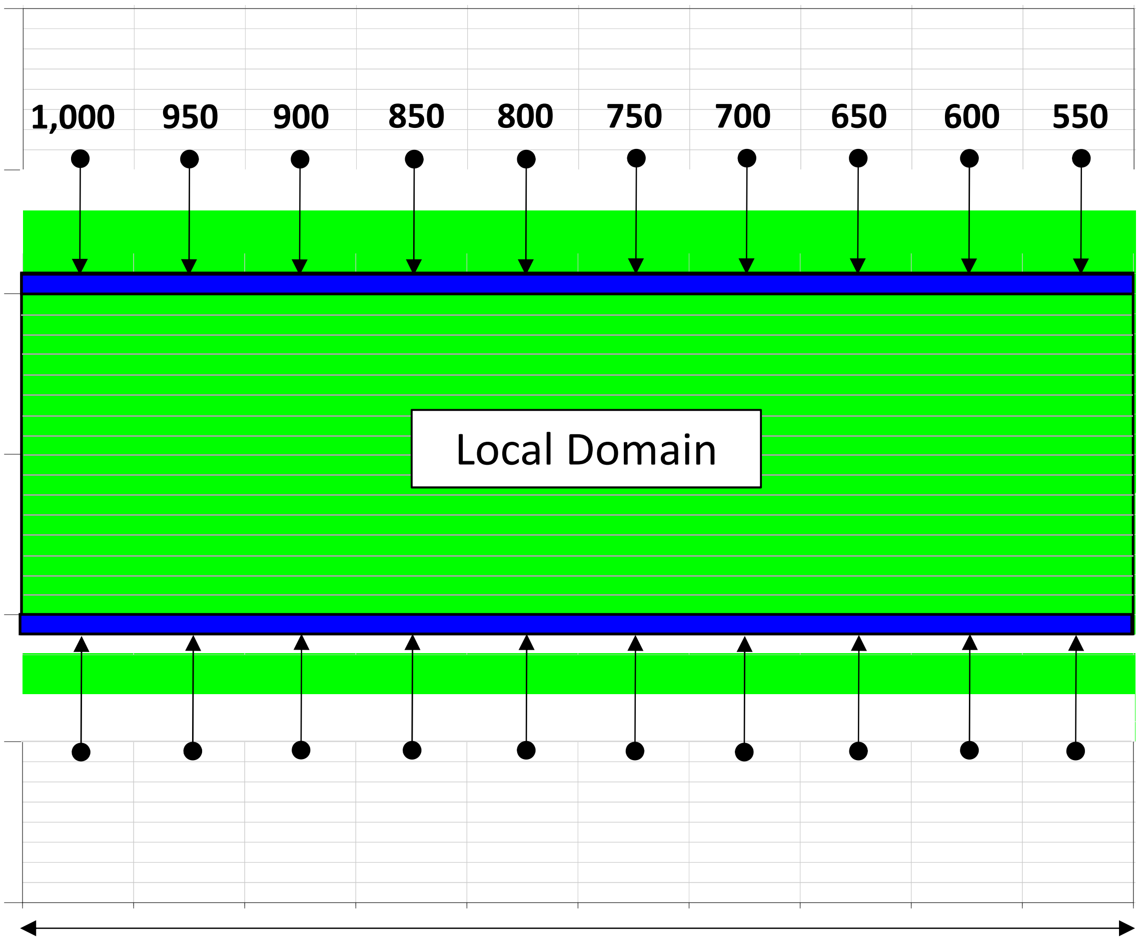
Example Scenario A

Local domain has larger horizontal grid spacing.

Example C:

