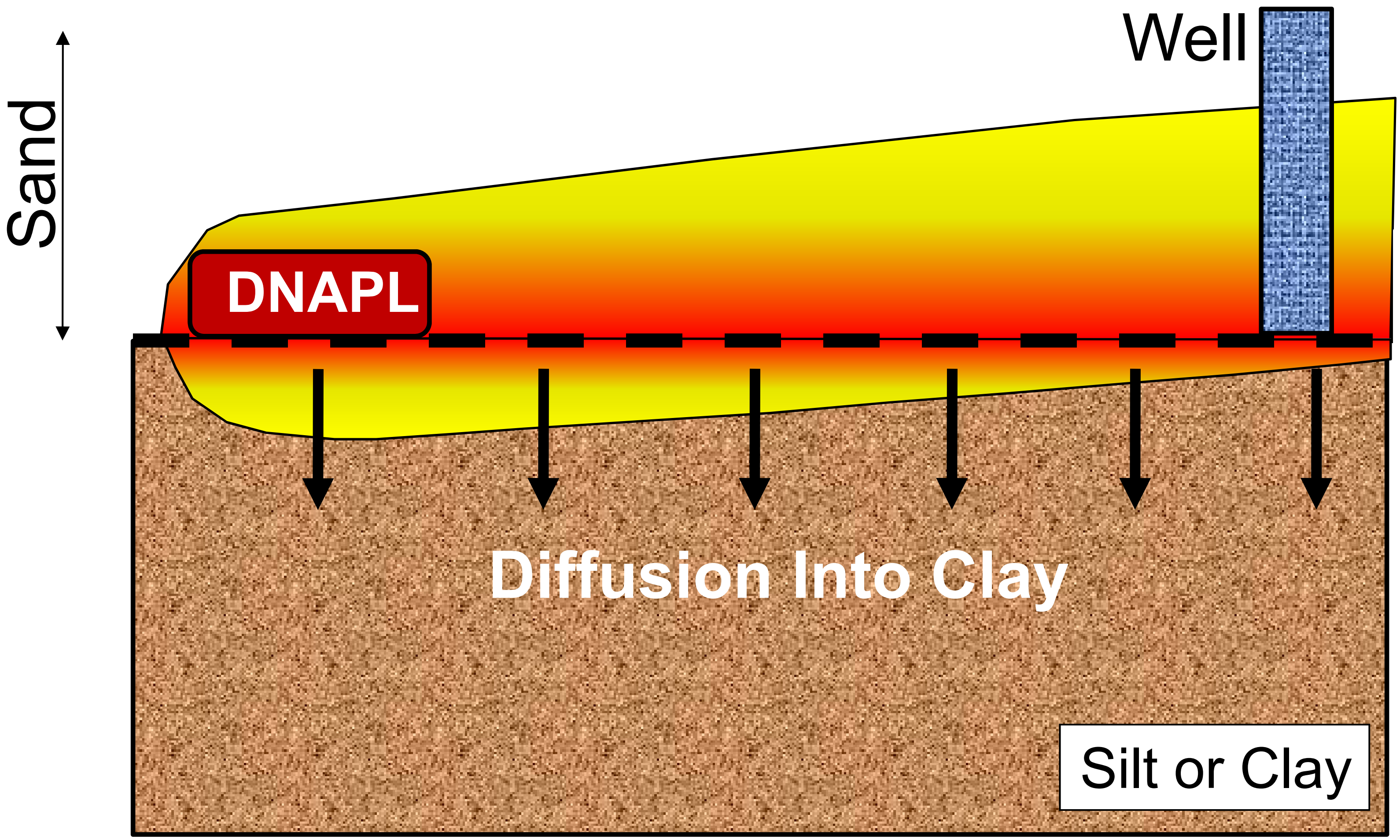
REMTEC
REMEDIATION TECHNOLOGY SUMMIT
THE FUTURE OF REMEDIATION TECHNOLOGY

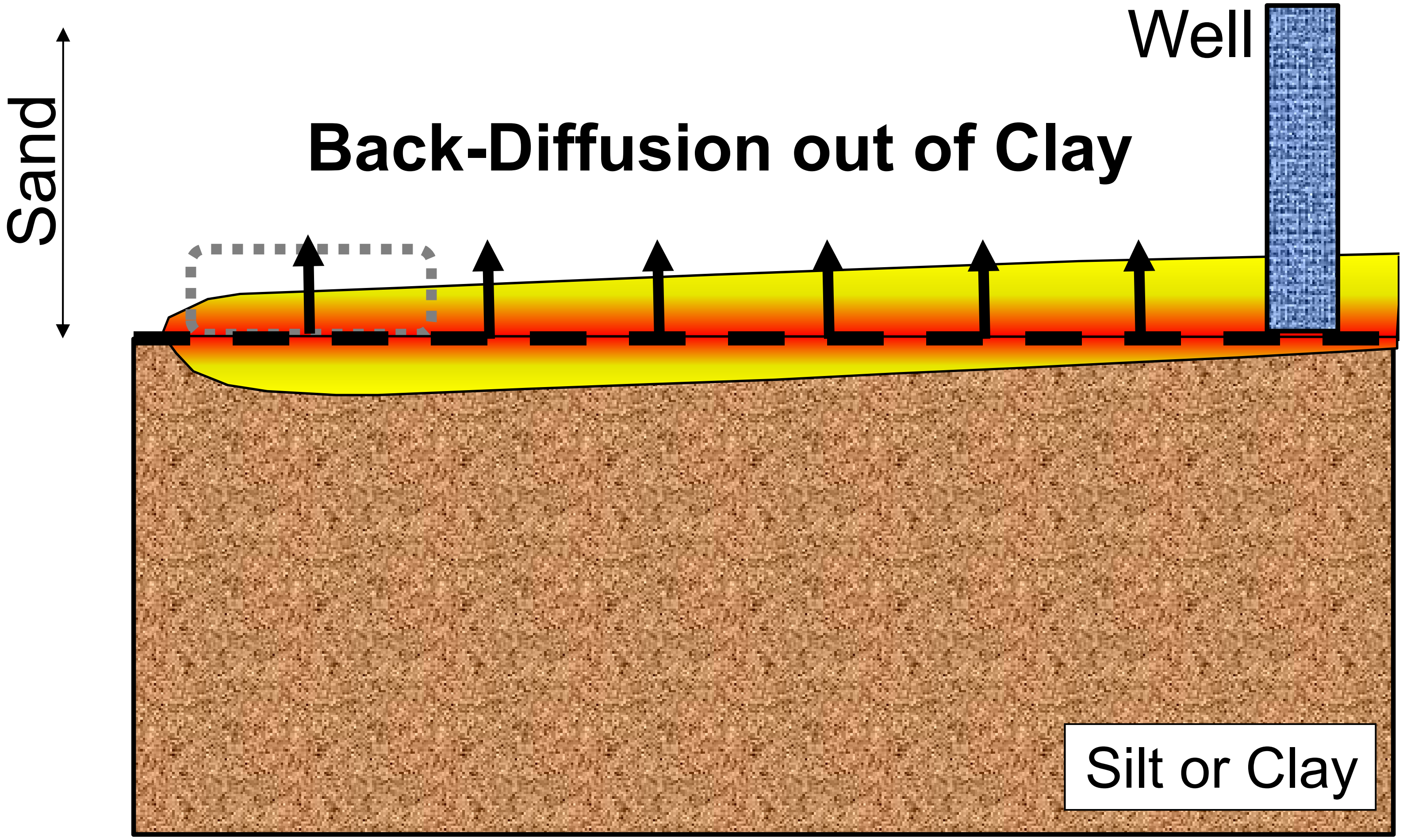
ISR-MT3DMS for Modeling Back-Diffusion Timeframe

Grant R. Carey
President
Porewater Solutions

Forward Diffusion



Back-Diffusion



Remediation Timeframe?

Influencing factors:

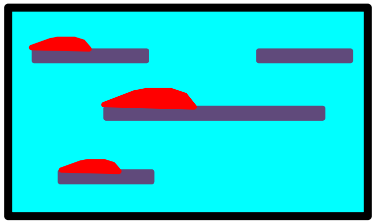
- Velocity
- Thickness
- Retardation
- Diffusion rate
- Transverse dispersion
- Length of clay lens
- Biodegradation
- Contact time

THICK silt/clay:

- Sale et al., 2008
- Matrix Diffusion ToolKit (ESTCP, www.gsi-net.com)

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: new approach

Introduction

- **Case Study #1** – Model limitations
- **ISR-MT3DMS** overview
- **Case Study #2** – Florida site (thin clay)
  - Model input estimation
  - ISR-MT3DMS proof of concept, verification
  - Timeframe sensitivity analysis

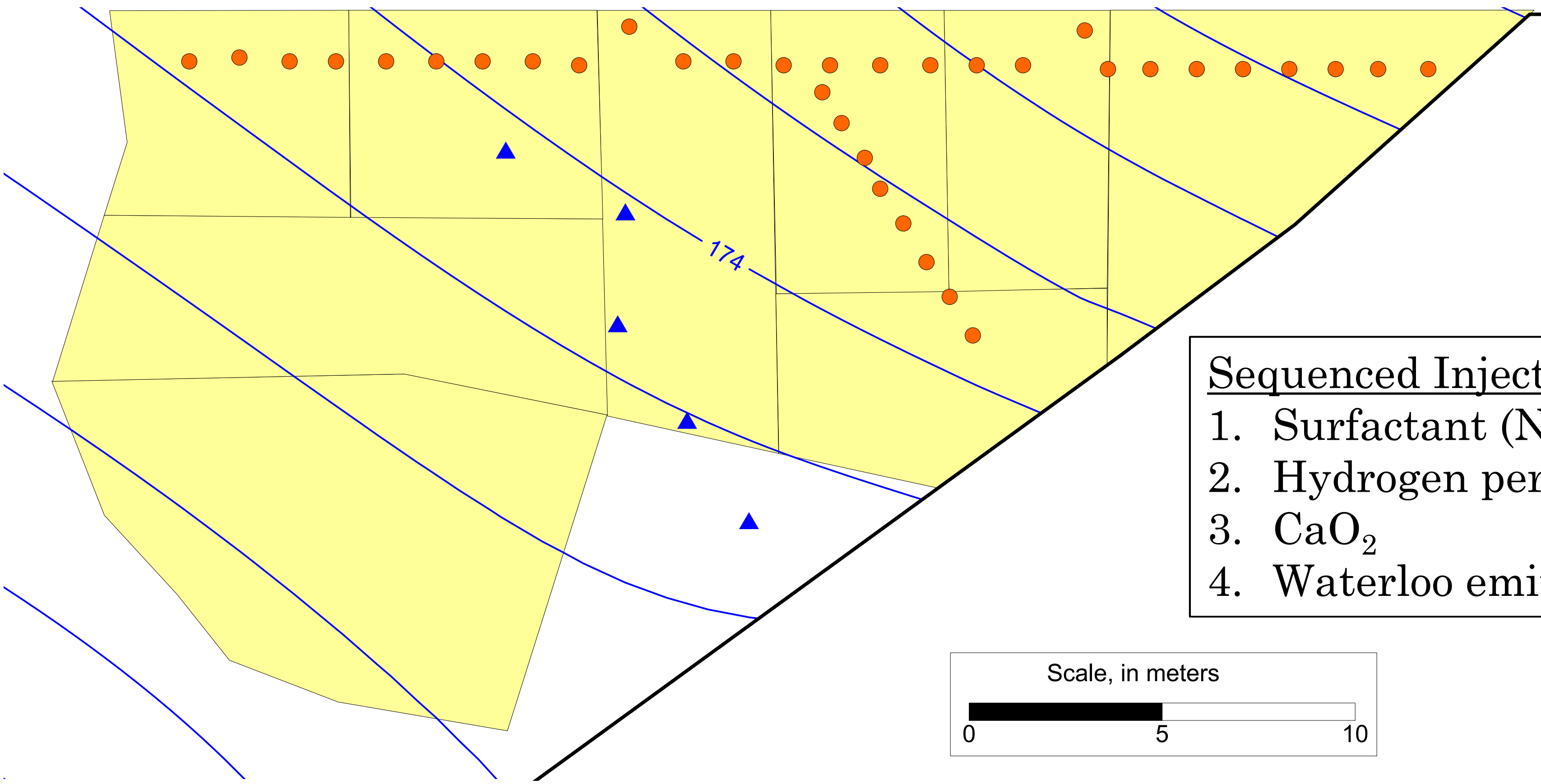
Case Study #1 – Ontario Site

Acknowledgement:

Rick McGregor, President
InSitu Remediation Services Limited

rickm@IRSL.ca

Case Study #1 – Ontario Site



Sequenced Injections:

1. Surfactant (NAPL)
2. Hydrogen peroxide
3. CaO_2
4. Waterloo emitters

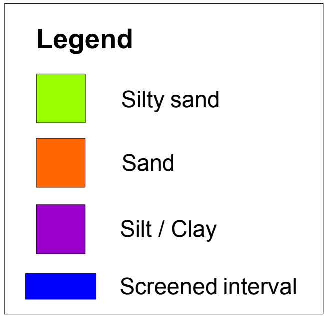
Treatment zone

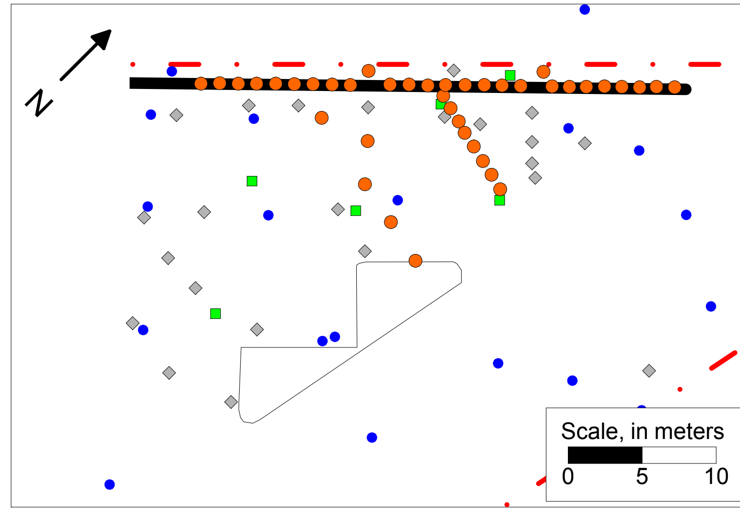
Groundwater elevation contour

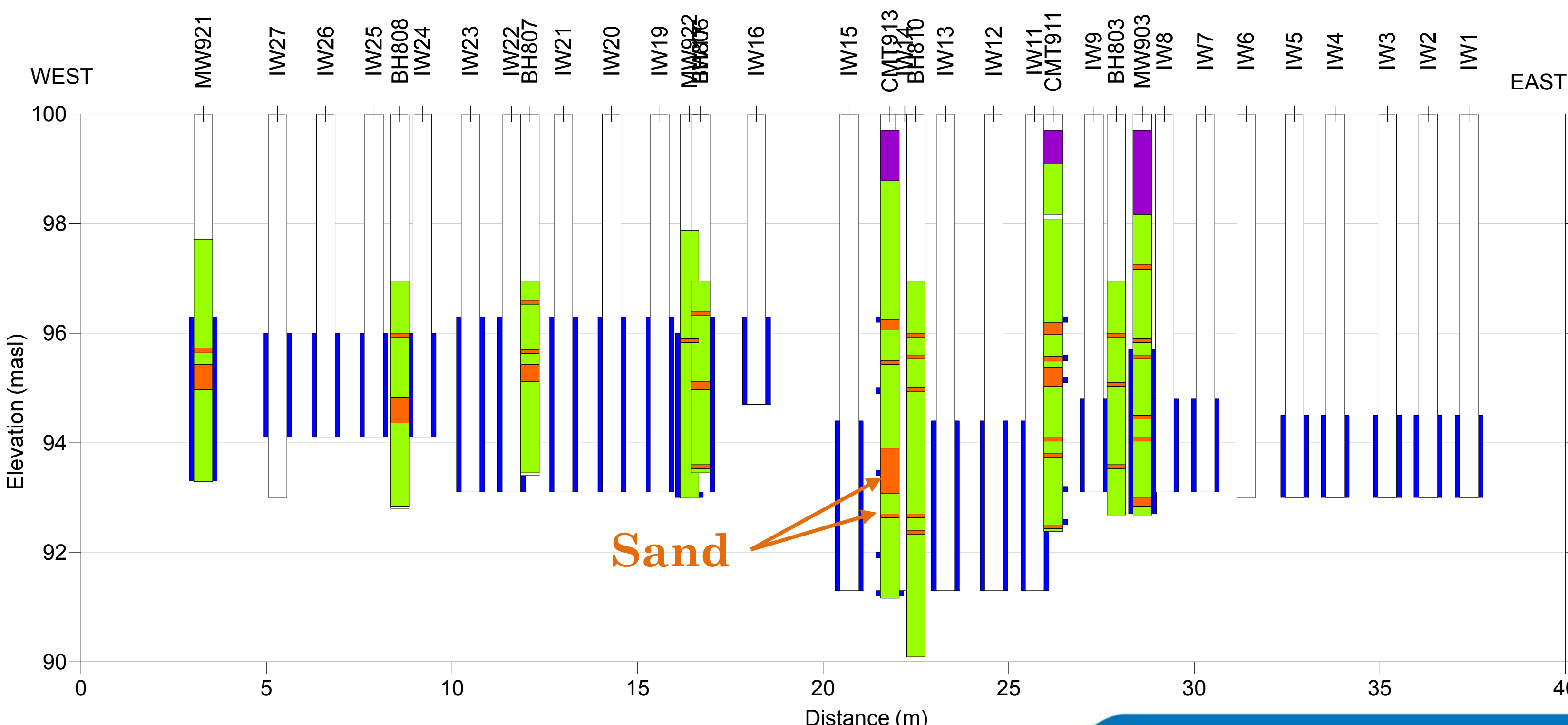
Waterloo Emitter

Other injection well

Section K-K'


Legend
Silty sand
Sand
Silt / Clay
Screened interval


N
Scale, in meters
0
5
10


WEST
EAST
MW921
IW27
IW26
IW25
BH808
IW24
IW23
IW22
BH807
IW21
IW20
IW19
IW16
IW15
BH810
IW13
IW12
IW11
CMT911
IW9
BH803
MW903
IW8
IW7
IW6
IW5
IW4
IW3
IW2
IW1
Elevation (masl)
Distance (m)
Sand
100
98
96
94
92
90
0
5
10
15
20
25
30
35
40

