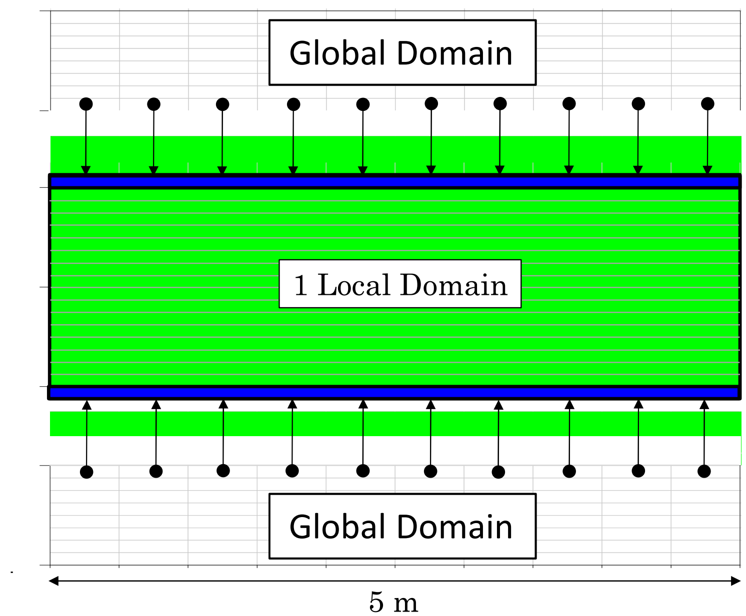
In-Situ Remediation (ISR-MT3DMS™) Local Domain Approach



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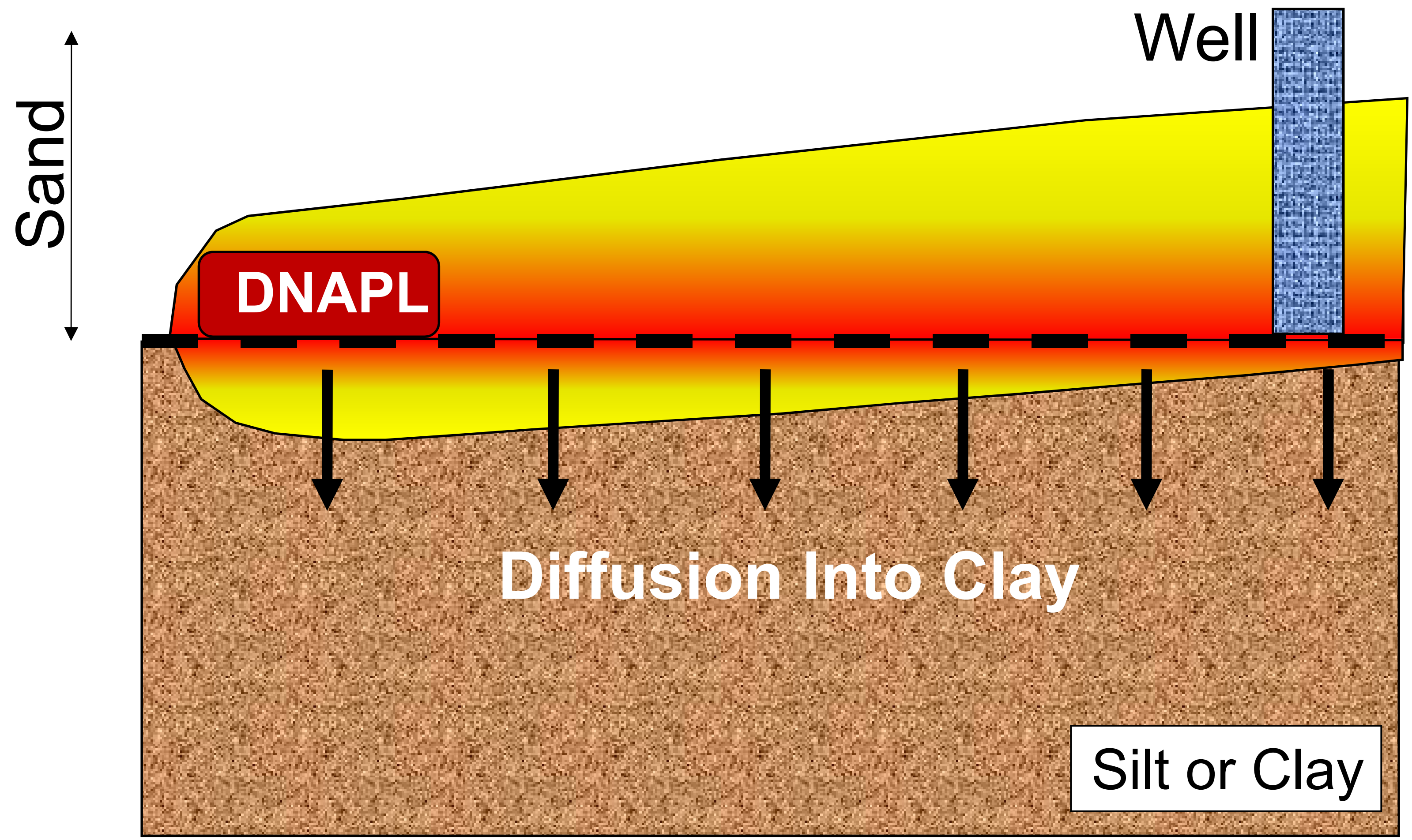
Forward Diffusion