Avg. C=775



Global model

Global model

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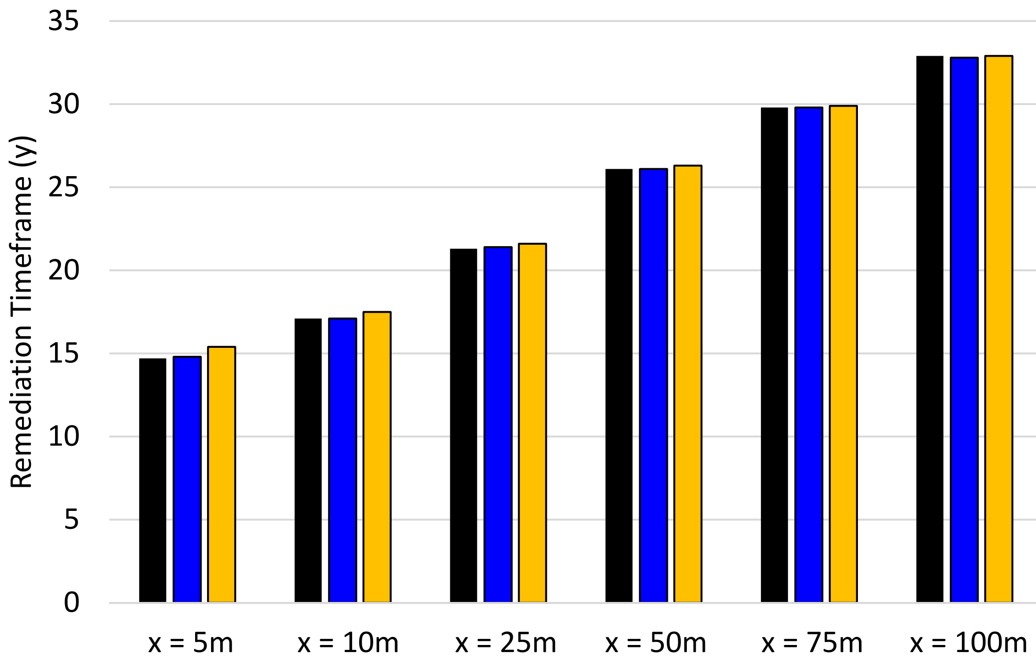
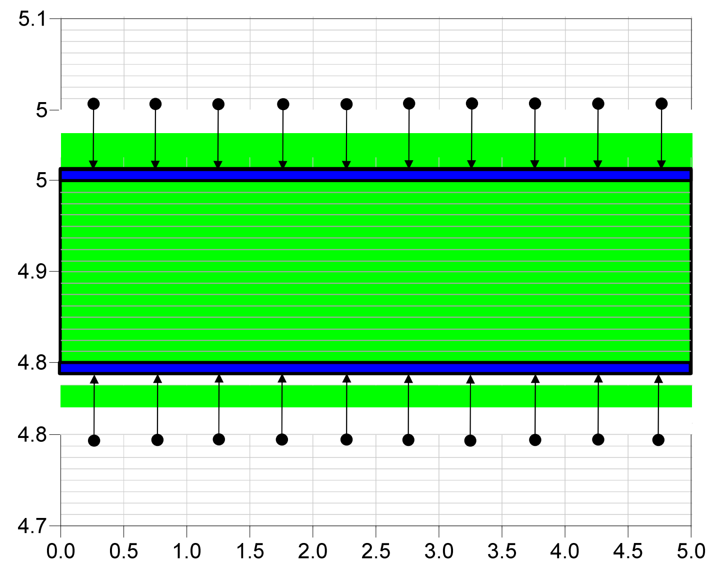
Local Domain Discretization

Mass balance = 0.04% | Mass balance = 0.04% | Mass balance = 0.07%

No Local domains | 200 Local domains $\Delta x = 0.5$ m | 20 Local domains



20 Local domains, $\Delta x = 5$ m



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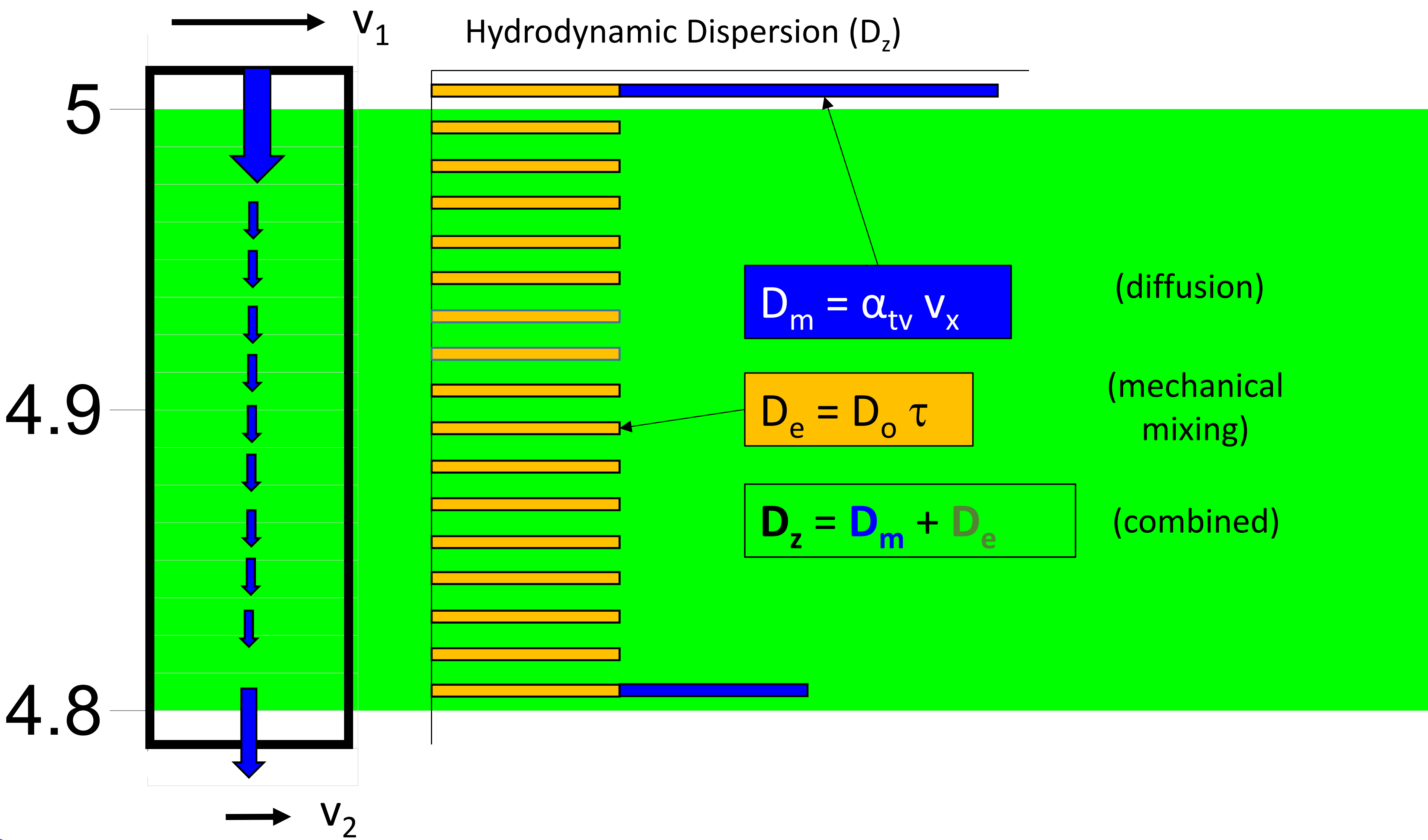
Vertical Dispersion at Sand-Clay Interface