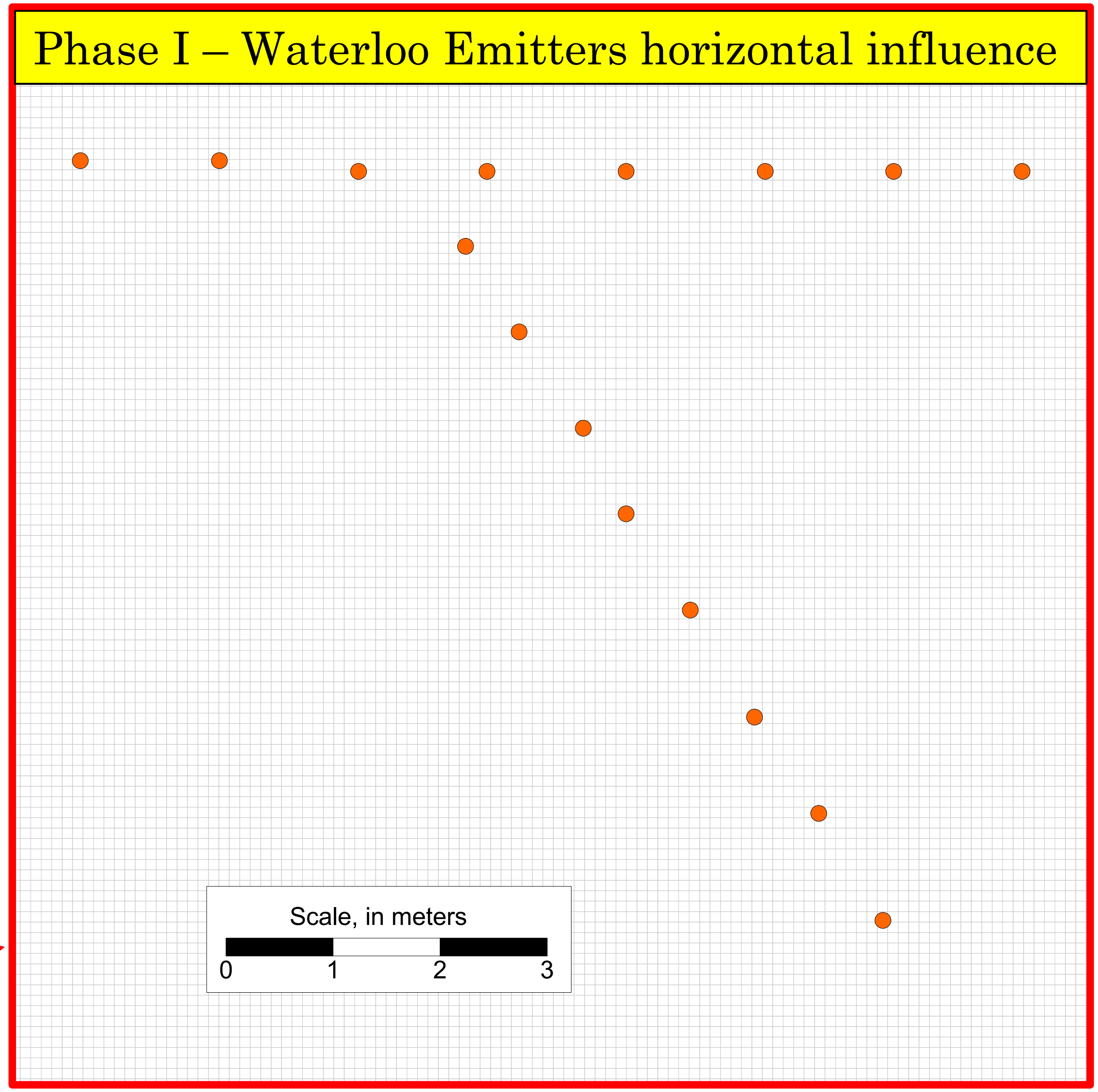
Model Grid

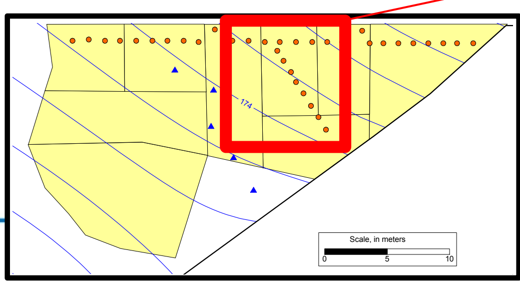
Minimum spacing = 4 inches (Waterloo Emitter diameter)

2-D: 450 columns, 280 rows

Time step = 0.05 d

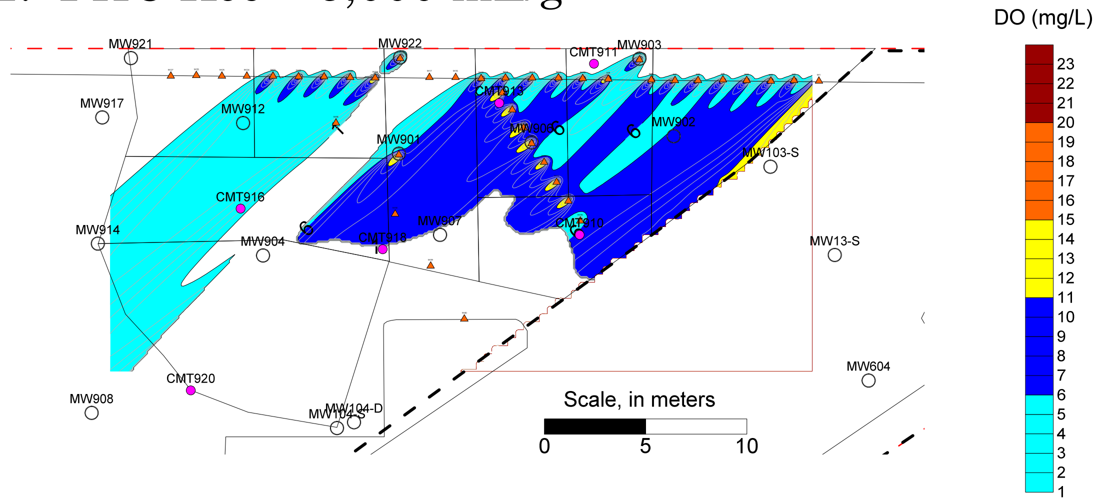
Phase I – 5 solutes (4-hour run-time)



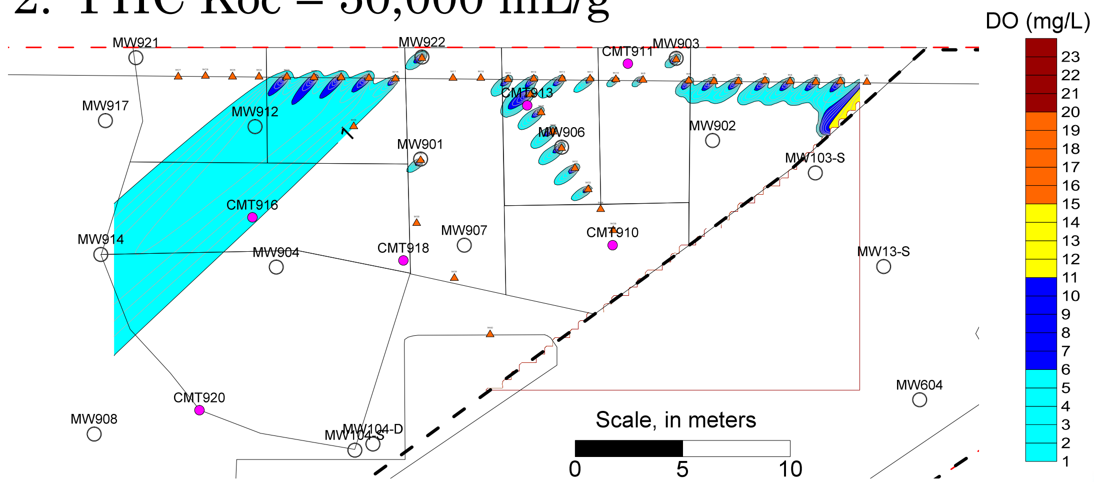


Phase I: Waterloo Emitters (t=3y)

Case 1: PHC Koc = 5,000 mL/g



Case 2: PHC Koc = 50,000 mL/g



Electron Donors:

- GRO, DRO, Fe(II)

Electron Acceptors:

- DO, $Fe(III)_s$

Reactions:

- Instantaneous or first-order
- Reductive dissolution

Phase II model:

- Hydrogen peroxide
- CaPO
- GRO/DRO Conc. ↓
- **Diffusion into silt**

In Situ Remediation (ISR-MT3DMS)

MT3DMS v5.3

Dr. Chunmiao Zheng

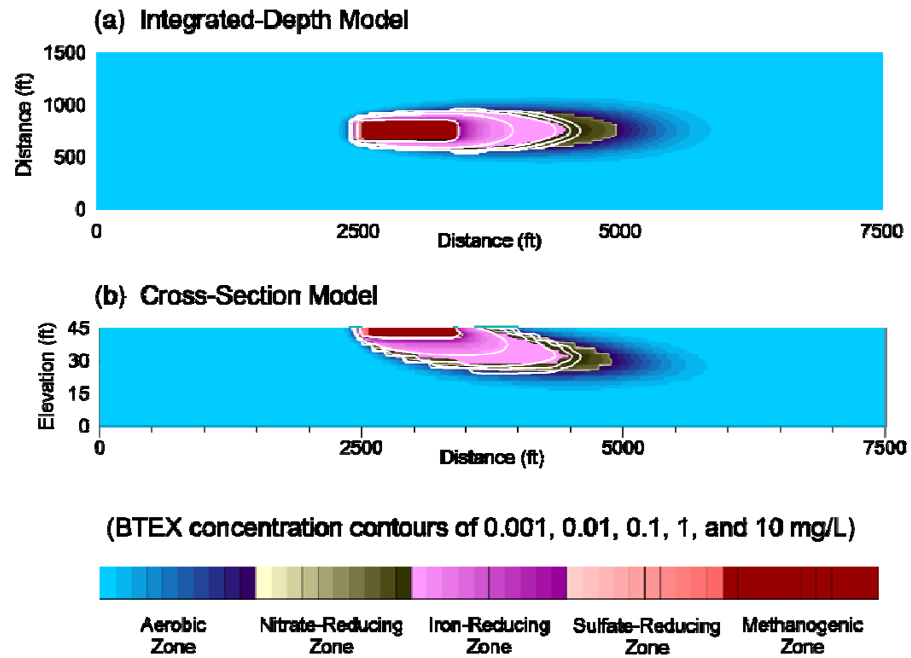
PUBLIC DOMAIN

Carey, Van Geel, and Murphy (1999)

In Situ Remediation (ISR-MT3DMS)

MT3DMS v5.3

BioRedox RCT package



- Flexible reaction framework
- Redox zone visualization
- Mineral precip./dissolution
- Rate stimulation/inhibition

Carey, Van Geel, and Murphy (1999)

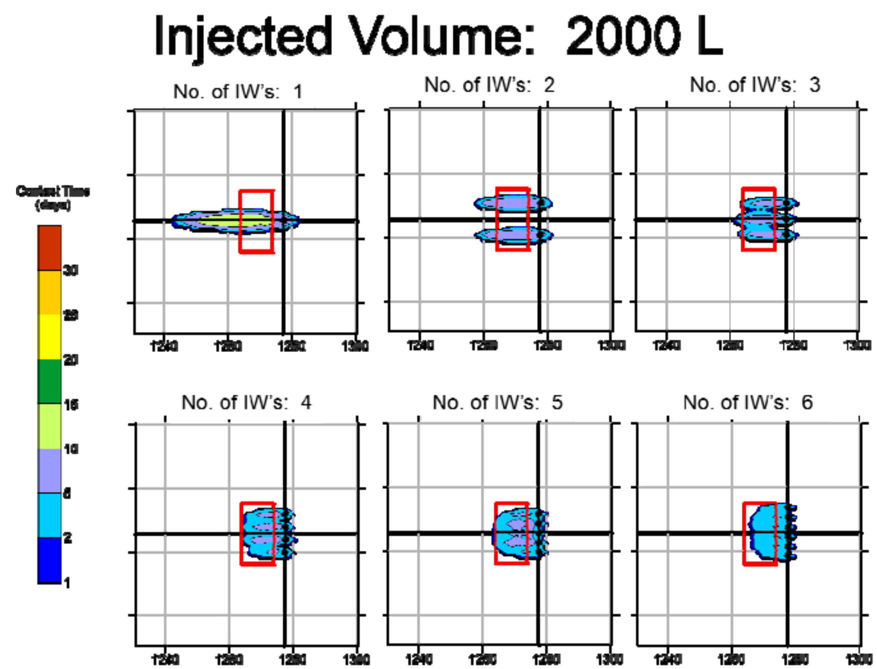
In Situ Remediation (ISR-MT3DMS)

MT3DMS v5.3

BioRedox RCT package

Contact Time Calculator

Optimization Metric



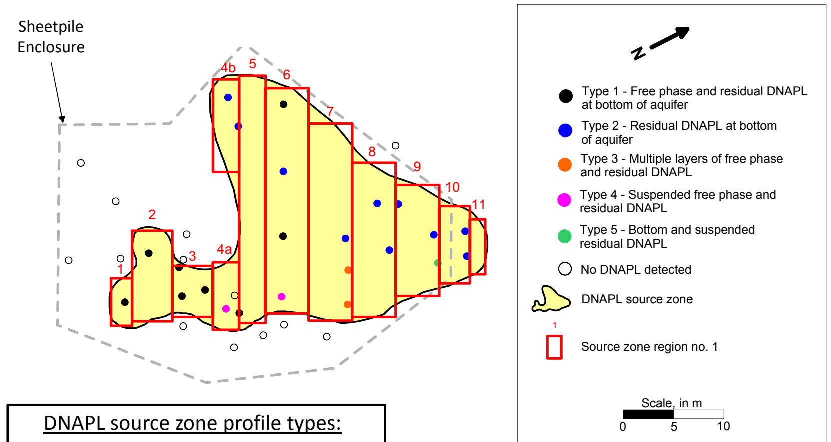
In Situ Remediation (ISR-MT3DMS)

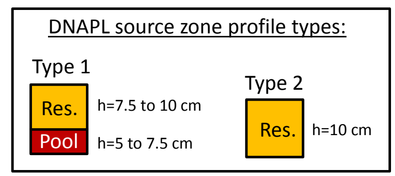
MT3DMS v5.3

BioRedox RCT package

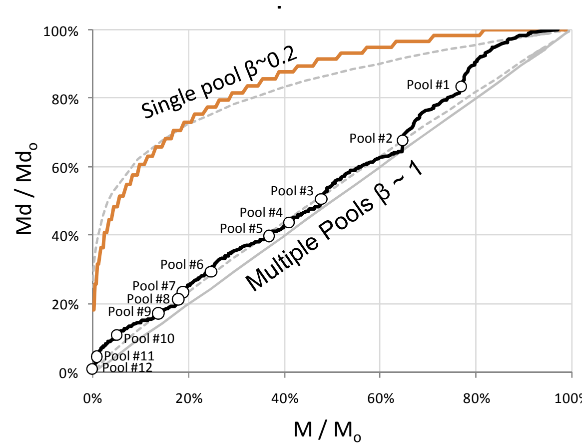
Contact Time Calculator

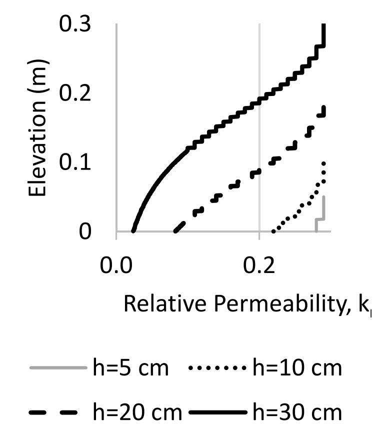
NAPL Depletion Model





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

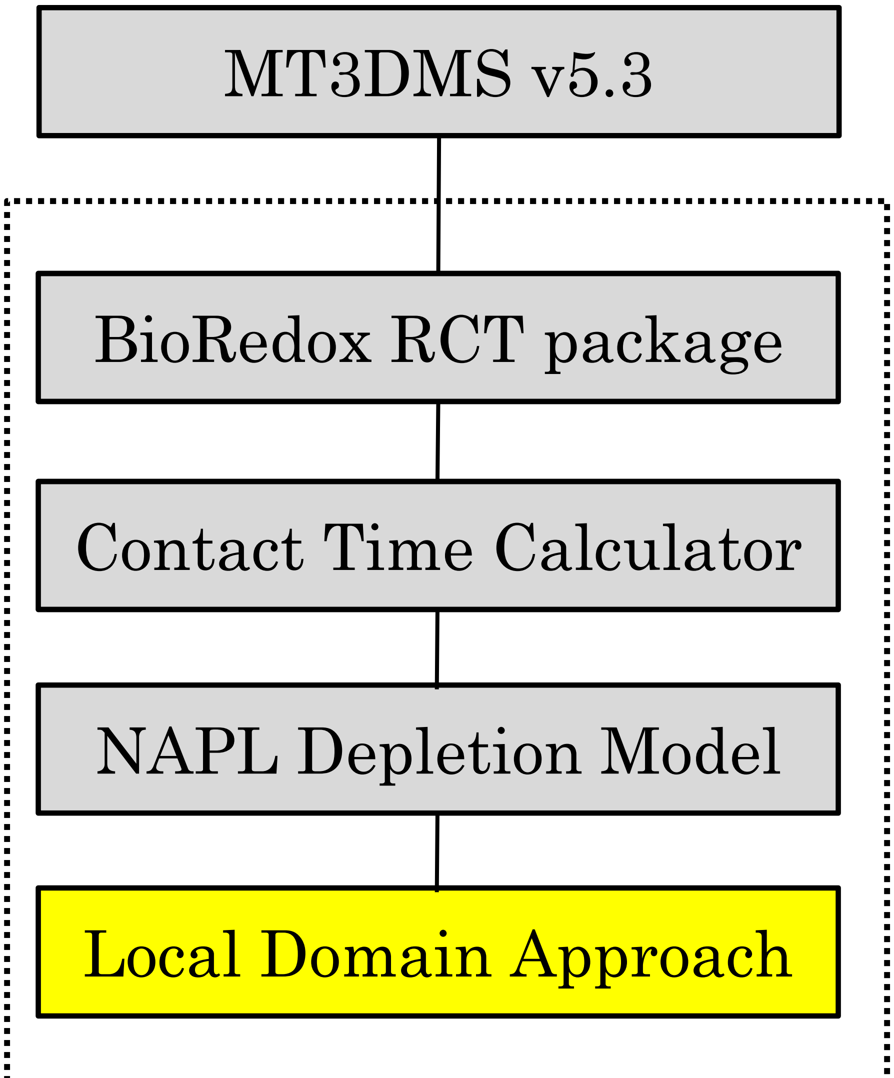




REMTEC REMEDIATION TECHNOLOGY SUMMIT THE FUTURE OF REMEDIATION TECHNOLOGY

Carey, McBean, and Feenstra (2014a,b; 2015a,b,c)

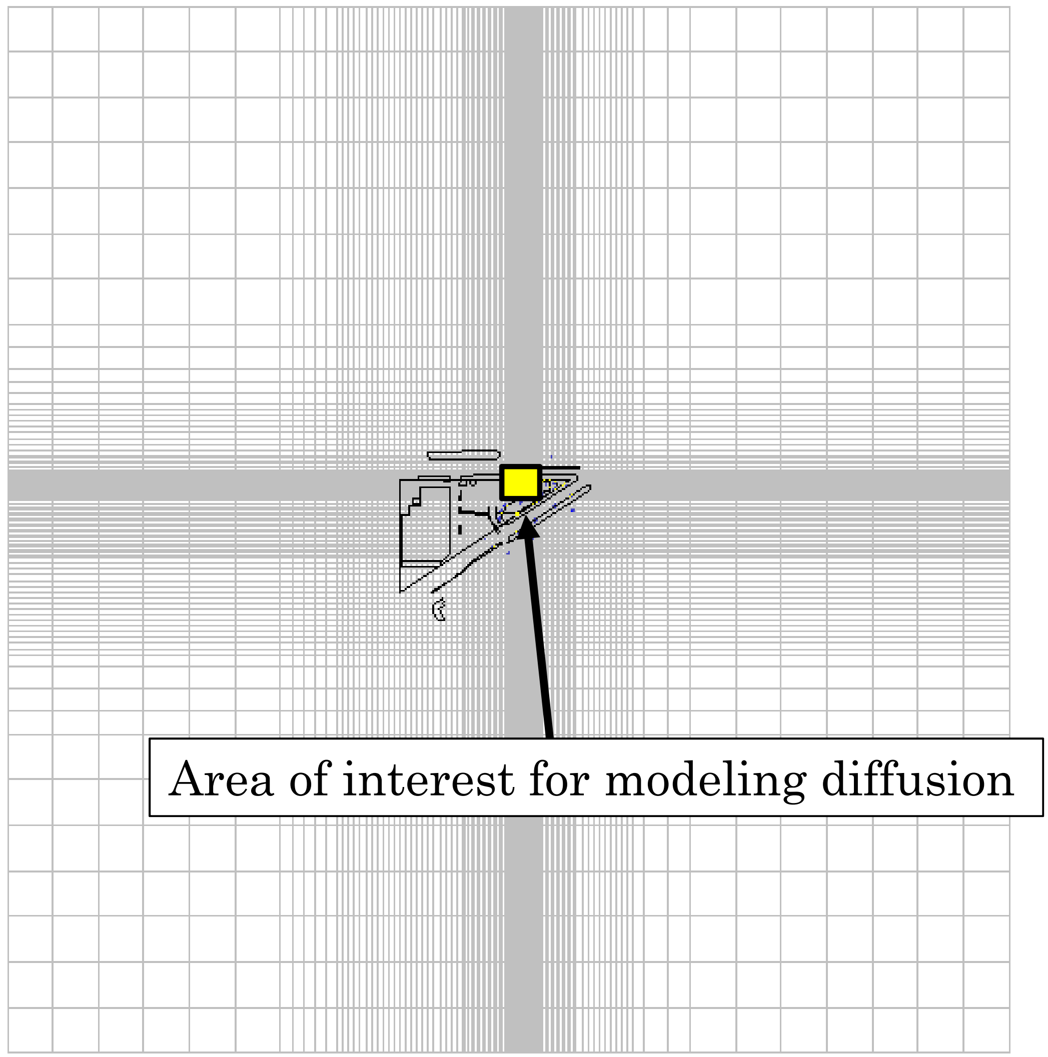
In Situ Remediation (ISR-MT3DMS)