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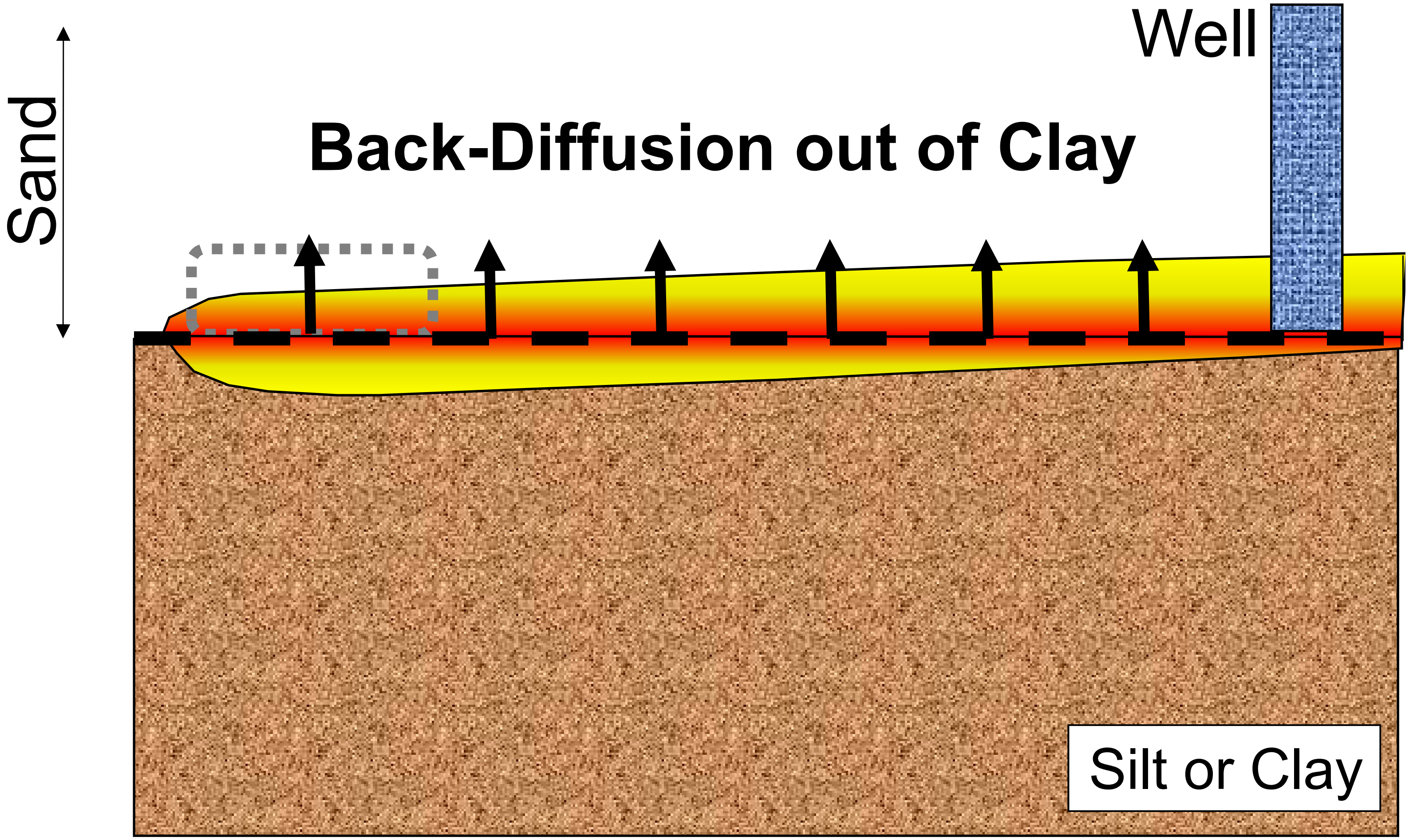
Back-Diffusion