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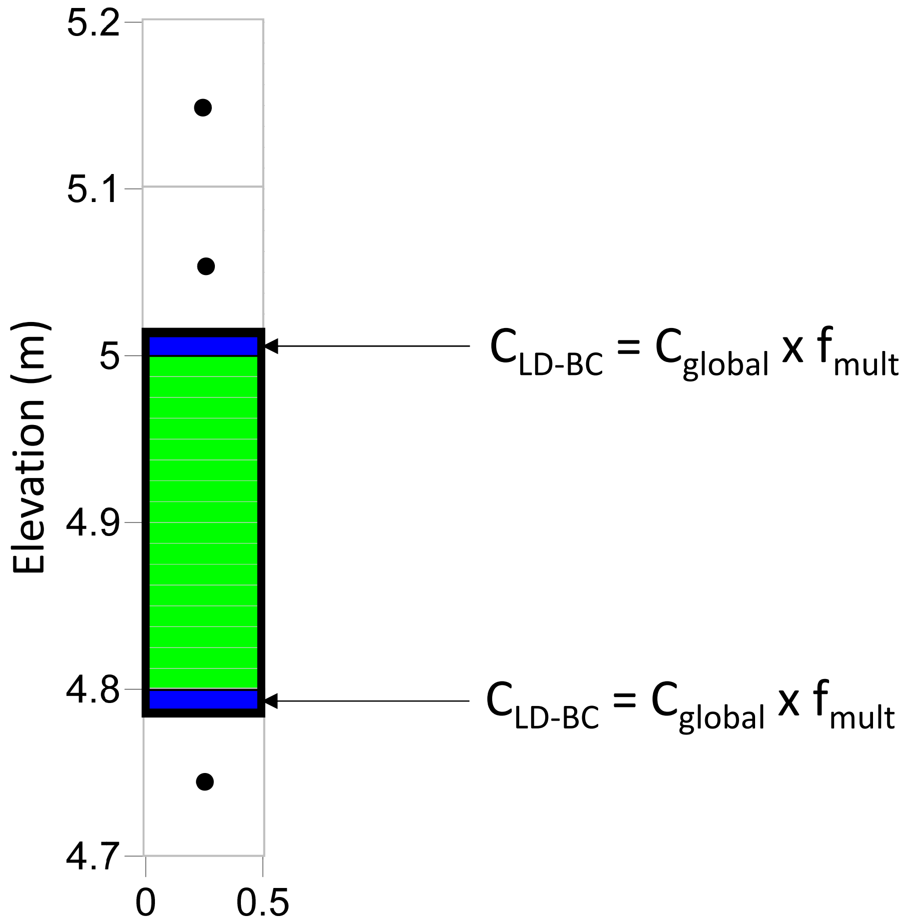
Example Scenario B

Global domain has larger vertical grid spacing.