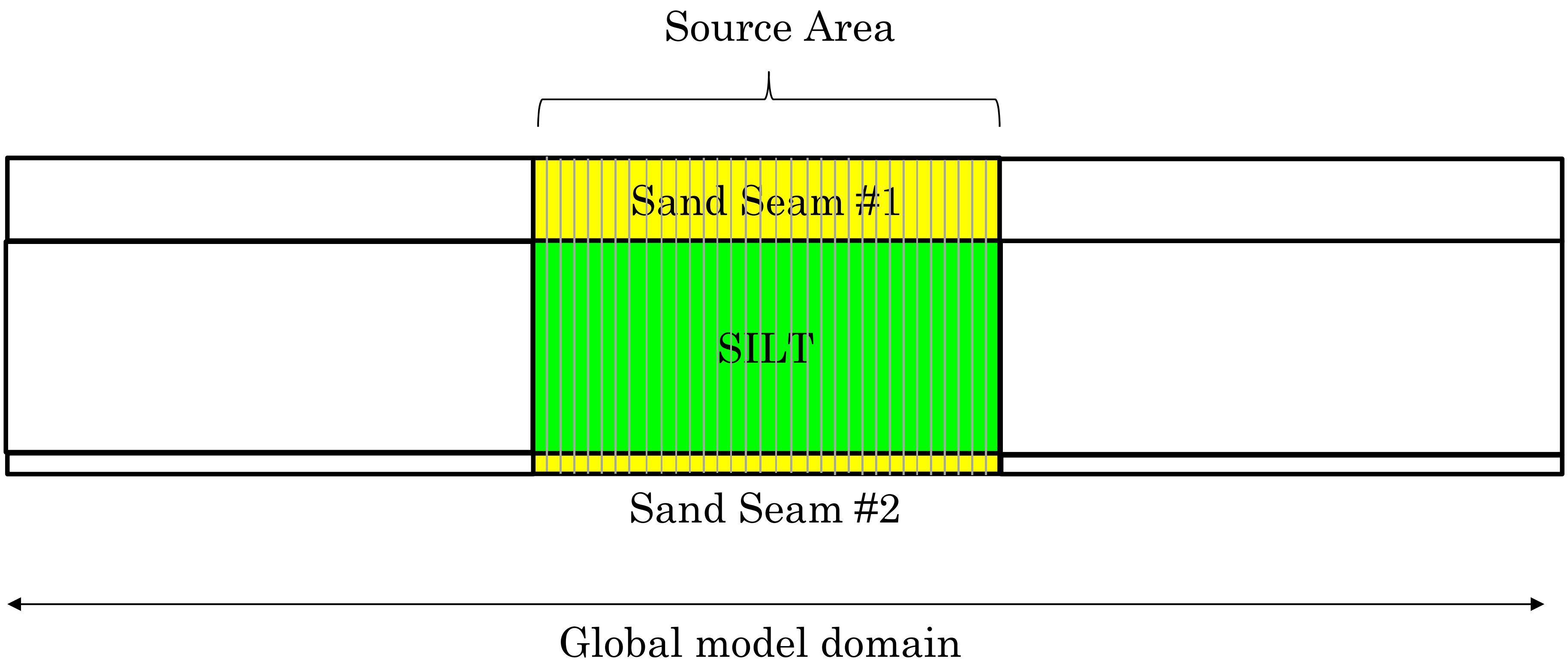
Large model linked to local 1-D model(s).

Local Domain Approach

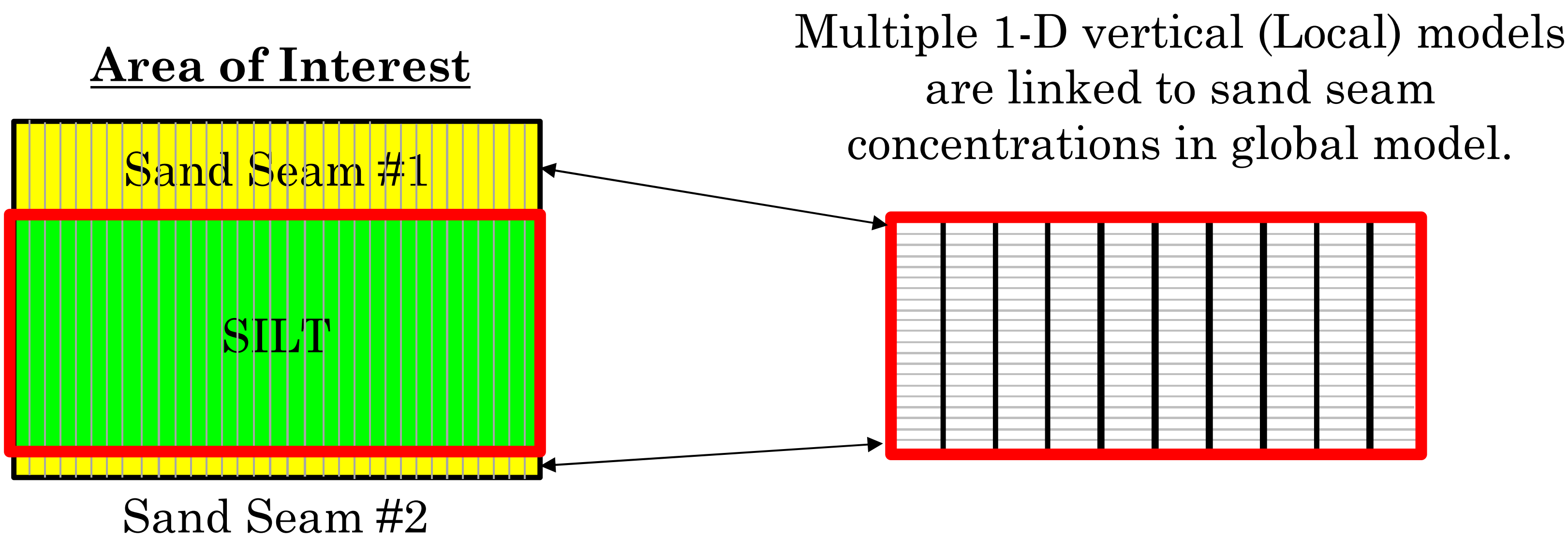
Global Model Domain



Cross-Section in Global Model (3 layers)

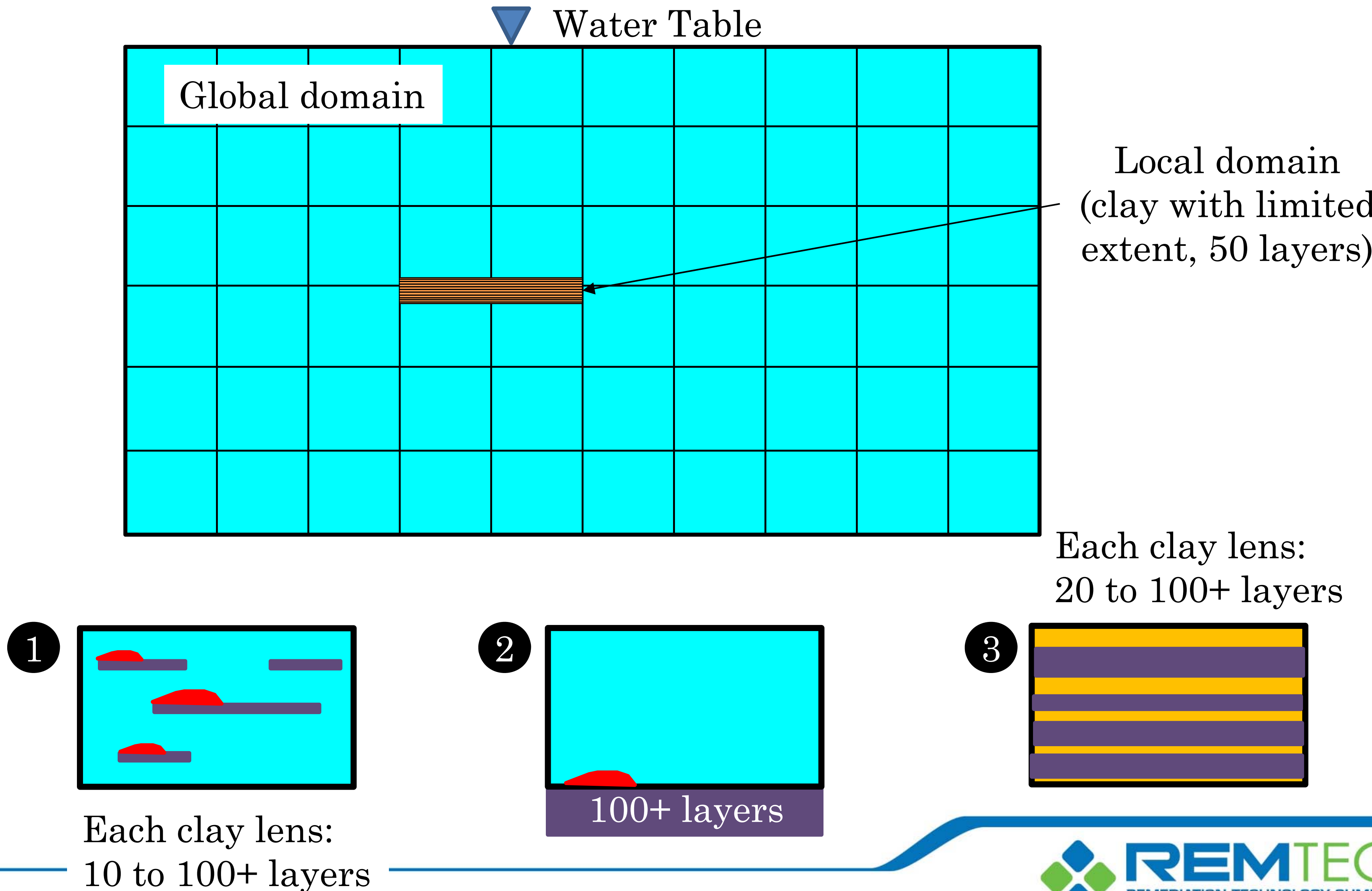


Local Model Domains for Silt (1-D Diffusion)

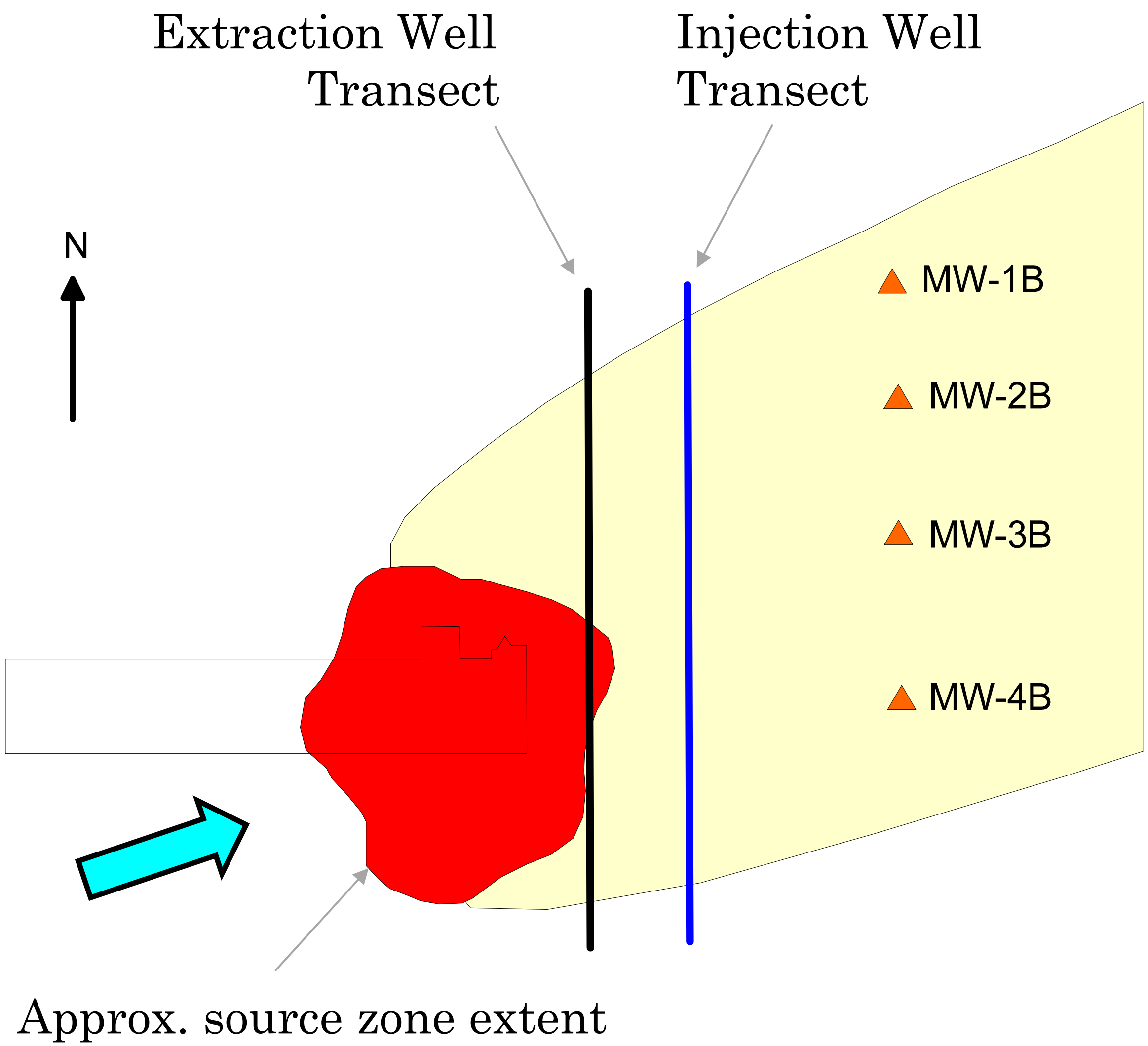


Silt layer is inactive to transport in global model.