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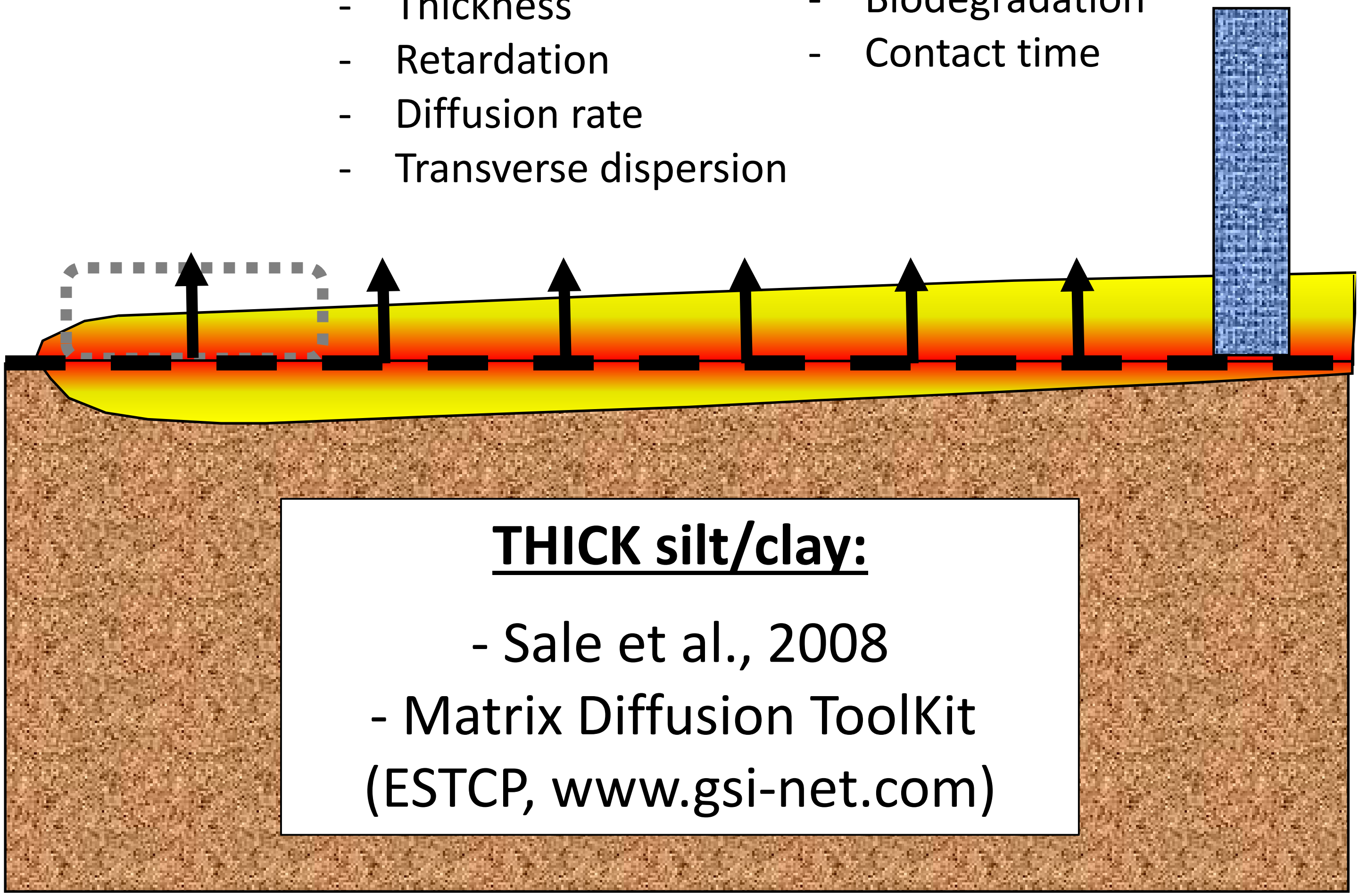
Factors Influencing Remediation Timeframe