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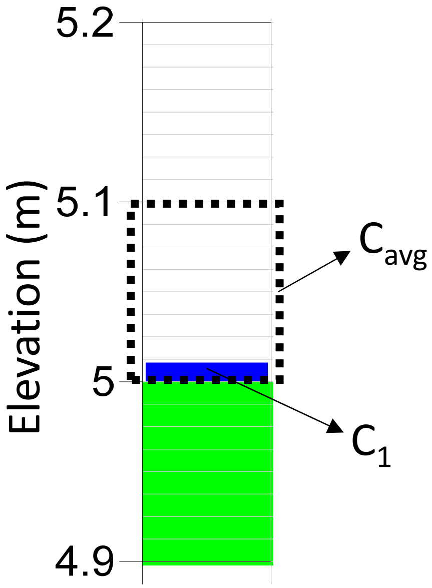
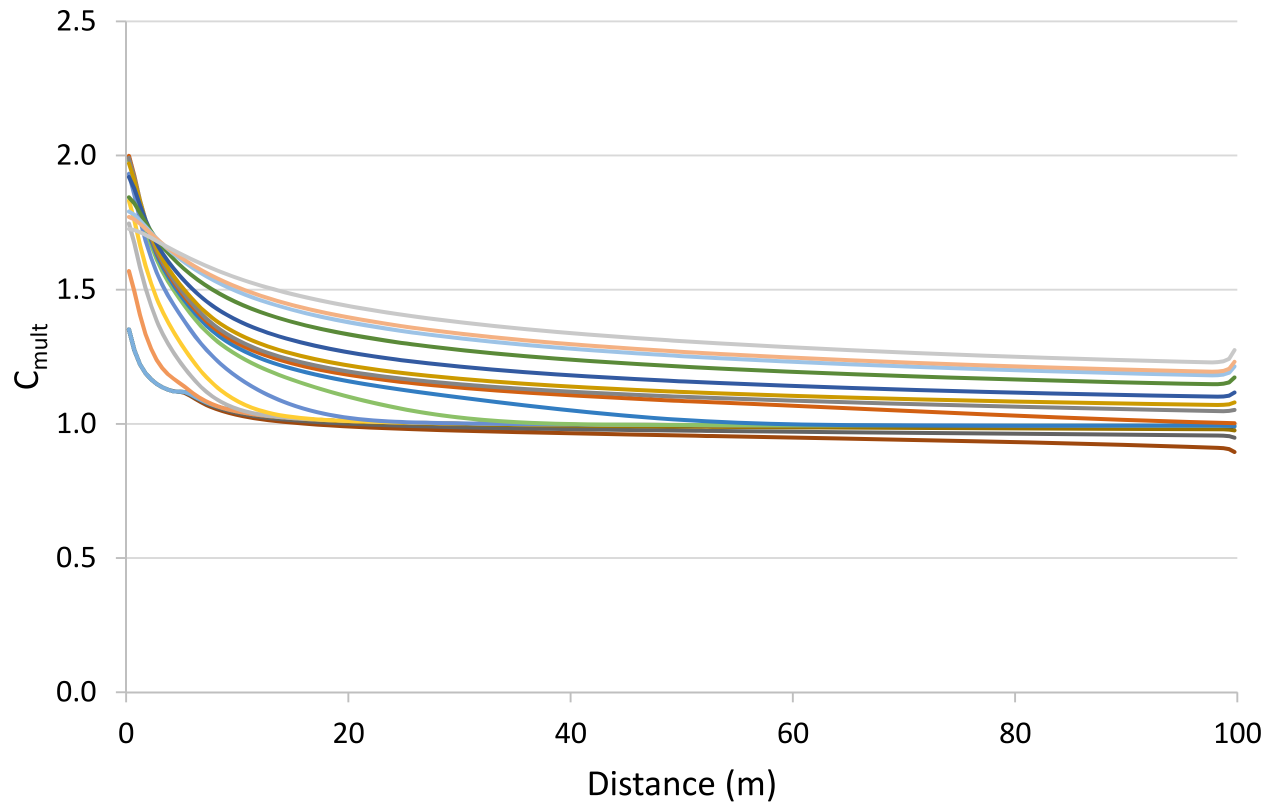
f_{mult} Trends (t = 3 to 85 y)



$f_{mult} = C_1 / C_{avg}$

(travel time from source to d/g boundary ~ 2.5 years)



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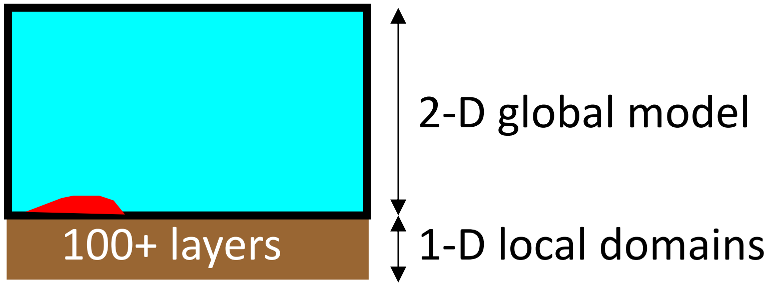
Next Steps

- Sensitivity of f_{mult} to:
  - Concentration
  - Site characteristics
  - Time
- Scenarios where global vertical discretization can be coarsened using local domains and f_{mult} *(x,t)*
  - Forward diffusion
  - Back-diffusion



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Questions?

Grant Carey, Ph.D.
Porewater Solutions, and Adjunct Professor at University of Toronto

613-270-9458
gcarey@porewater.com
www.porewater.com

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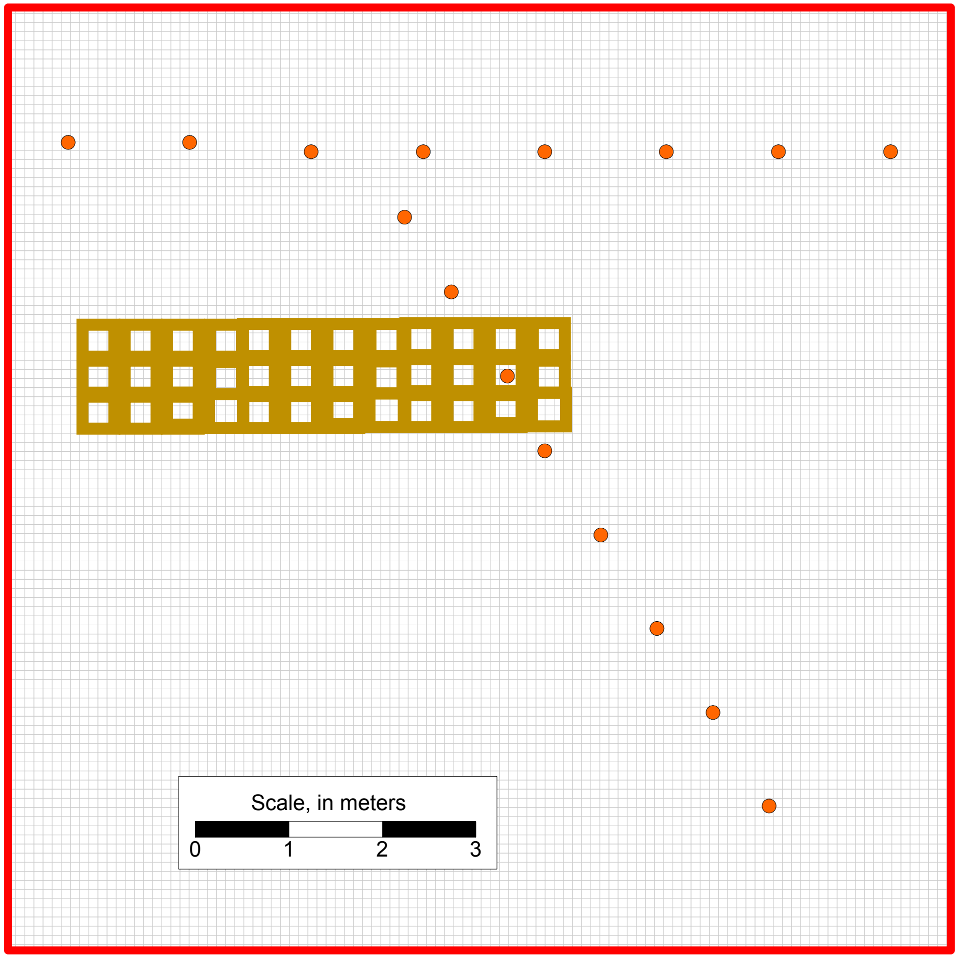
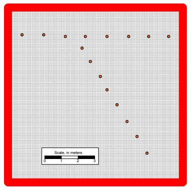
Back-Up Slides