Local Domain Approach



Case Study #2 – Florida Site

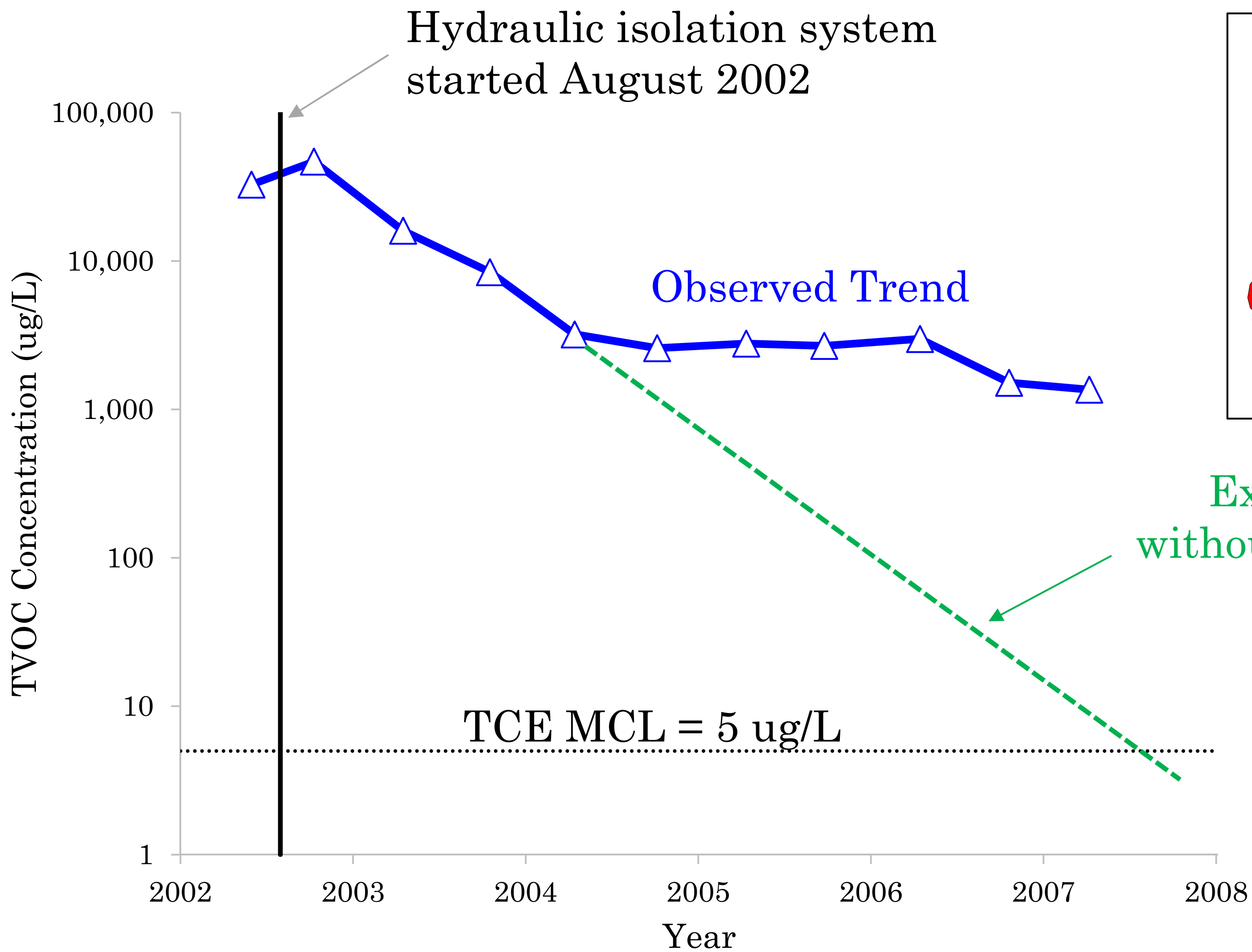


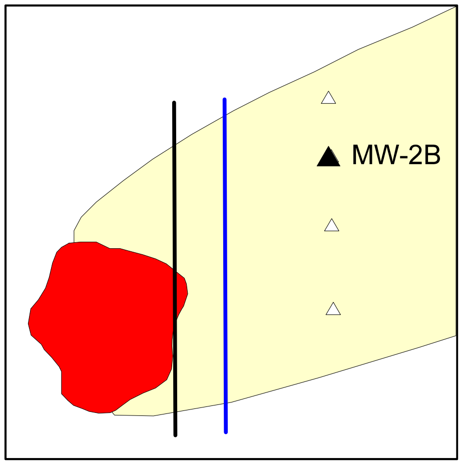
Site Characteristics

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

Source: Modified from Parker et al., 2008

TVOC Trend at MW-2B

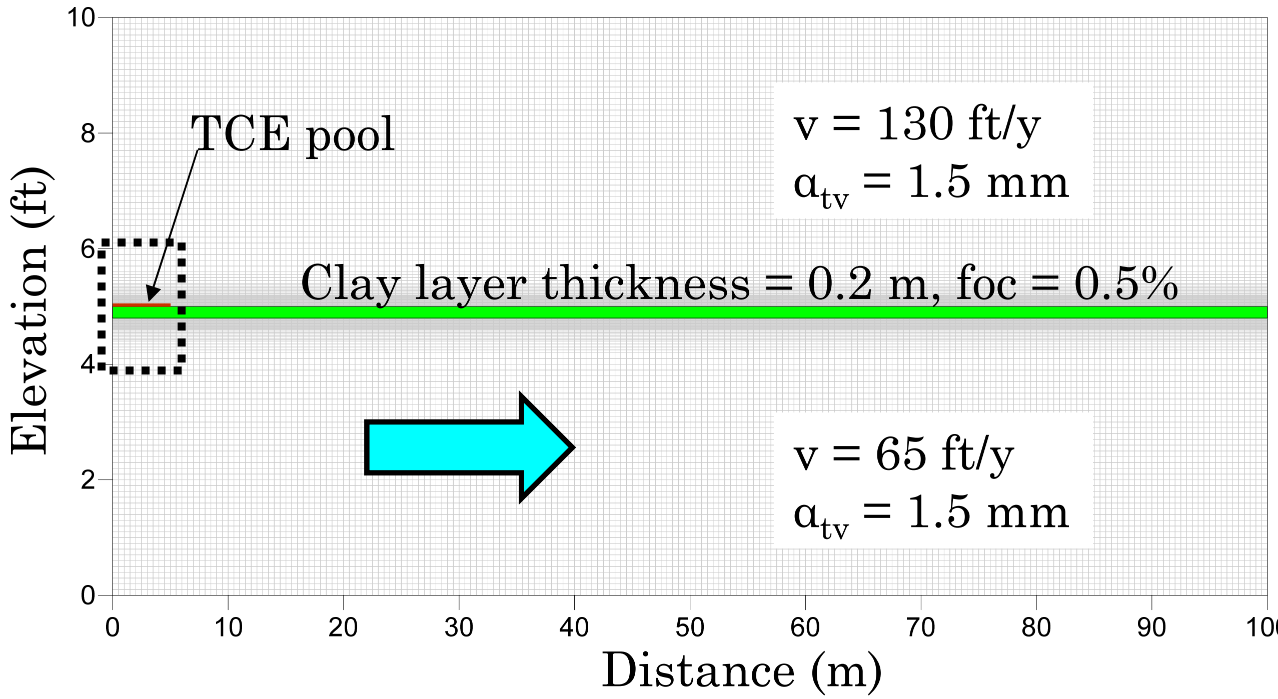




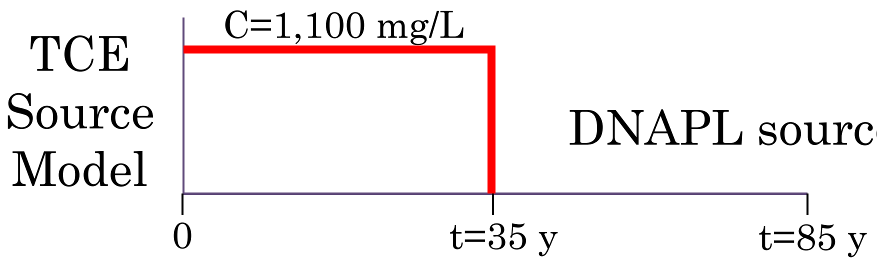
Source: Modified from Parker et al., 2008

2-D Model Grid

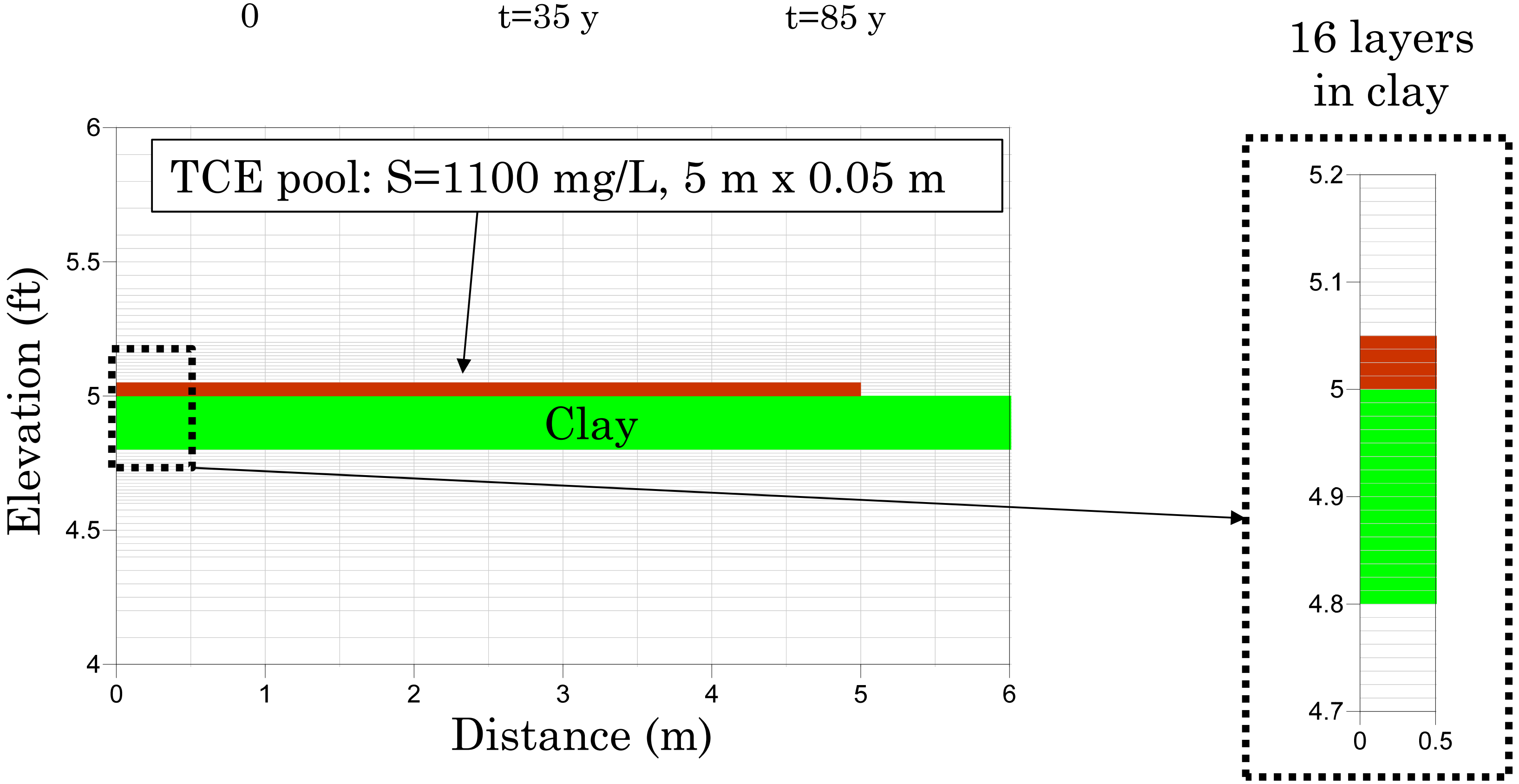
200 columns, 158 rows (layers)
Minimum grid spacing: Δz = 1.25 cm, Δx = 0.5 m
Run-time = 45 minutes for 85-y simulation (Δt = 0.24 d)



2-D Model Grid

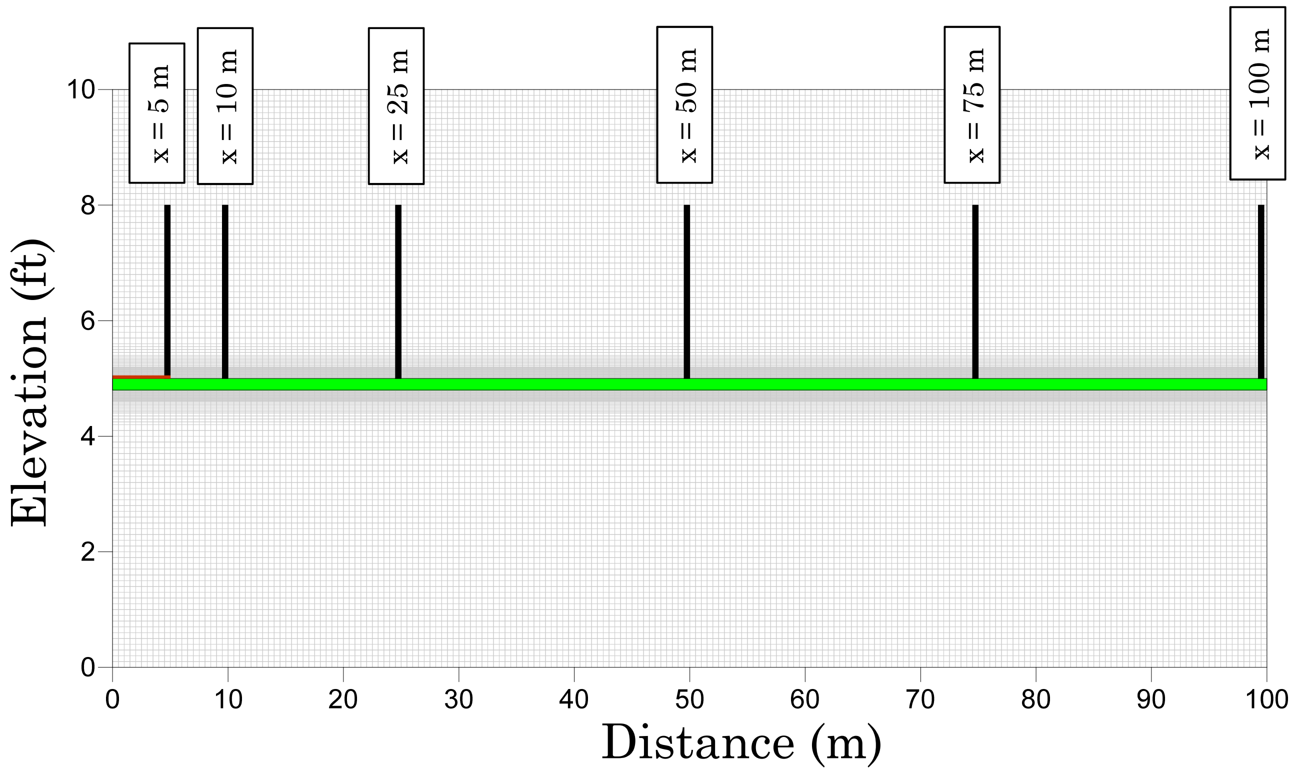


DNAPL source removed at t=35 y.



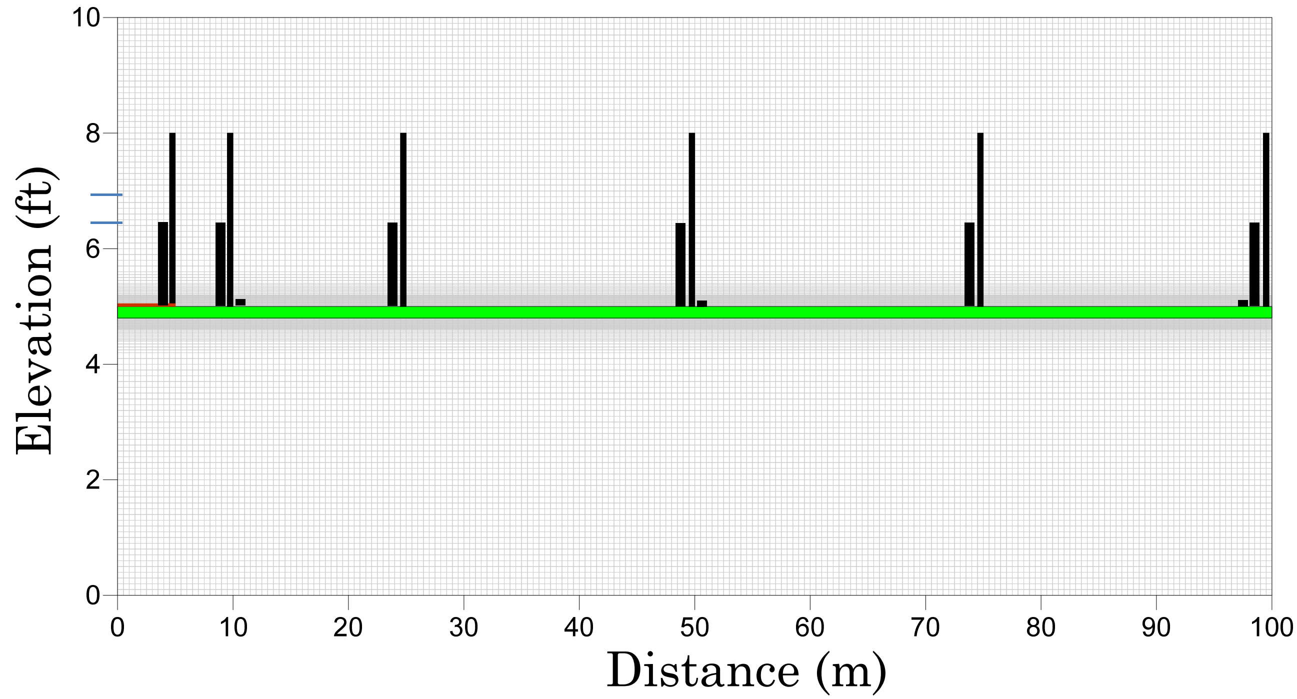
2-D Model: Horizontal Wells

RTF versus clay layer length? (C < 0.005 mg/L)



Multiple Well Screen Lengths

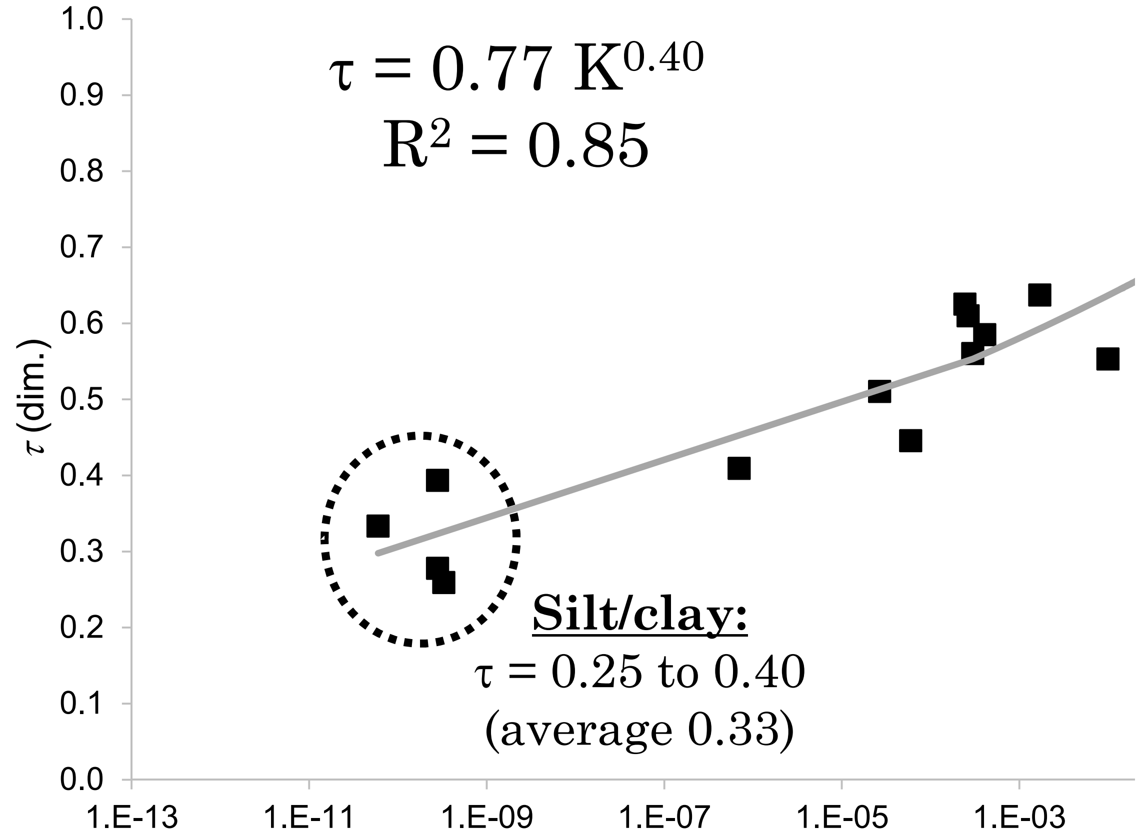
Influence of screen length on remediation timeframe?