Influencing factors:

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

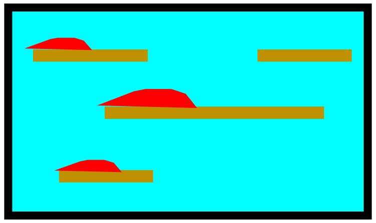


THICK silt/clay:

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

Introduction

- Modeling diffusion-dominated transport may require the addition of dozens to hundreds of layers to a model, depending on the thickness of silt/clay layers. This can have prohibitive costs, particularly for 3-D models which already incorporate a large number of rows and columns.

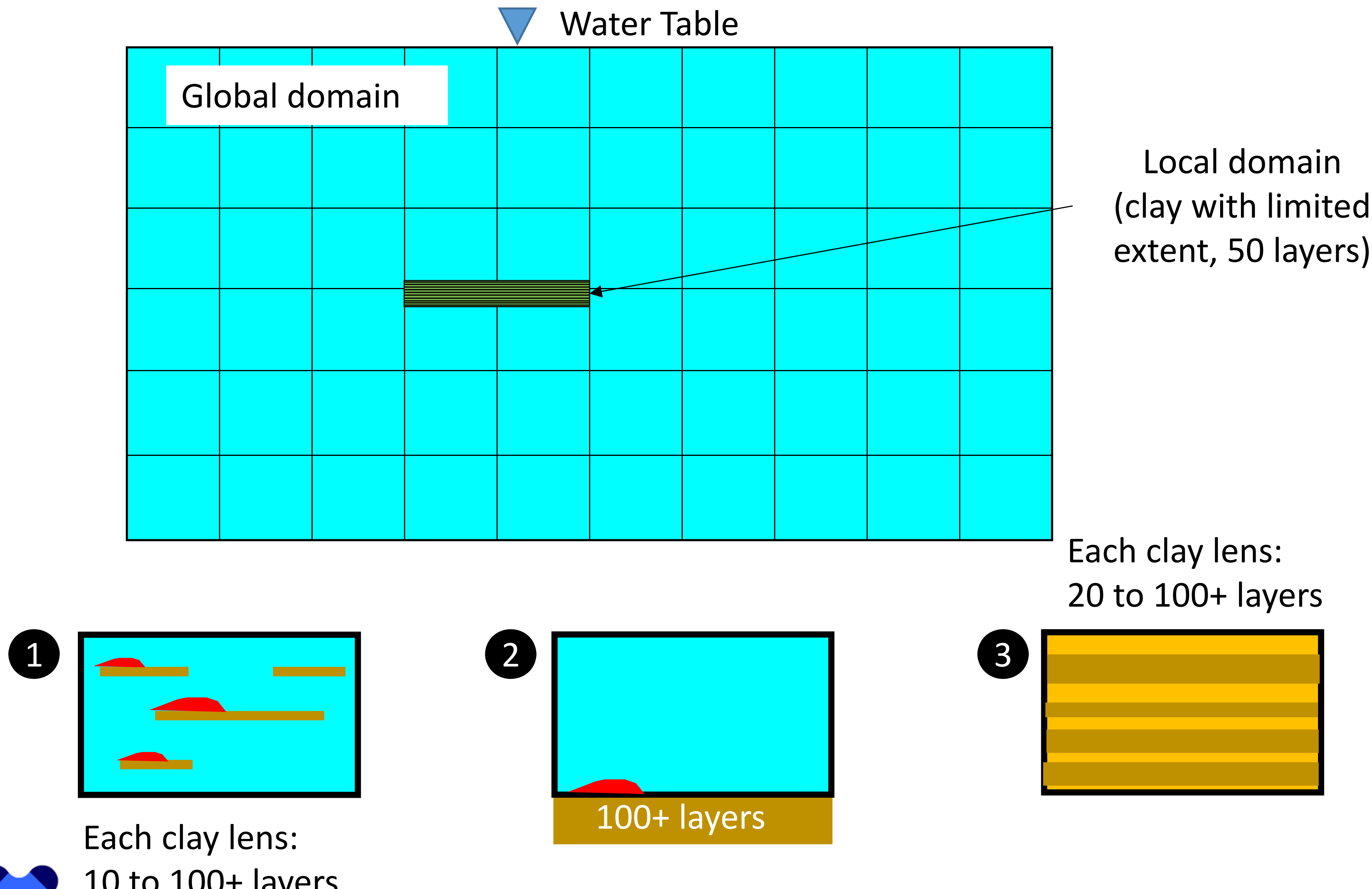


- While there are analytical solutions for simulating diffusion in thicker layers of silt/clay, a numerical model is often needed for thinner silt/clay layers, or when complex degradation reactions occur.