Example Application

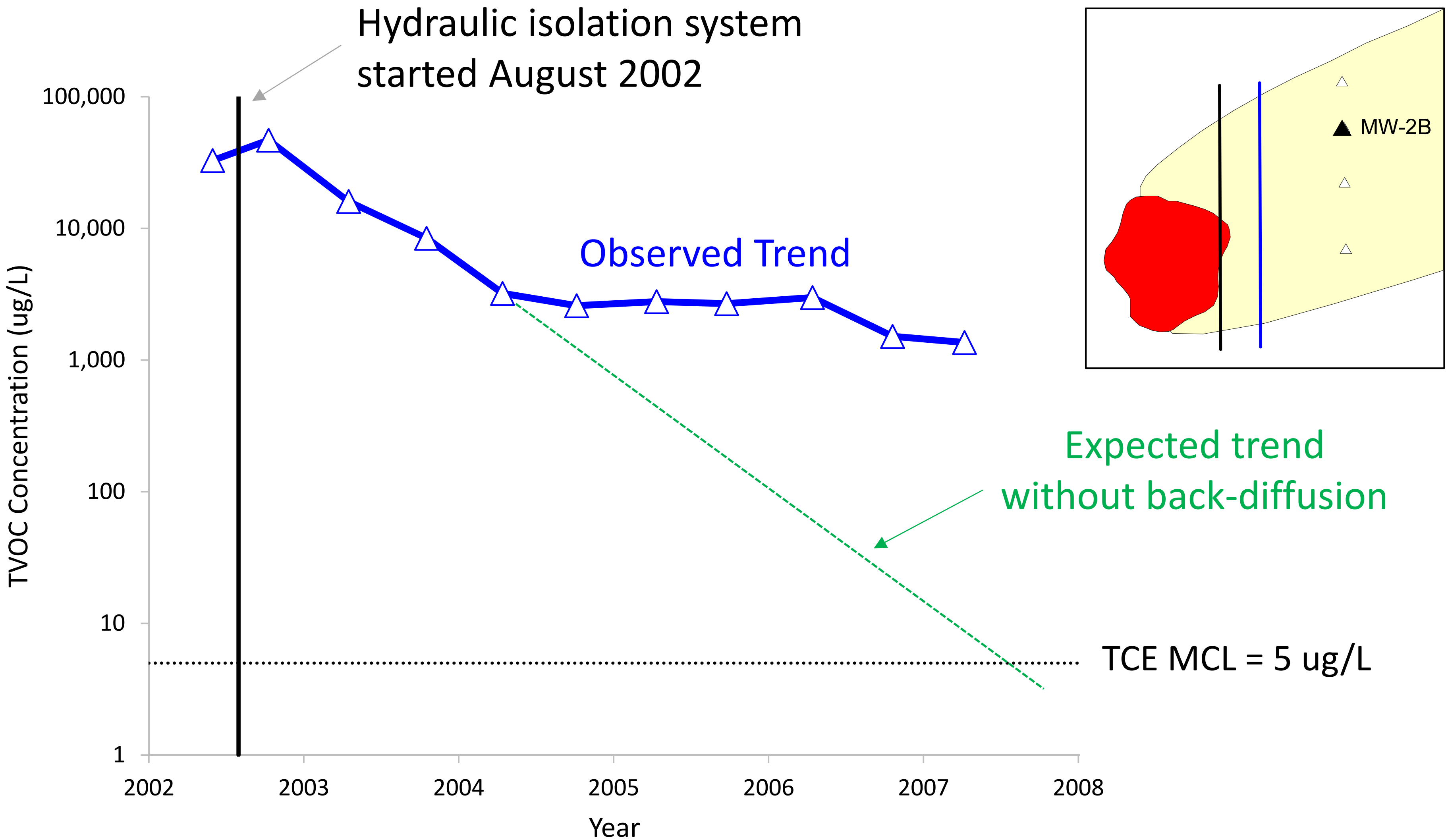




Global domain

Local domain

TVOC Trend After Source Containment



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