Well lengths = 0.1, 1.5, and 3 m

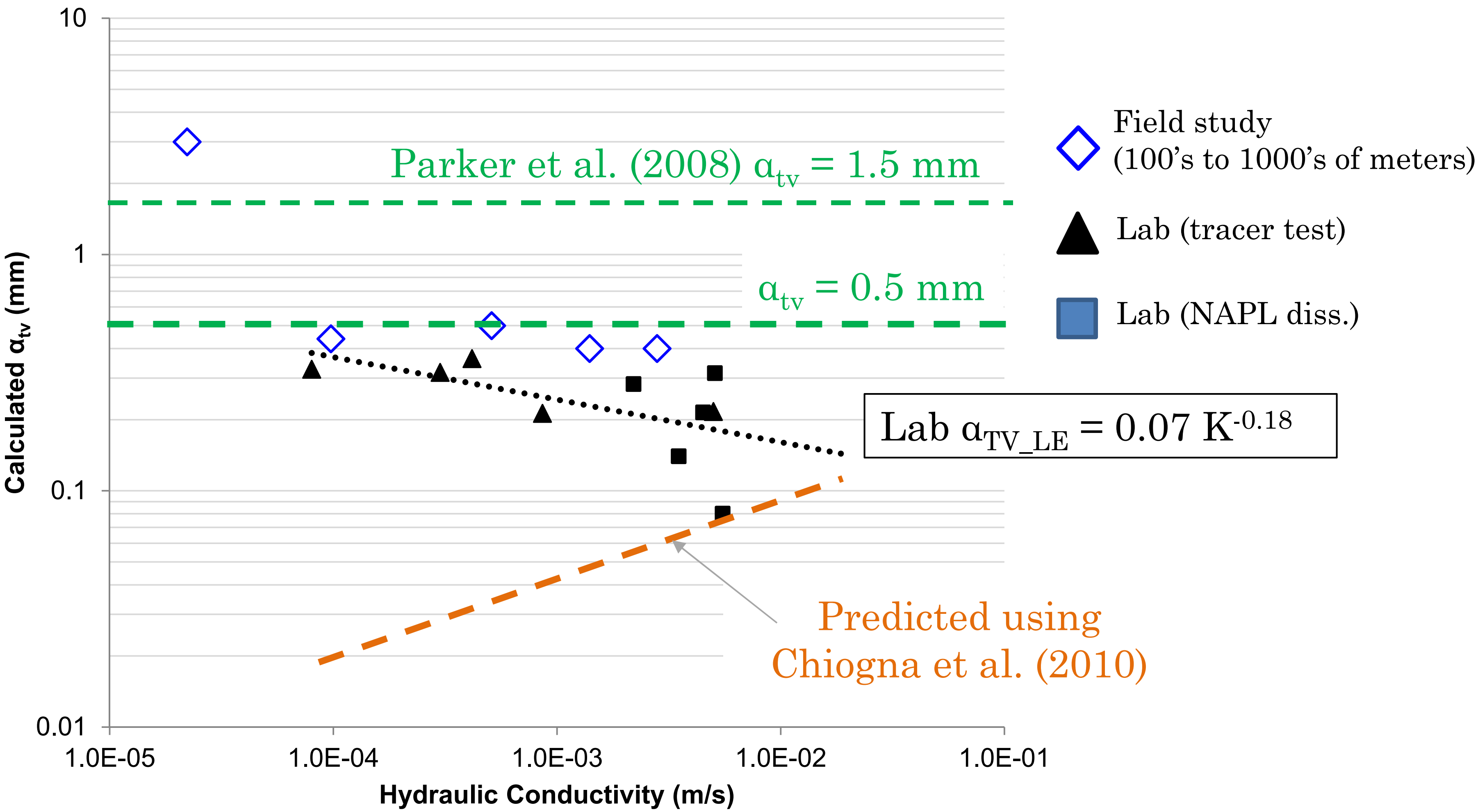
Tortuosity Coefficient

τ proportional to θ_e (not θ_t)



Carey, McBean, and Feenstra, 2015d

Transverse Dispersivity (LE) vs. K

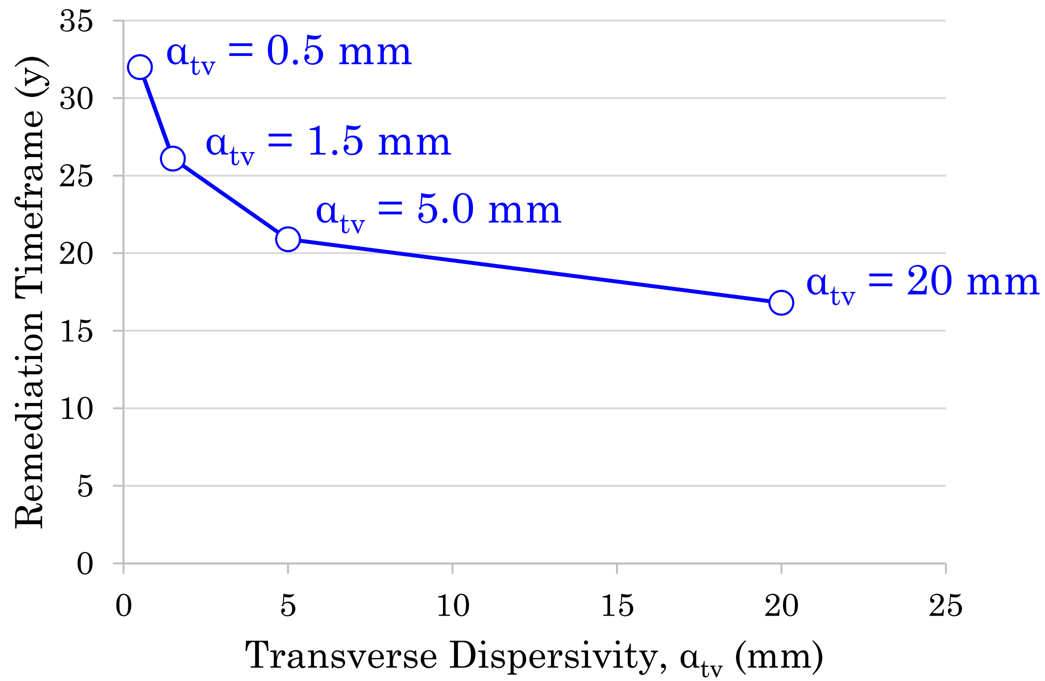


Note – results not shown for glass bead studies.
LE = Local equilibrium.

Carey, McBean, and Feenstra, 2015e

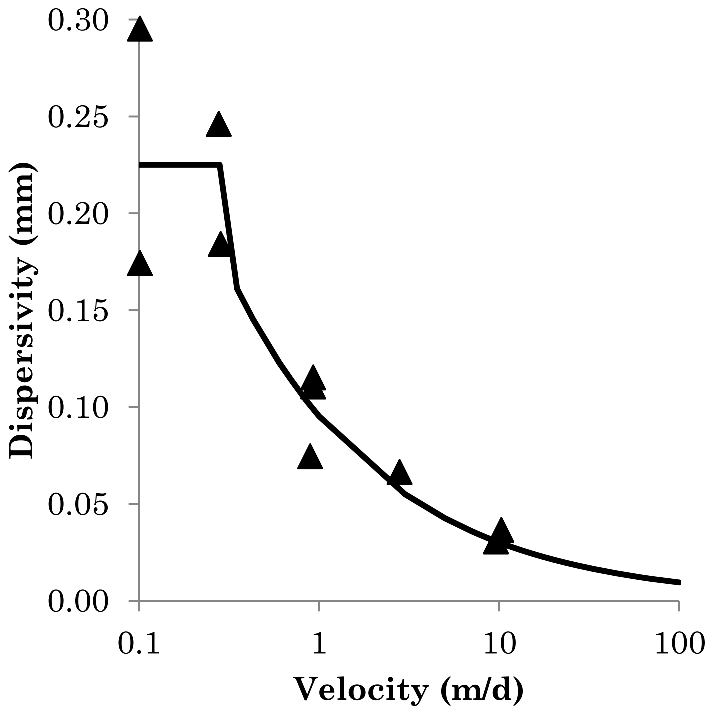
Dispersivity Influence on Remediation Timeframe

X = 50 m, Well screen length = 3 m



Transverse Dispersivity vs. Velocity

Re-calculated dispersivity based on Seagren et al., 1999 experiments.



$$\alpha_{TV} = \alpha_{TV\_LE}, v \leq vc$$

$$\alpha_{TV} = \alpha_{TV\_LE} 0.8\sqrt{v_c/v}, v > vc$$

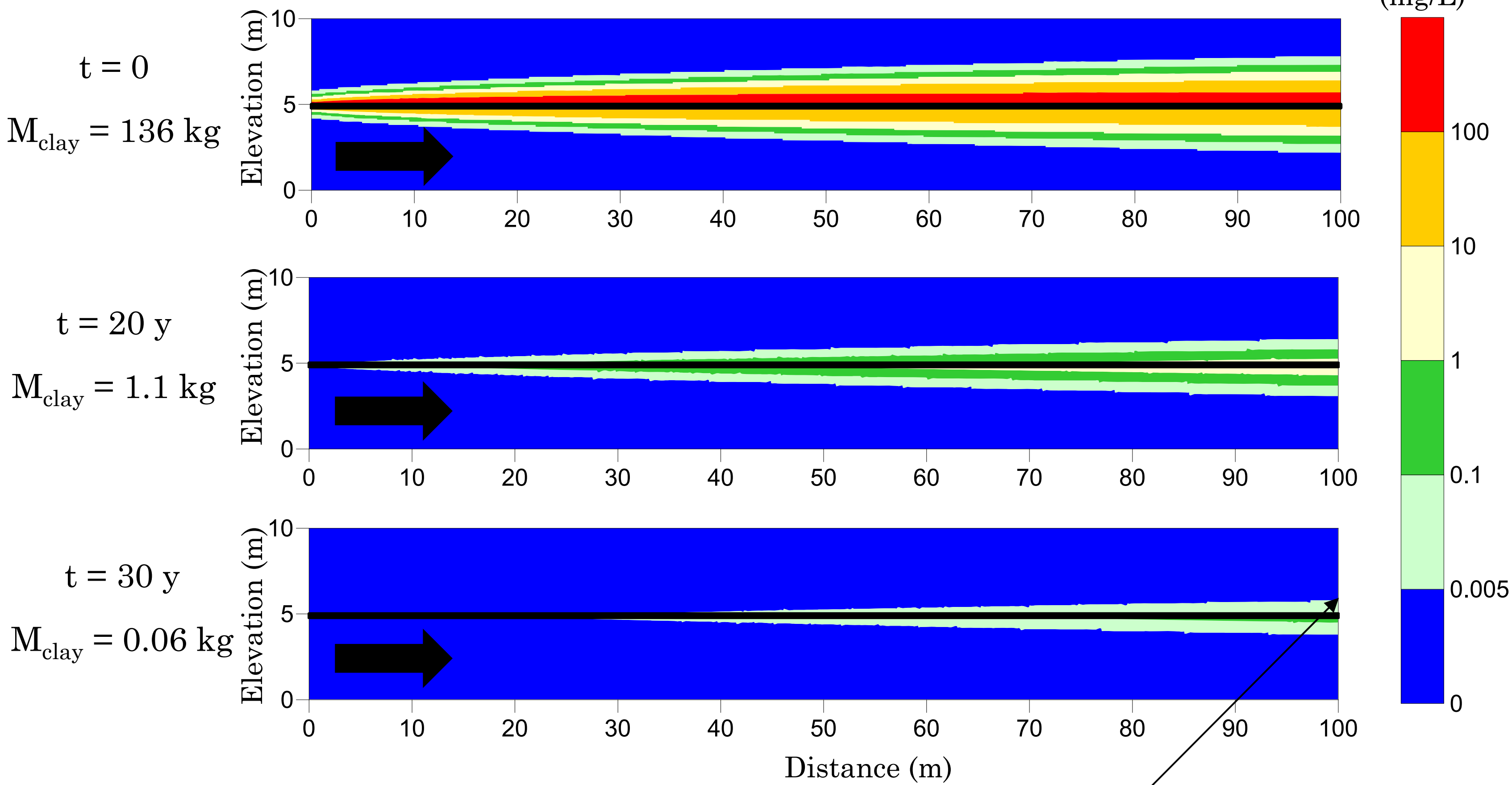
Non-equilibrium transverse dispersion at high velocity:

- Klenk and Grathwohl, 2002
- Chiogna et al., 2010

Carey, McBean, and Feenstra, 2015e

Simulated TCE After Source Removal

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

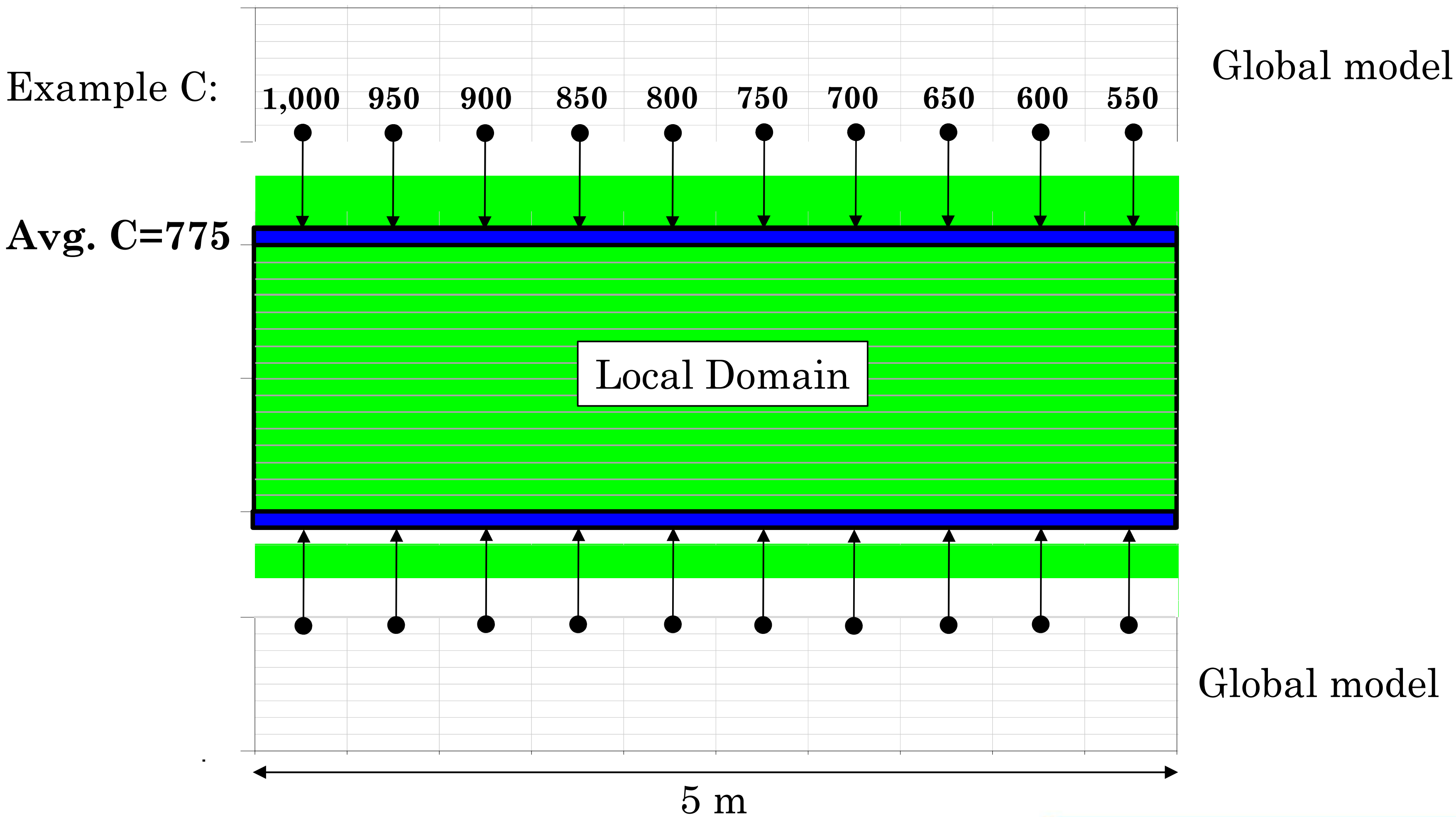


30 years after source removal:
99.96% mass depletion in clay, avg. C_{well} = 12 to 126 ug/L

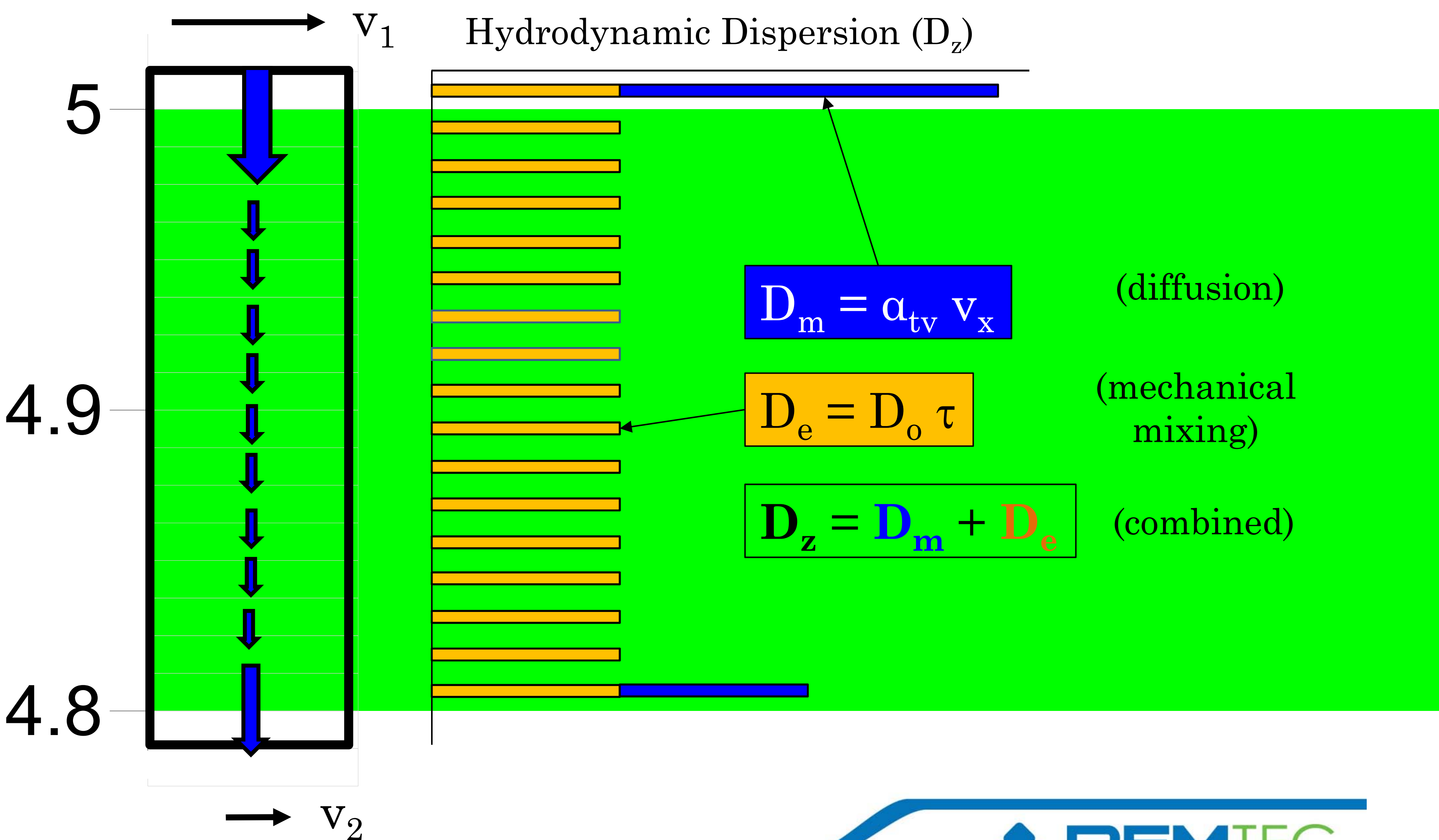
Md into top of clay = 15% to 40% of Md from DNAPL pool.

Local Domain Approach

Local domain Δx = 5 m, clay thickness varied.