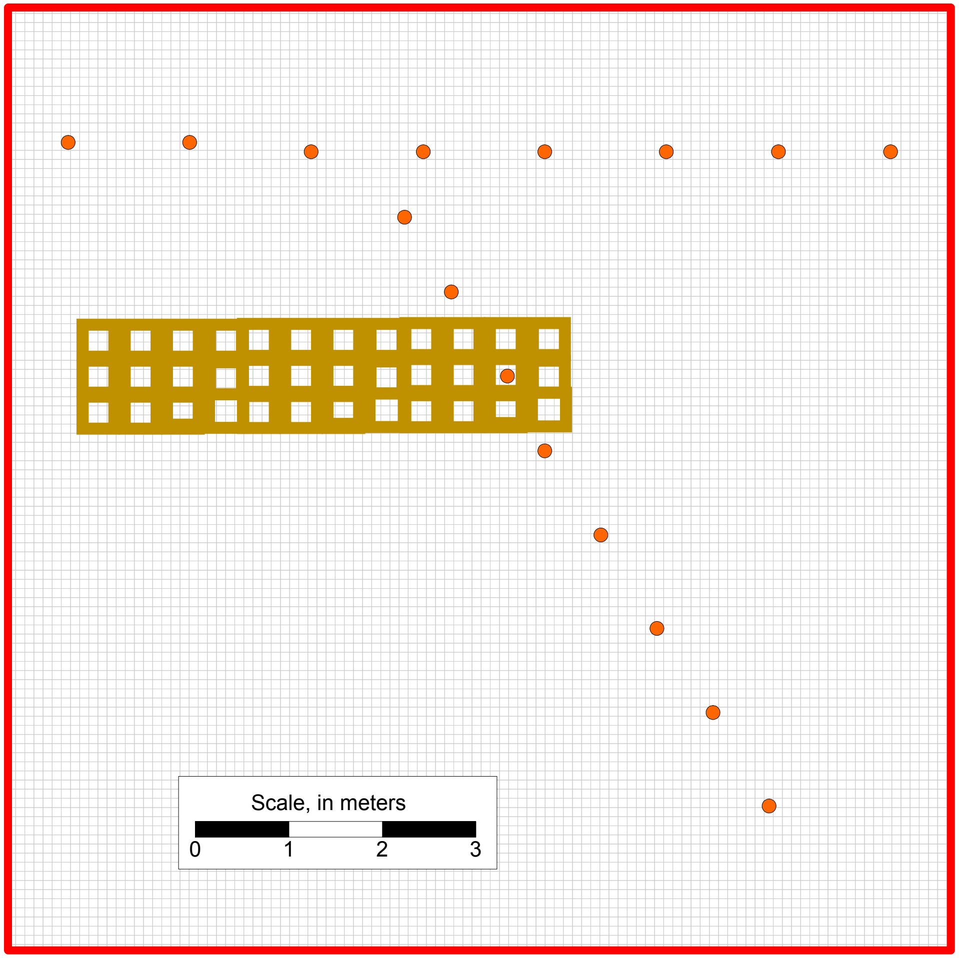
Introduction

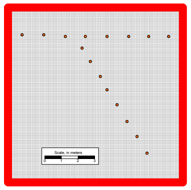
- ISR-MT3DMS™ offers the option to use local 1-D domains to represent diffusion-dominated transport. These 1-D domains are outside the global model grid, and thus may result in significant cost and time savings for some sites.
- The local 1-D domains incorporate the same reaction options that are available for the global model, so the effects of in-situ bioremediation or ISCO, for example, may be simulated in silt/clay layers.
- Users also have the option to specify different horizontal and temporal discretization for the local 1-D domains, relative to the global model.