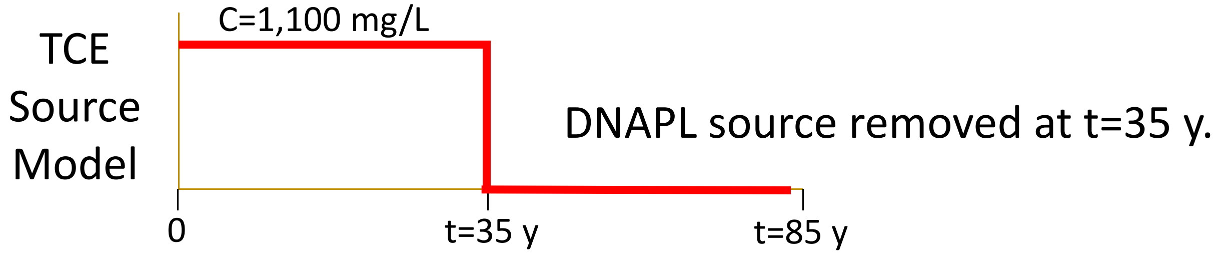
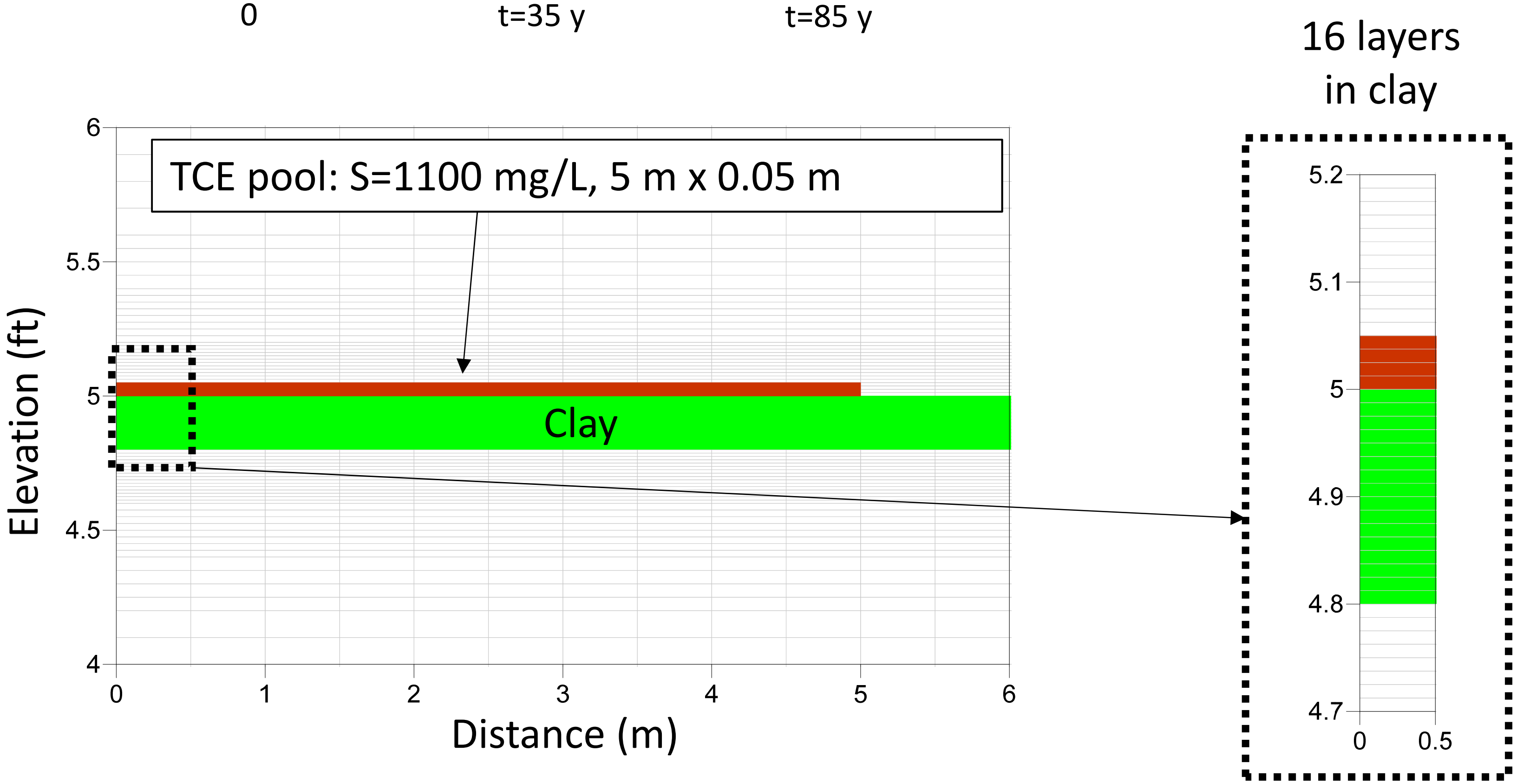
Carey et al. (2015)

Source Characteristics





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Carey et al. (2015)