Local Domain Dispersion



$D_m = \alpha_{tv}\, v_x$ (diffusion)

$D_e = D_o\, \tau$ (mechanical mixing)

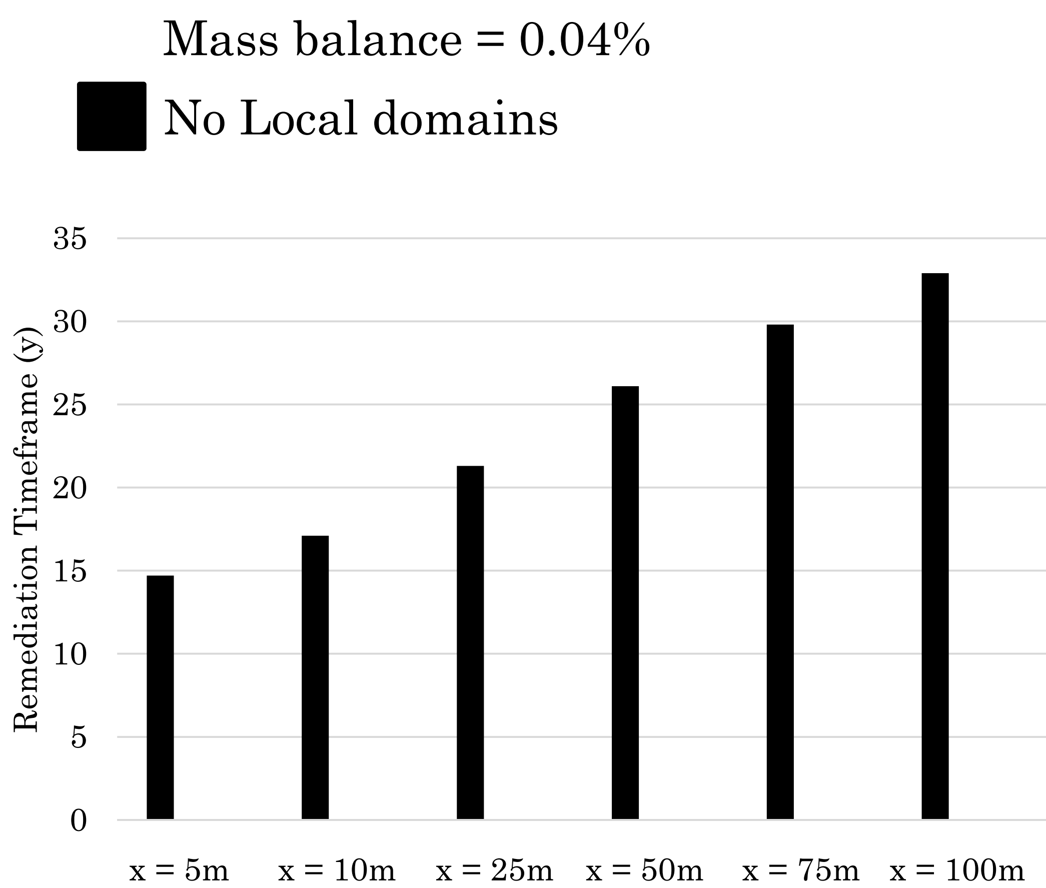
$\mathbf{D_z = D_m + D_e}$ (combined)

Influence of Mechanical Mixing

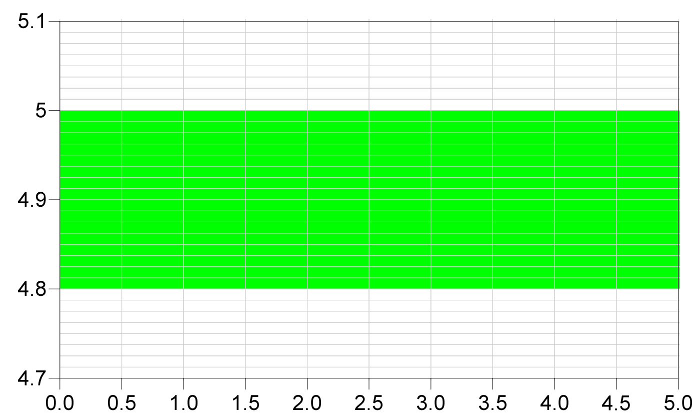
- Horizontal velocity above clay - increases transverse dispersion and mass flux into/out of clay (3x higher at this site)
- 1-D models or flux calculations typically based on D_e (D_m assumed to be zero)
  - May substantially underestimate mass flux into and out of clay

$$\text{Flux} = -D_z\ \theta\ \Delta C / \Delta x$$

Remediation Timeframe



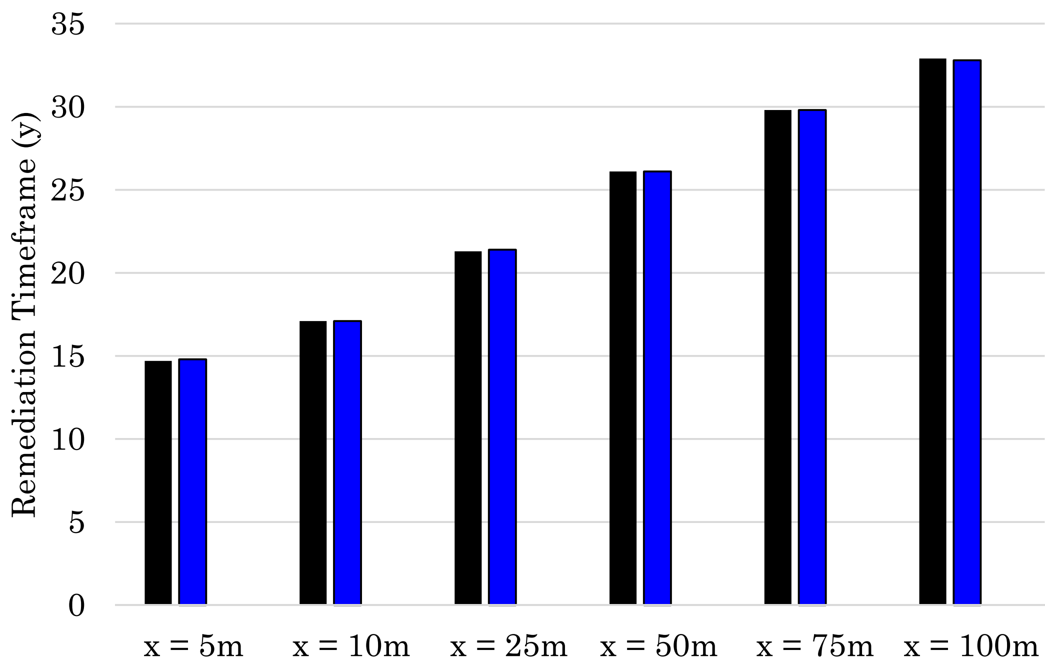
Global domain only



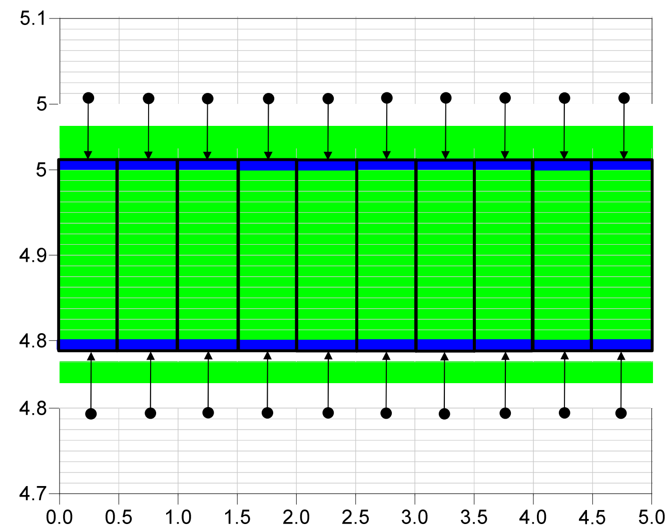
Remediation Timeframe

Mass balance = 0.04%   Mass balance = 0.04%

No Local domains   200 Local domains



200 Local domains, $\Delta x = 0.5$ m

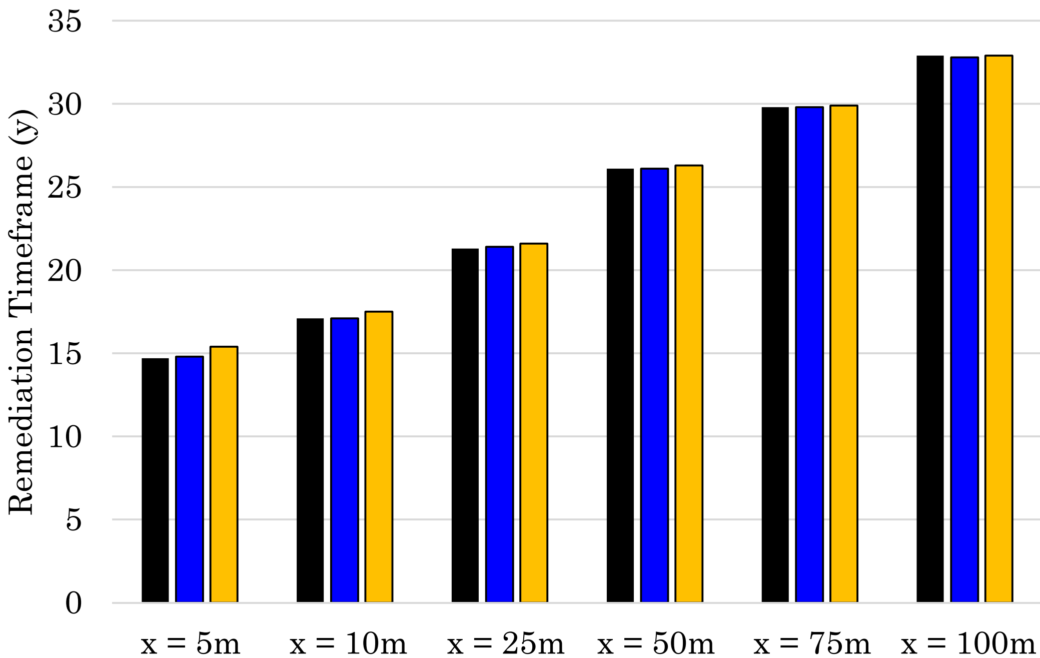


Remediation Timeframe

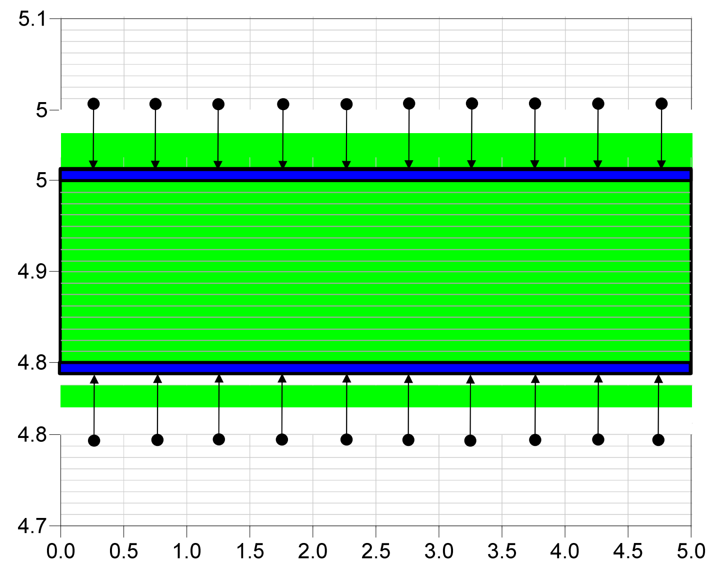
Mass balance = 0.04%   Mass balance = 0.04%   Mass balance = 0.07%

No Local domains   200 Local domains   20 Local domains

Δx = 0.5 m



20 Local domains, Δx = 5 m

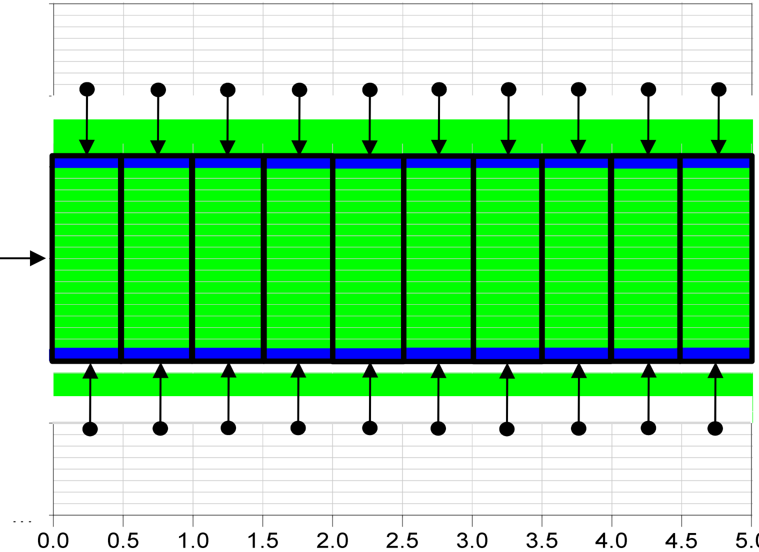


Influence of Thickness and R

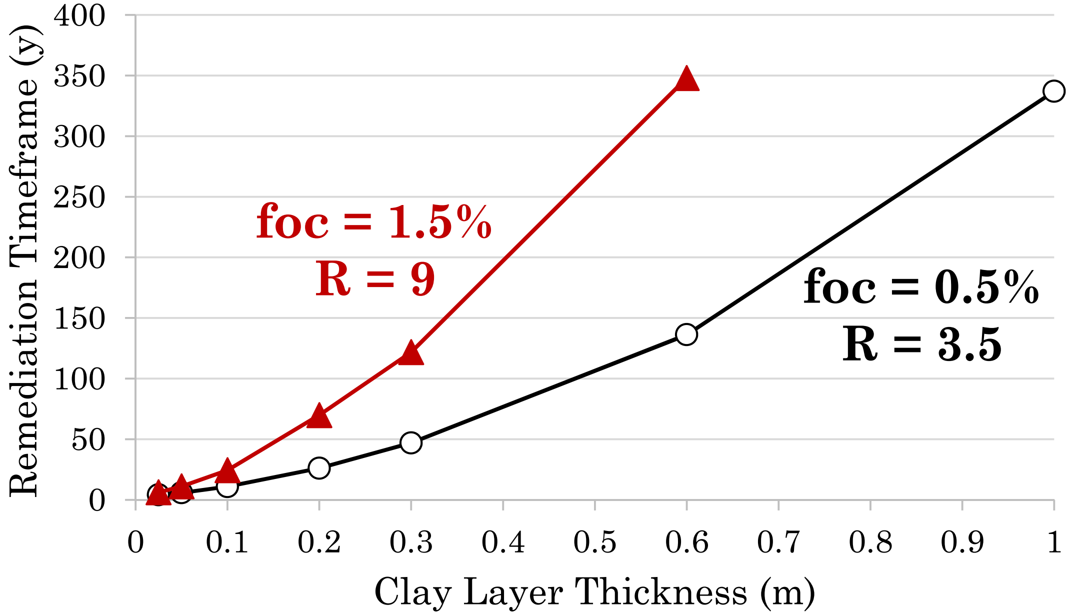
No. local domains = 200 (Δx = 0.5 m)

7 model runs with different clay thickness

- 0.025, 0.05, 0.1, 0.2, 0.3, 0.6, and 1 m



x= 50 m



Sensitivity Analysis:

Length of Clay Layer

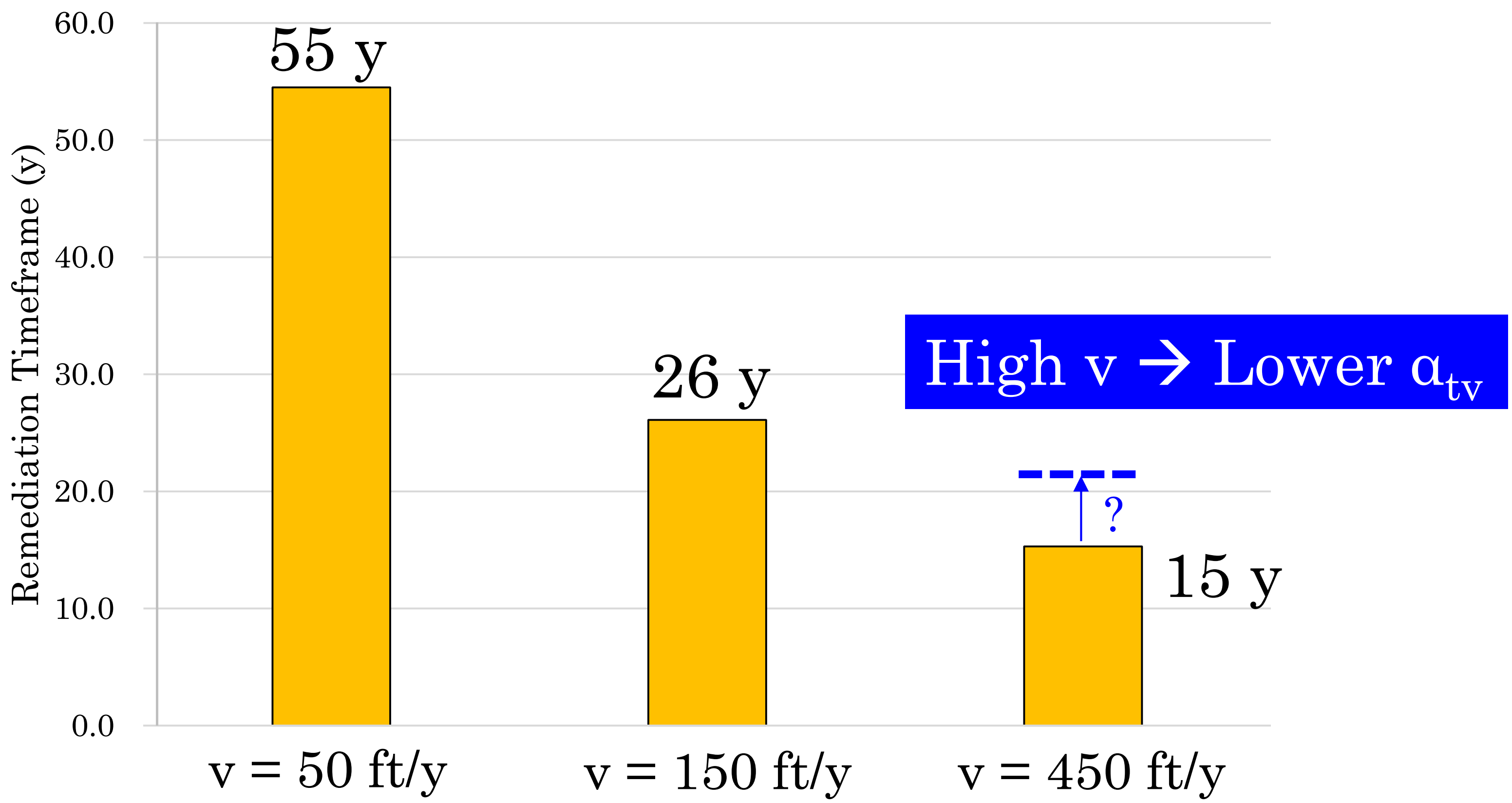
L_1 ~ 30 ft

L_2 ~ 300 ft

Length x 10 → RTF x 2

Sensitivity Analysis:

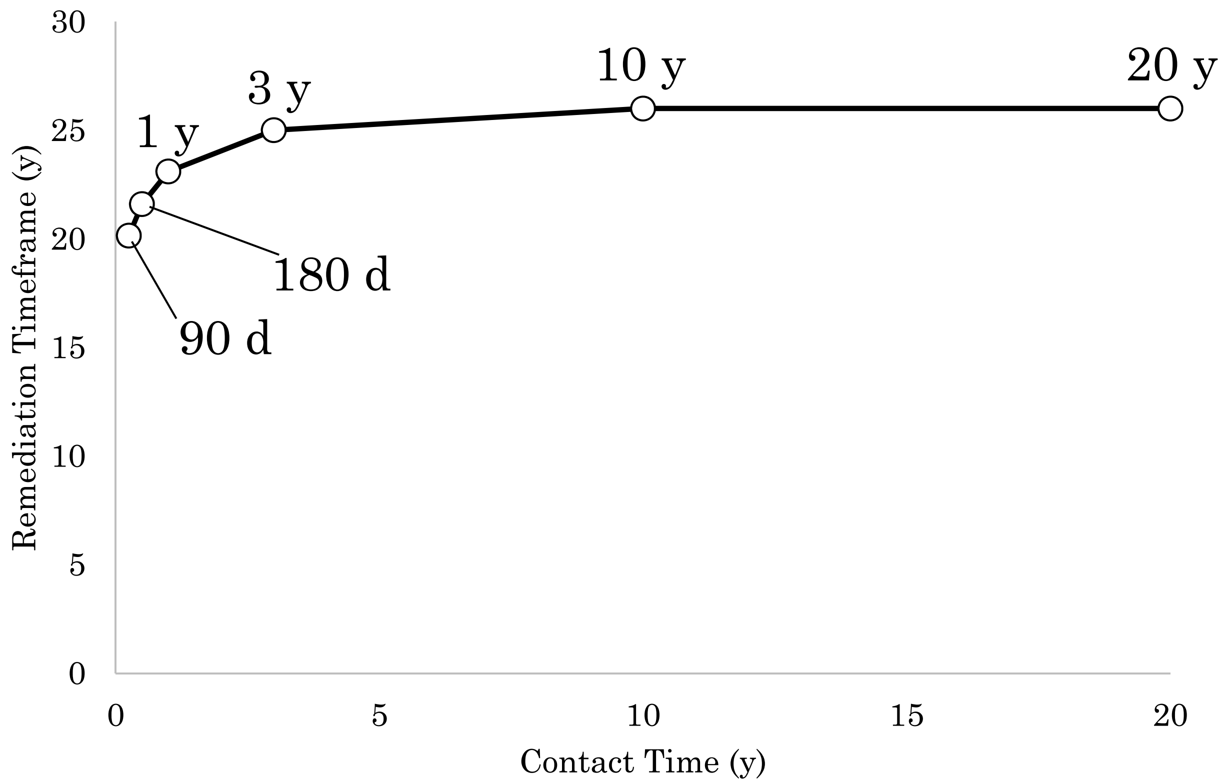
Velocity (x=50 m, scrn L=3 m)



Note – ISR-MT3DMS simulation did not consider potential decrease in α_{tv} at higher velocity.