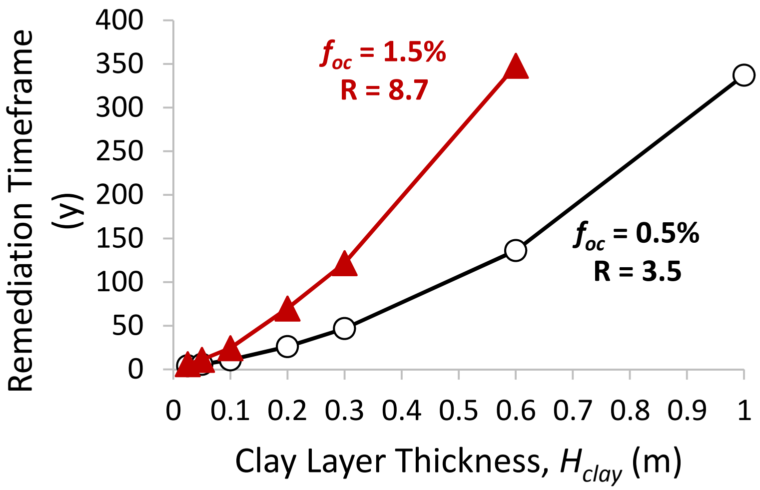
Remediation Timeframe Sensitivity Analysis

x = 50 m

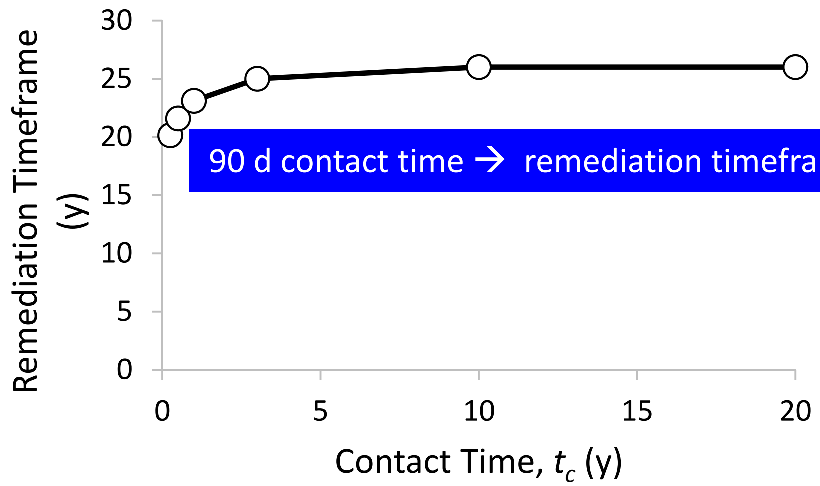
L_{screen} = 3 m

H_{clay} = 0.2 m

Clay layer thickness and f_{oc}



Contact time (DNAPL and clay)



90 d contact time → remediation timeframe = 20 y

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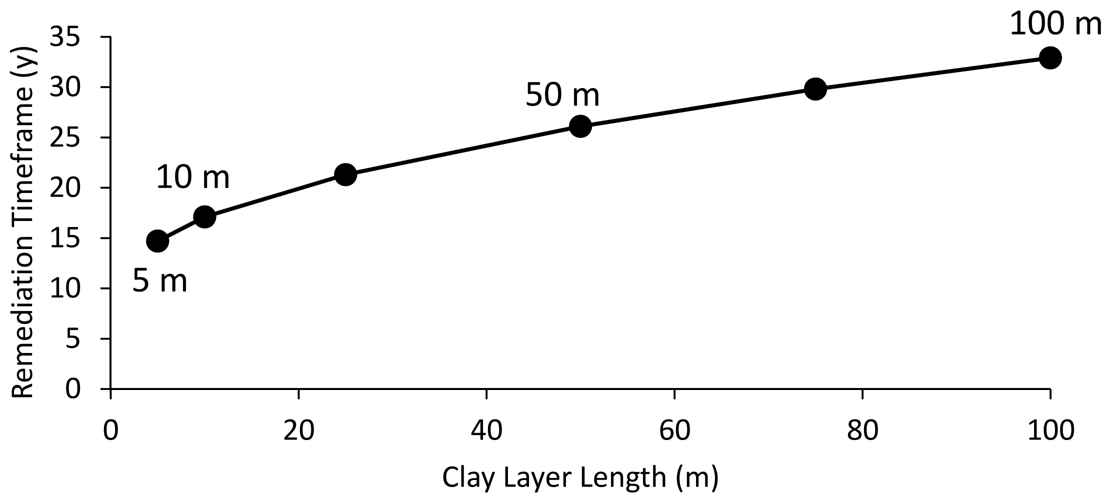
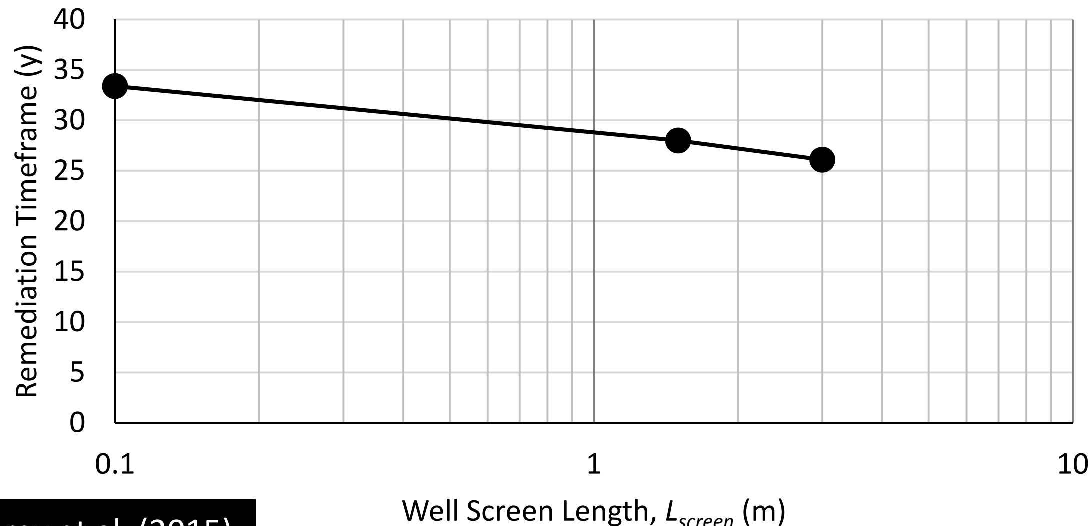
Remediation Timeframe Sensitivity Analysis