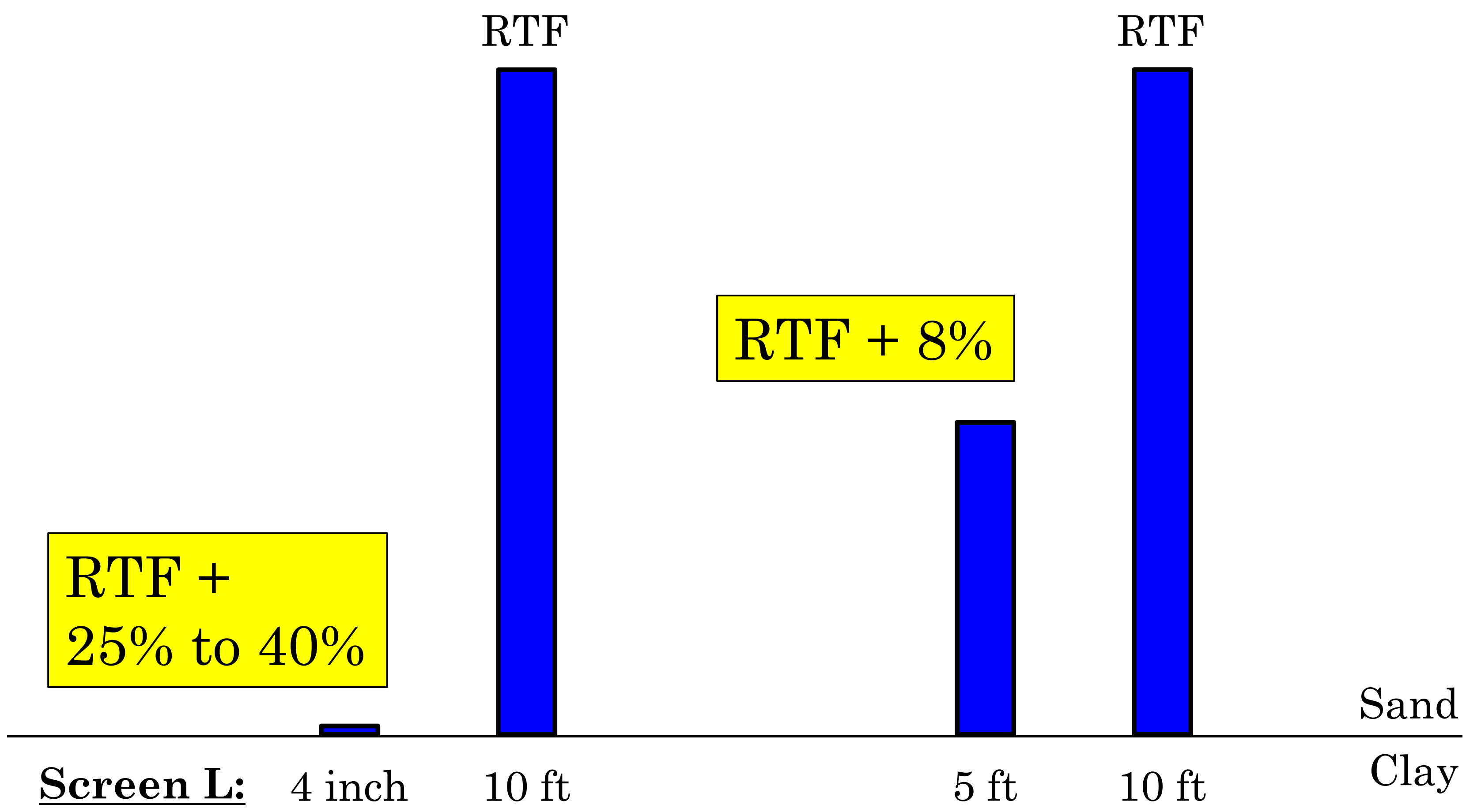
Influence of Contact Time (Thin Layer)

x = 50 m, Well screen L = 3 m



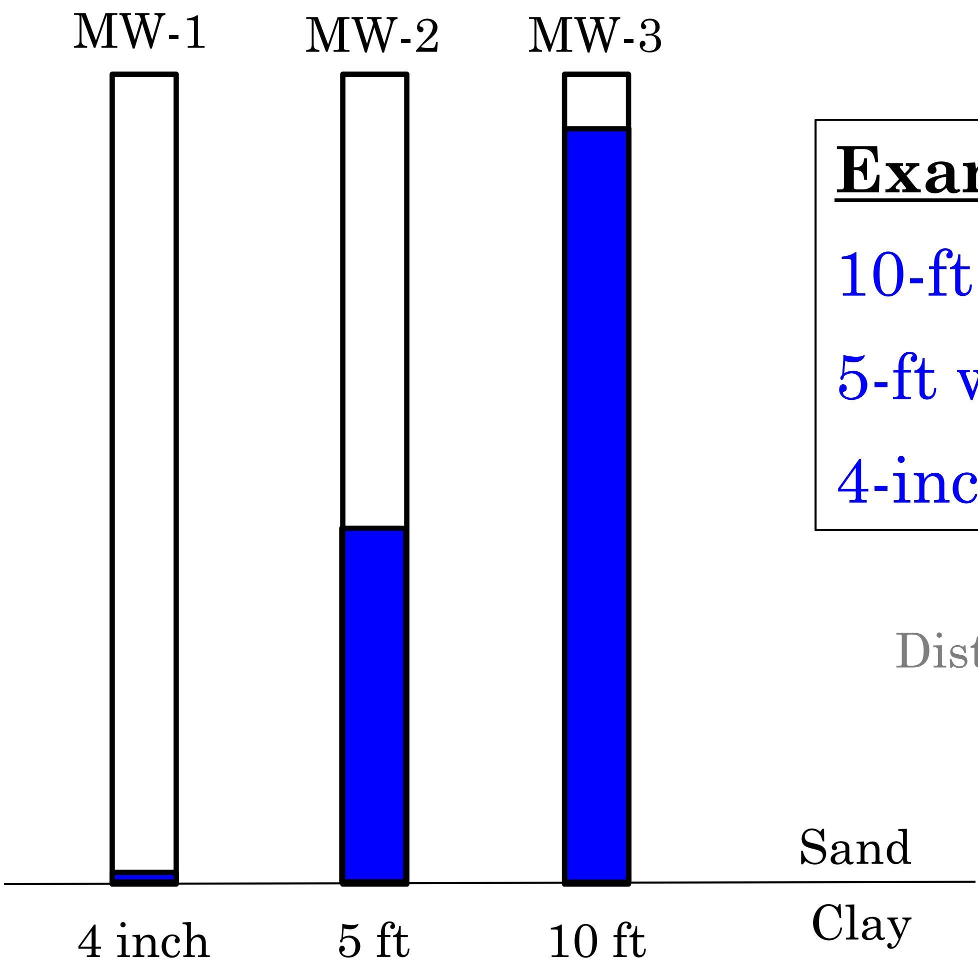
Contact time - between DNAPL and clay layer.

Sensitivity Analysis:
Well Screen Length



Shorter screen → Longer RTF

Sensitivity Analysis:
Well Screen Length



Example

10-ft well: **RTF = 30 y**

5-ft well: **RTF + 3 y**

4-inch well: **RTF + 8 to 12 y**

Distance of 15 to 300 ft from source.

REMTEC REMEDIATION TECHNOLOGY SUMMIT
THE FUTURE OF REMEDIATION TECHNOLOGY

Conclusions

- ISR-MT3DMS – Local Domain
  - Proof of concept, verification
- Model inputs: τ and α_{tv}
- Mechanical mixing vs. diffusion
- Back-diffusion in thin layers: RTF most sensitive to v, b, foc

ISR-MT3DMS Next Steps

- On-going development, verification

Demonstration sites (w/reactions) & beta testing

- Short course at Battelle symposium in May 2015
  - NDM and ISR-MT3DMS
  - Beta version release
- GUI Developers
- Target release date: 2016 (FREE)

Questions?

Porewater Solutions

Expertise • Experience • Innovation

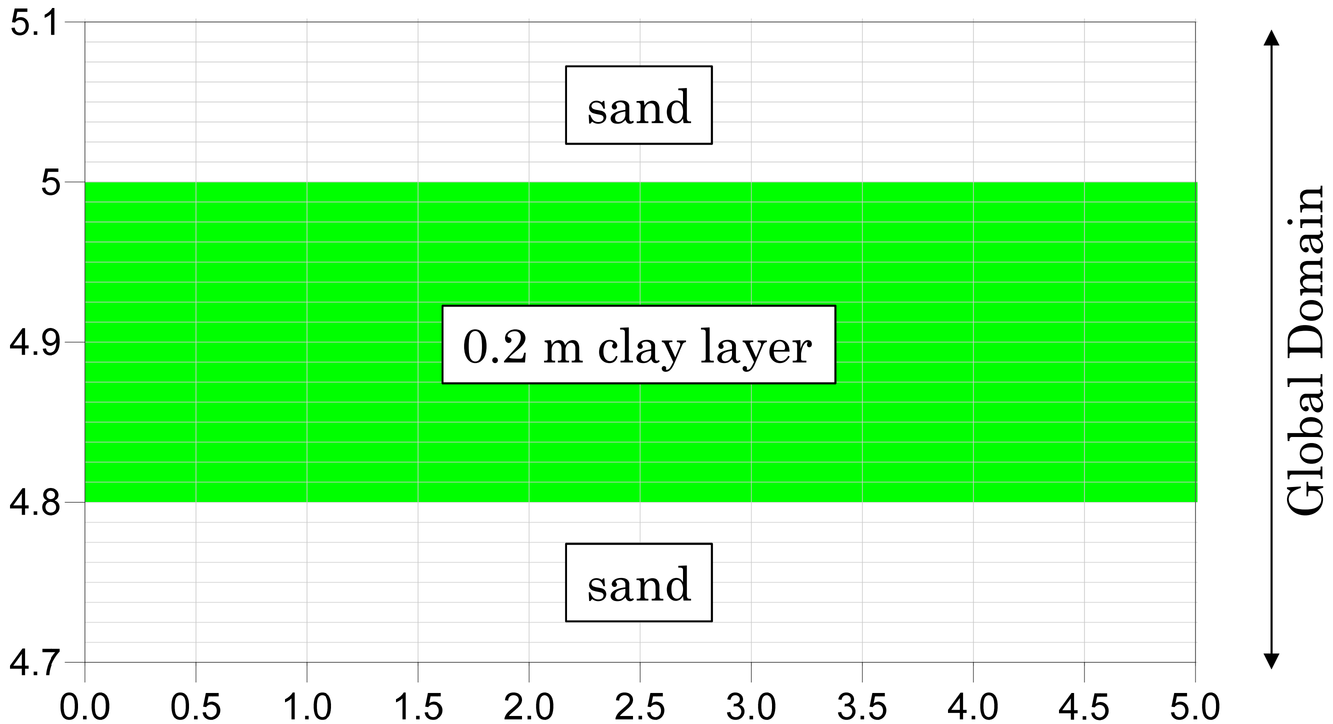
Grant Carey
Porewater Solutions

613-270-9458
gcarey@porewater.com

REMTEC
REMEDIATION TECHNOLOGY SUMMIT
THE FUTURE OF REMEDIATION TECHNOLOGY

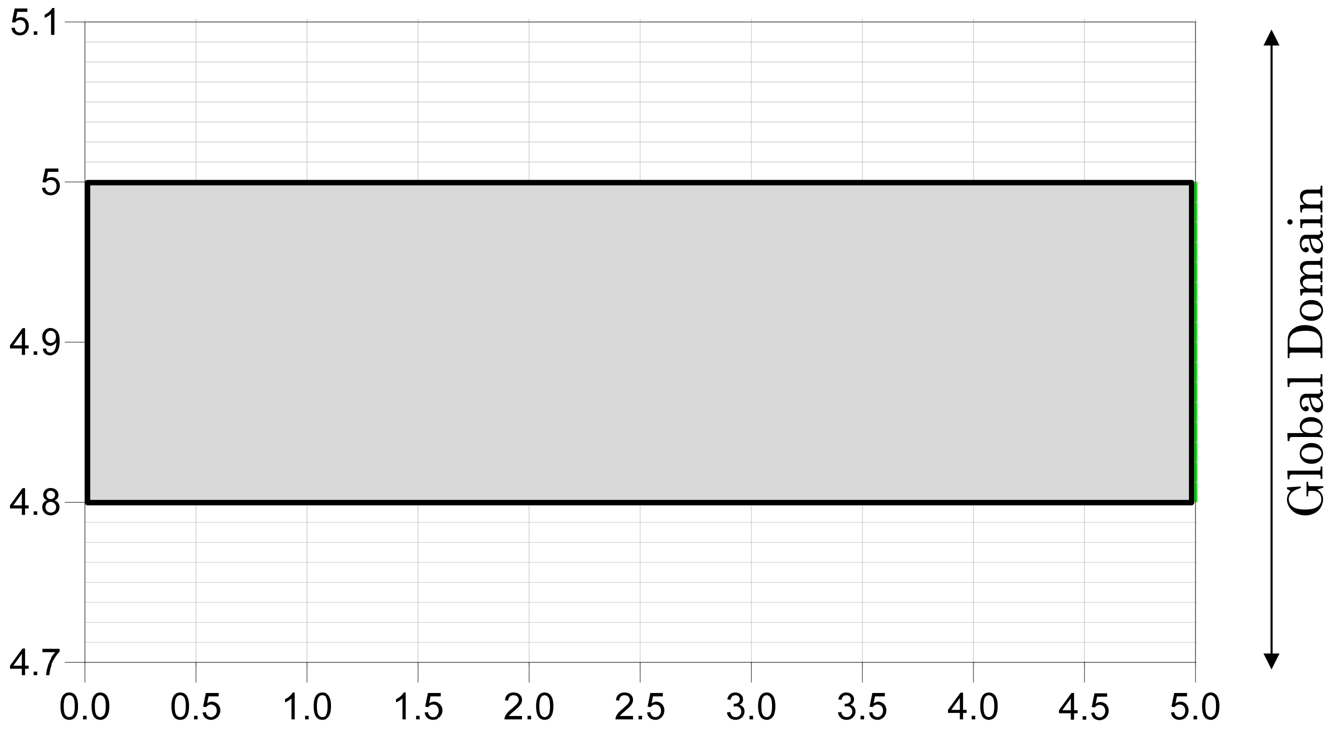
Local Domain Approach

1. Global domain section (example)



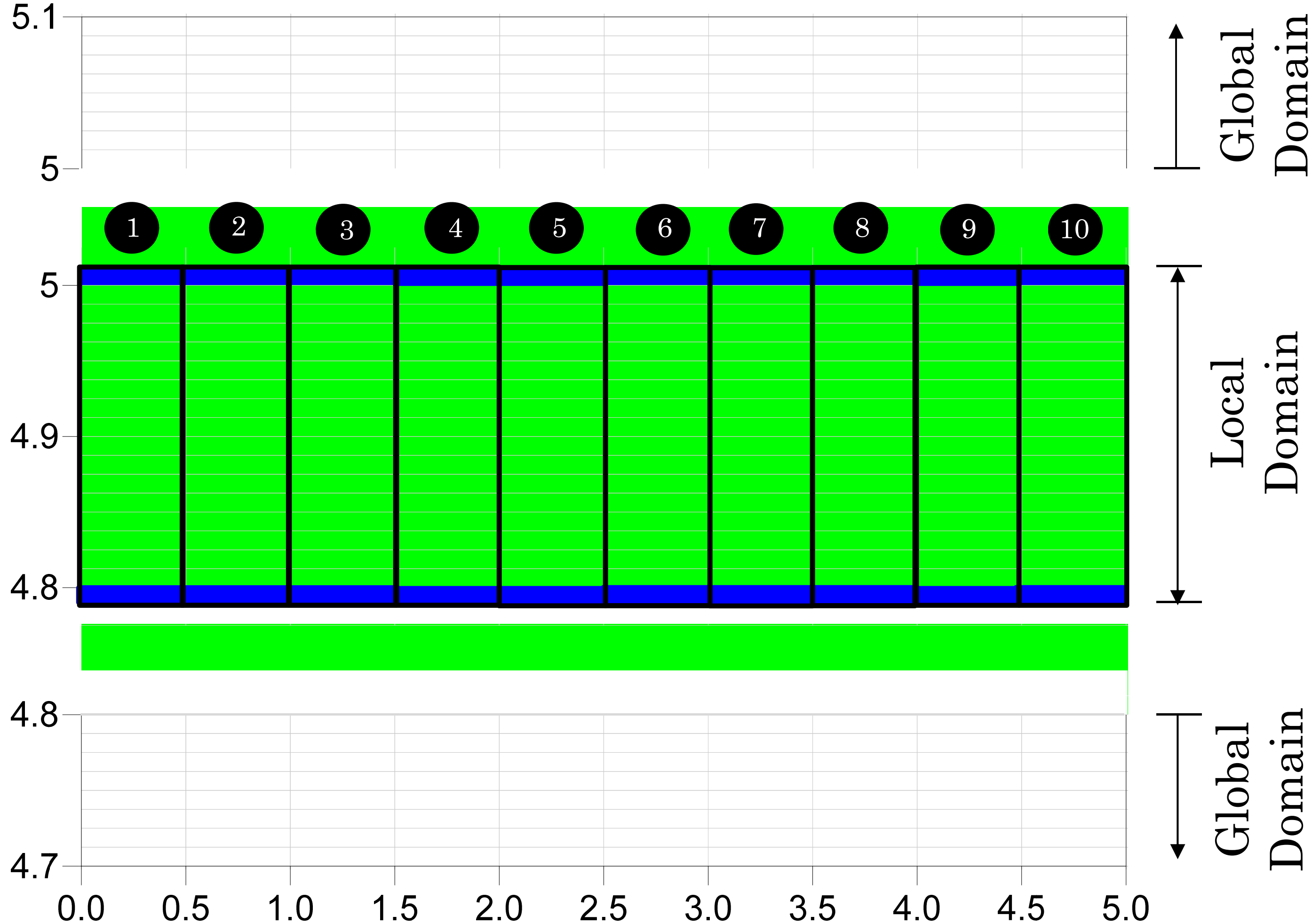
Local Domain Approach

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



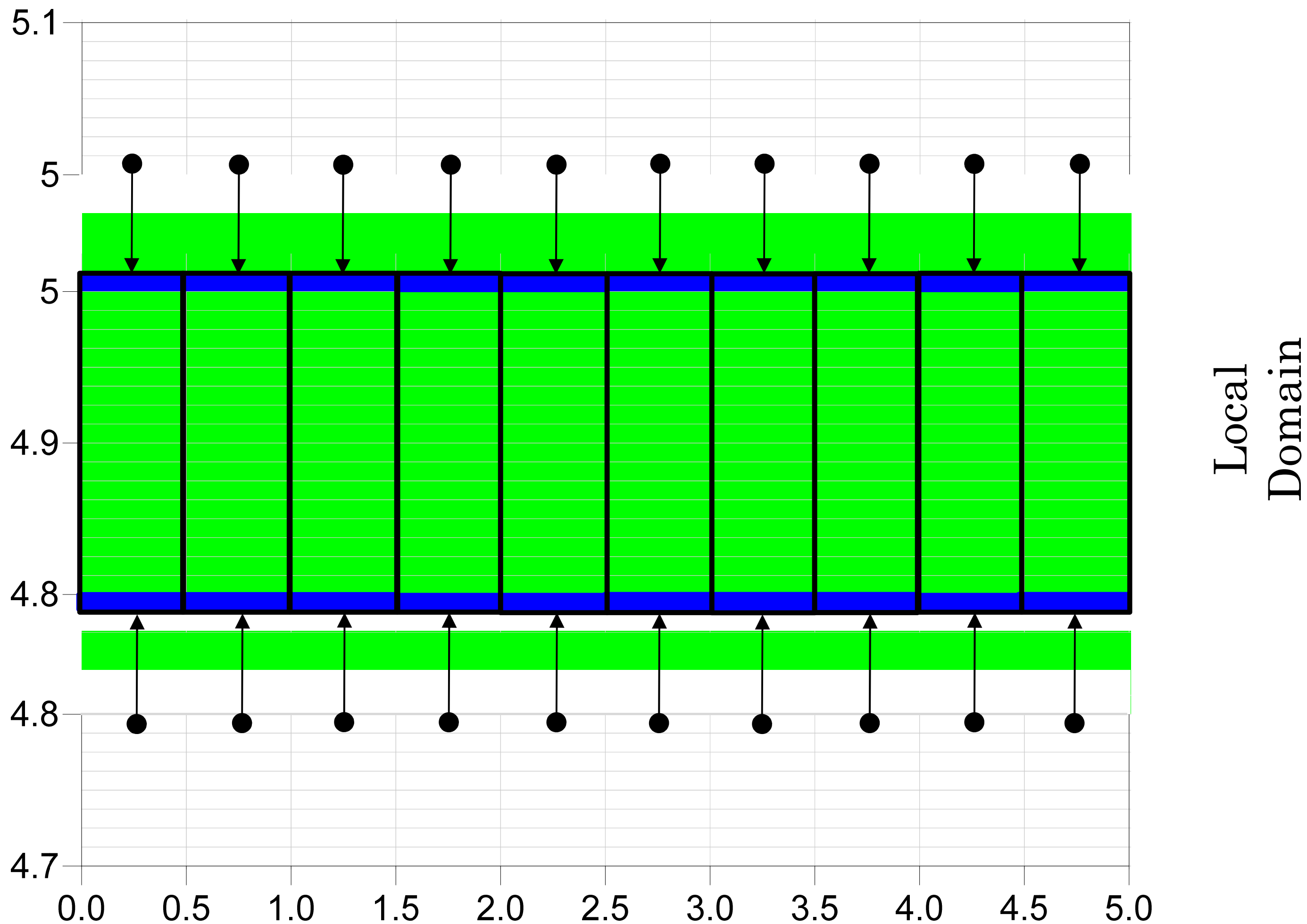
Local Domain Approach

3. Insert 200 local domains ($\Delta x = 0.5$ m, $\Delta z = 1.25$ cm).



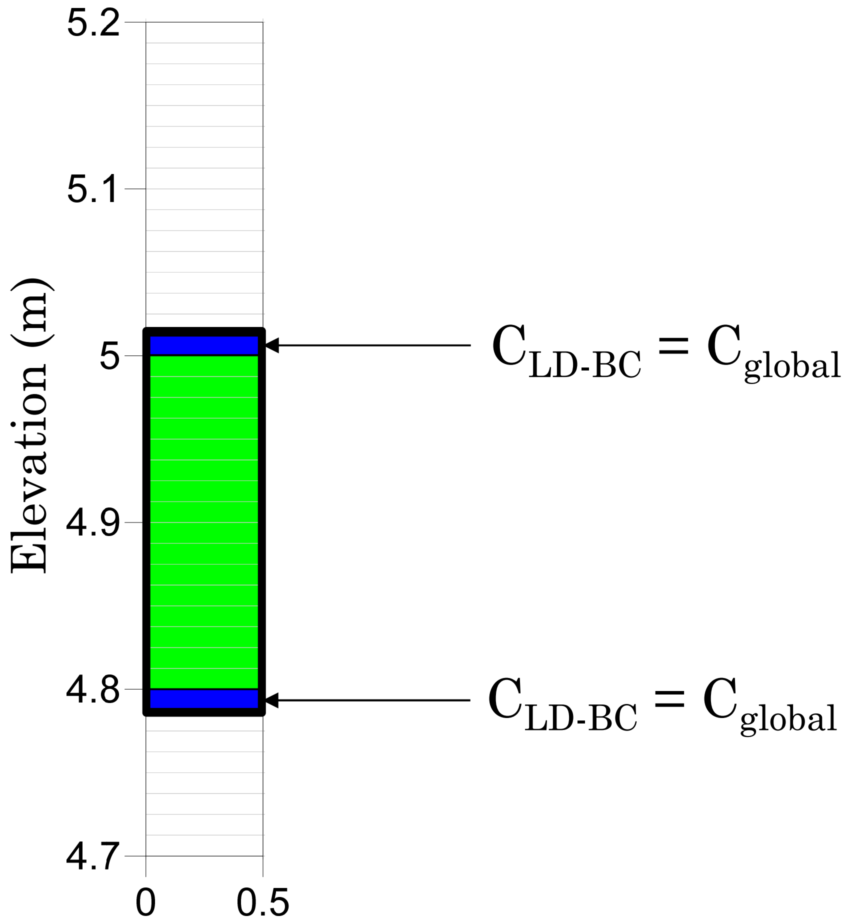
Local Domain Approach

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



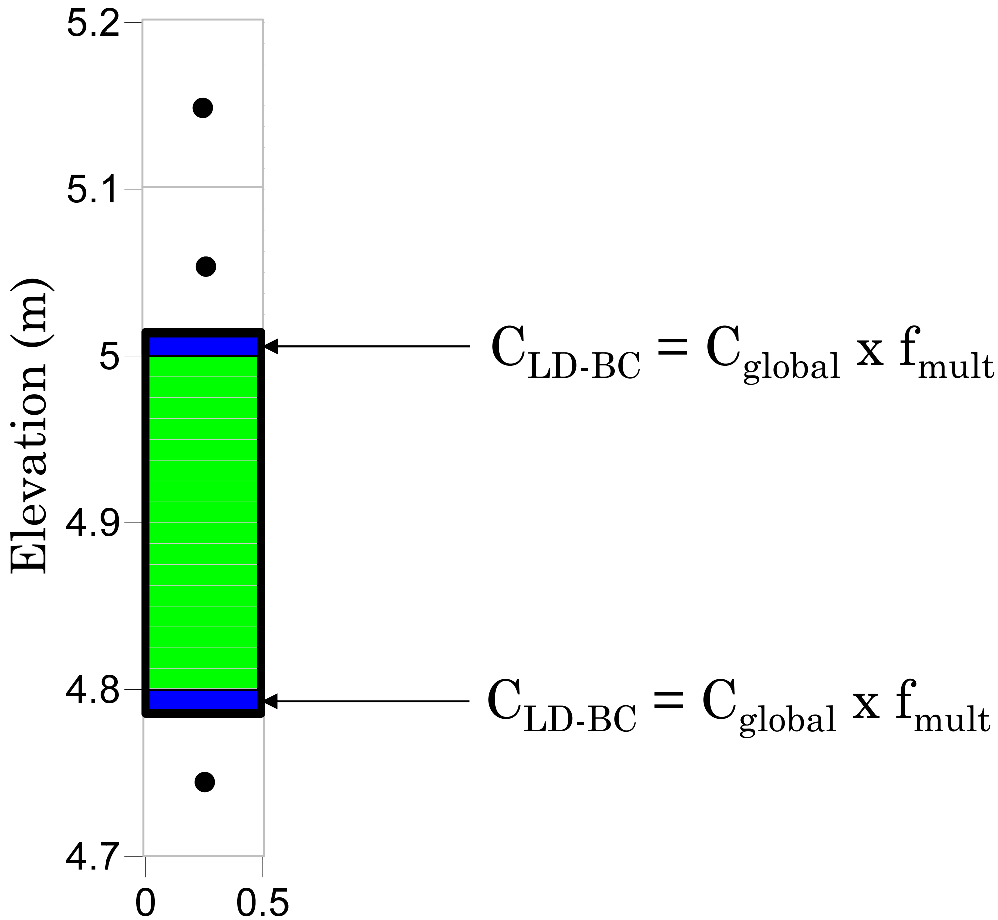
Local Domain Boundary Conditions

Scenario A – same vertical discretization in local and global domains

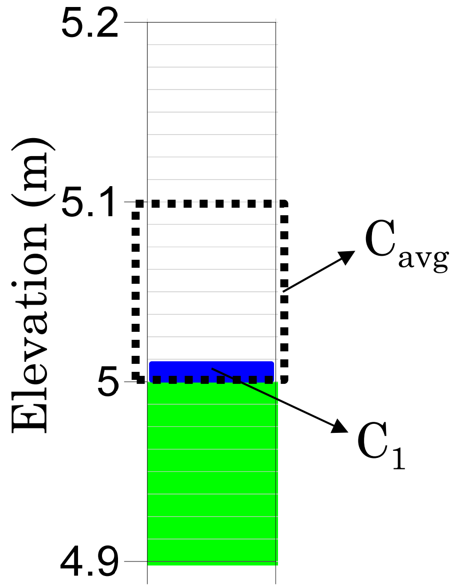


Local Domain Boundary Conditions

Scenario B – Global domain has larger vertical grid spacing.

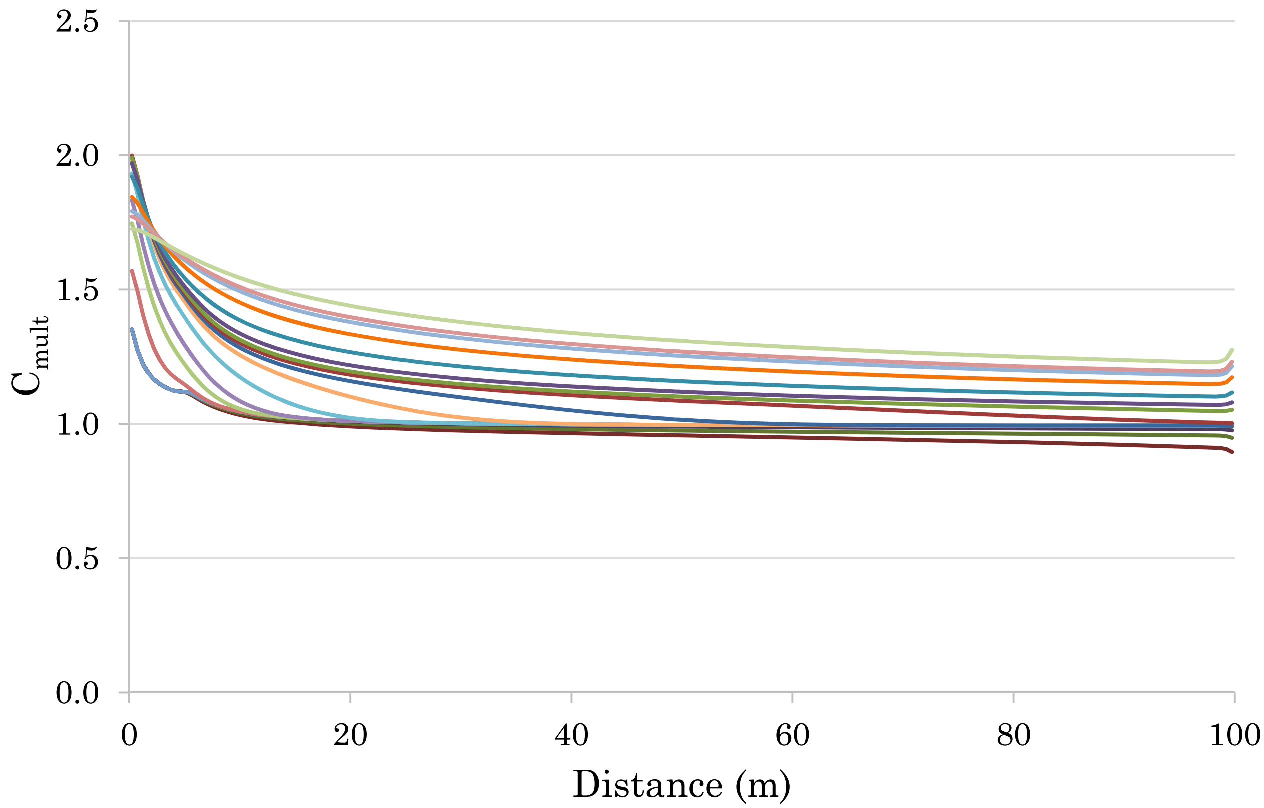


f_{mult} Trends (t = 3 to 85 y)



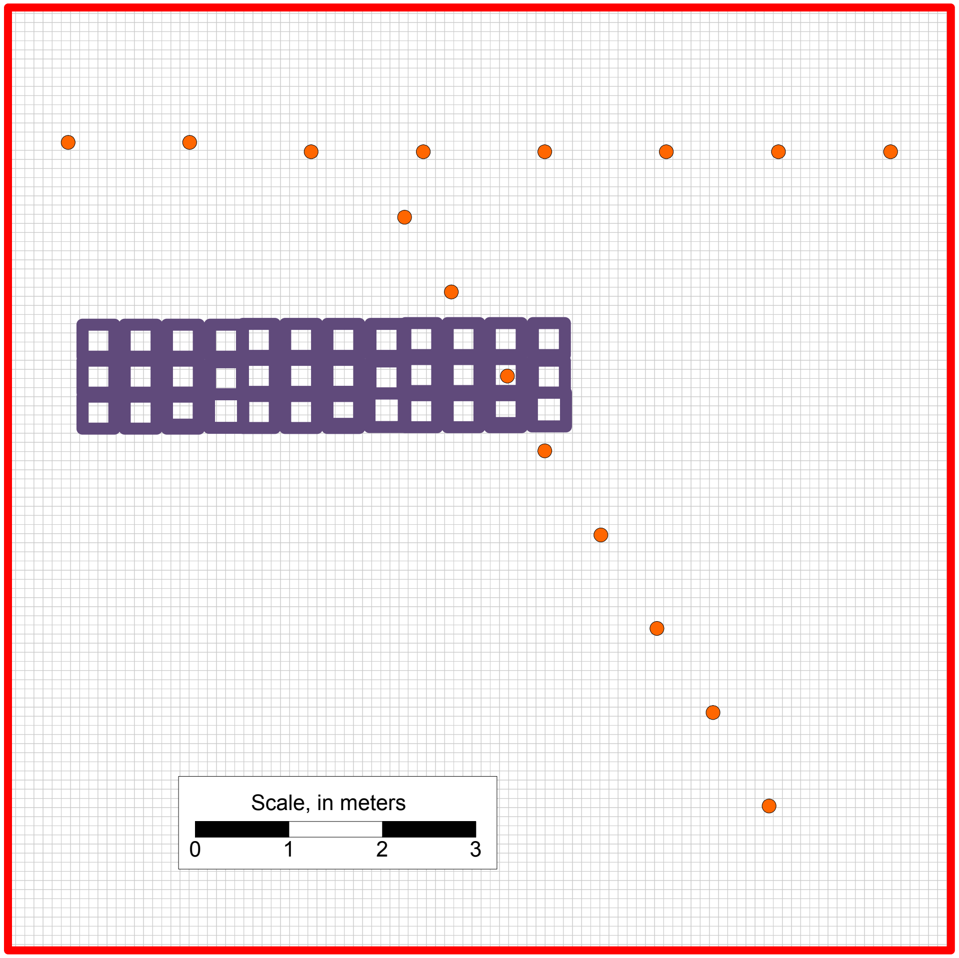
$f_{mult} = C_1 / C_{avg}$

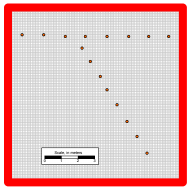
(travel time from source to d/g boundary ~ 2.5 years)



Narrow range in f_{mult} over x and time – suggests average may be used to define local domain boundary condition with coarser global domain grid spacing (to be confirmed).

Example Applications

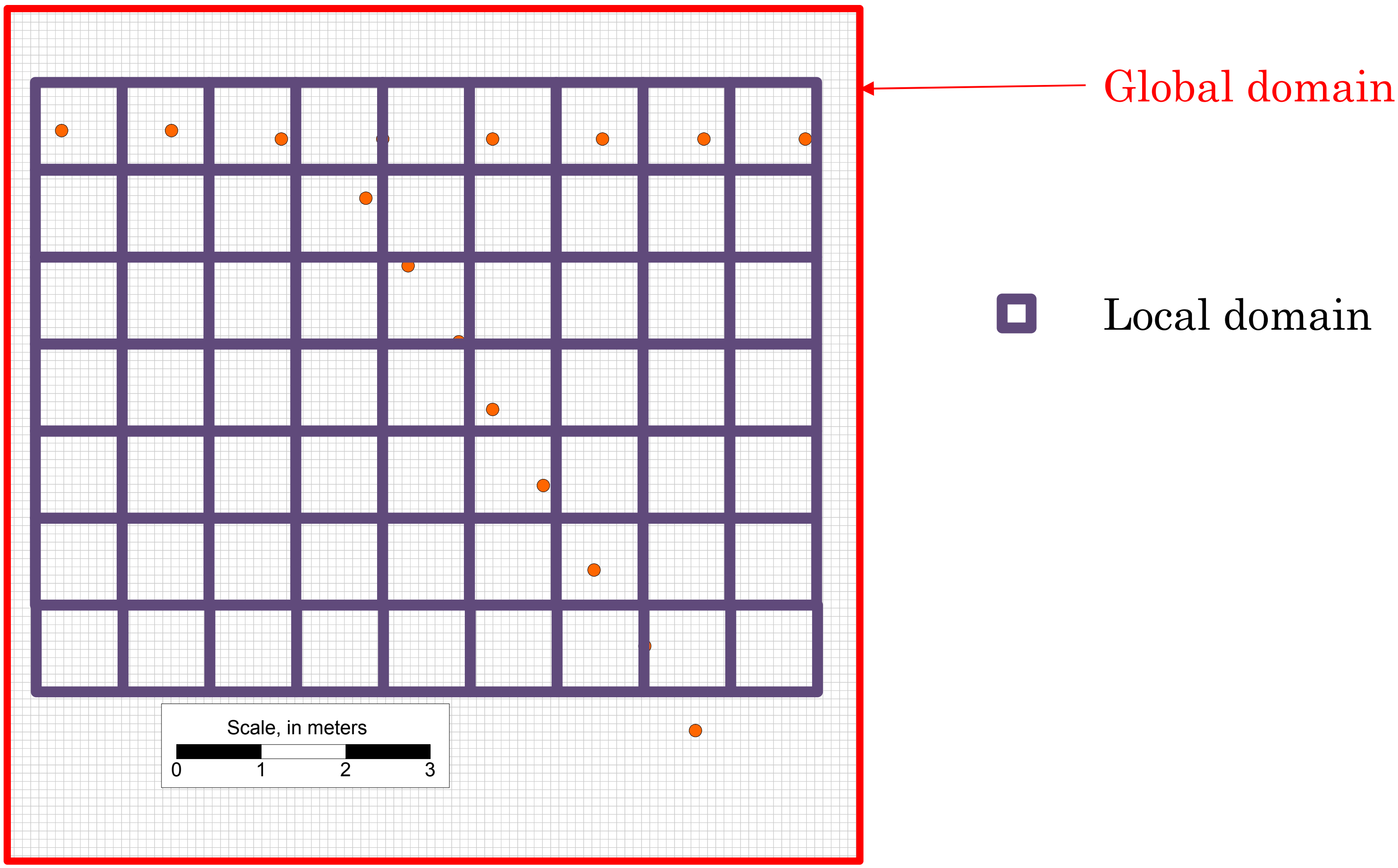




Global domain

Local domain

Example Applications



Modeling Goals at Complex Sites

- Improve process understanding

Interpretive Tool

- Optimize remediation performance
- Timeframe range (RTF)
    - Establish realistic expectations