(a) RTF vs. clay length
(Well screen=3 m)



(b) RTF vs. screen length
(x = 50 m)



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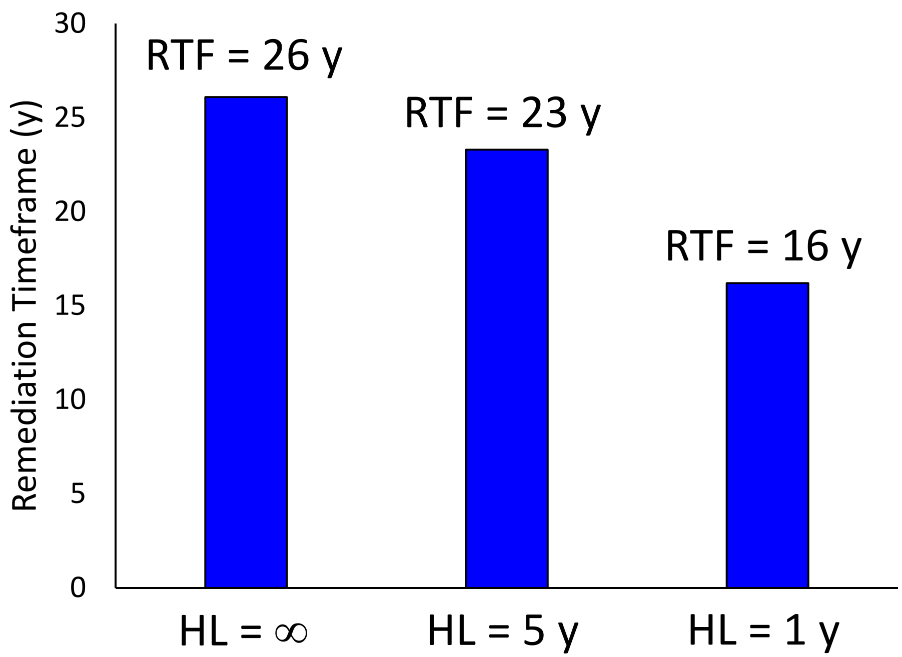
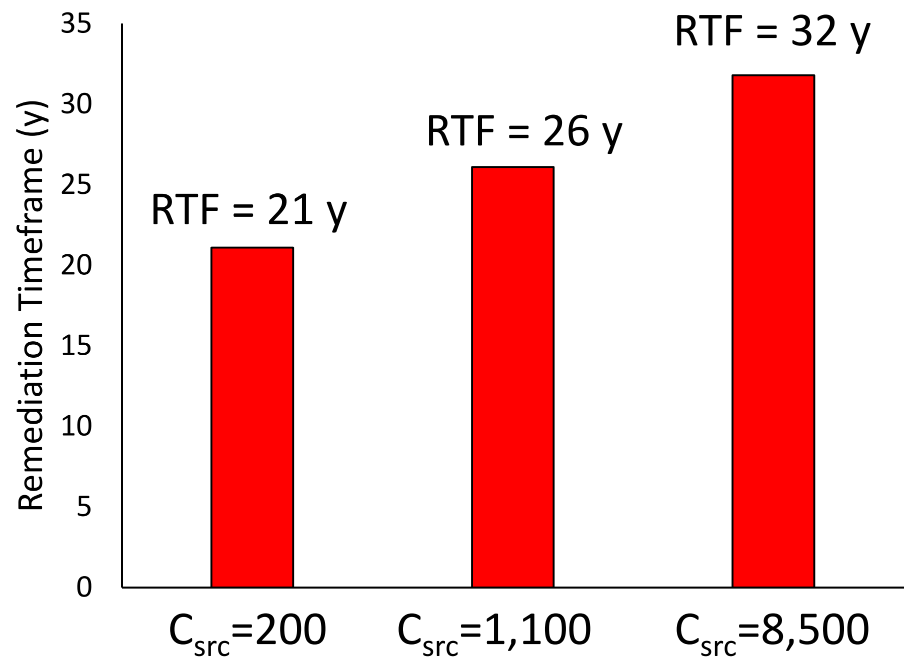
Remediation Timeframe Sensitivity Analysis

a) Biodegradation Half-life in Clay Layer



b) Source Concentration (mg/L)



Note: K_d uniform

Source conc. increase:	>4,000%
Timeframe increase:	50%

x = 50 m

L_{screen} = 3 m

H_{clay} = 0.2 m

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Carey et al. (2015)