Example Applications



Example Applications

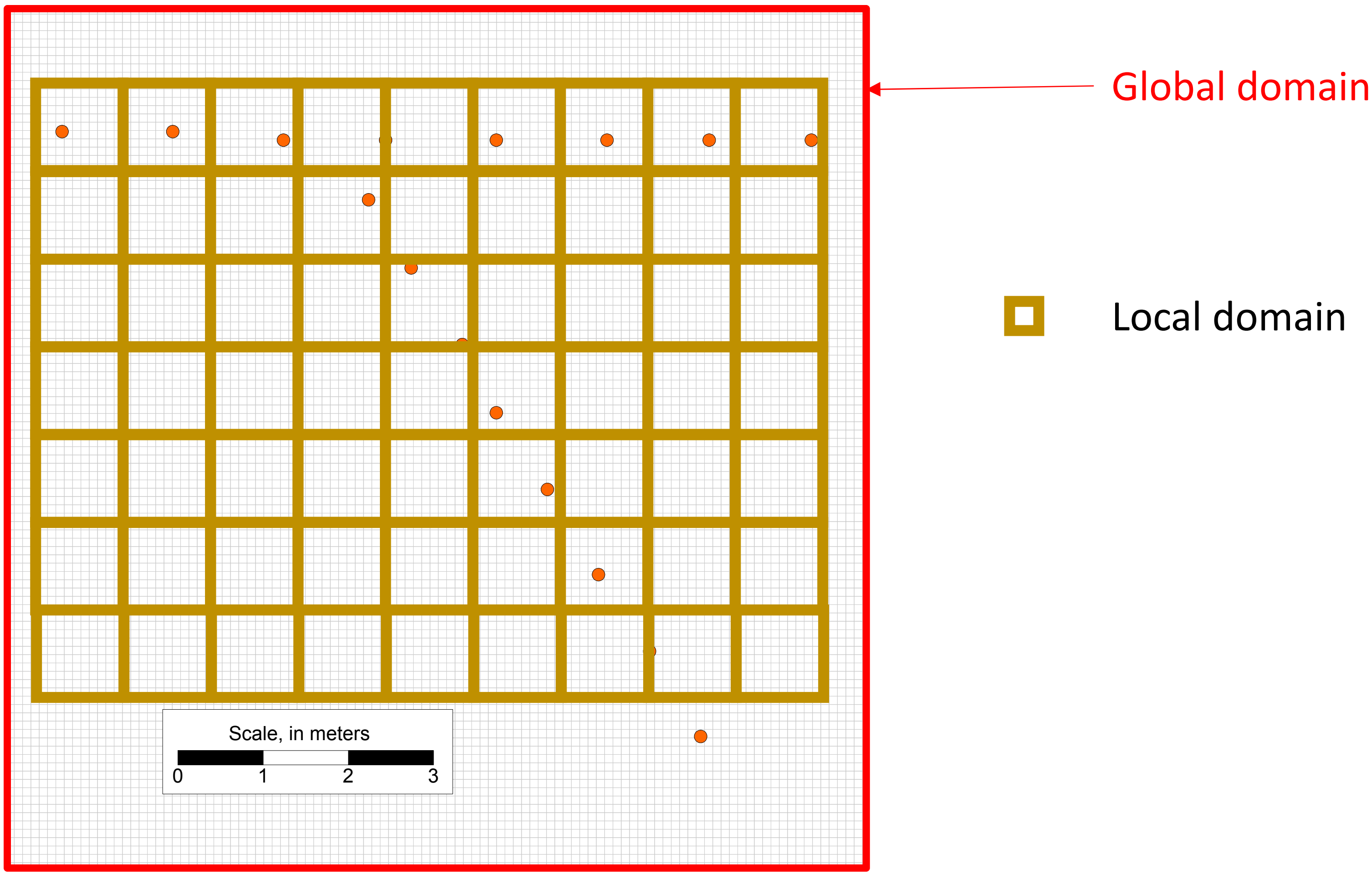




Global domain

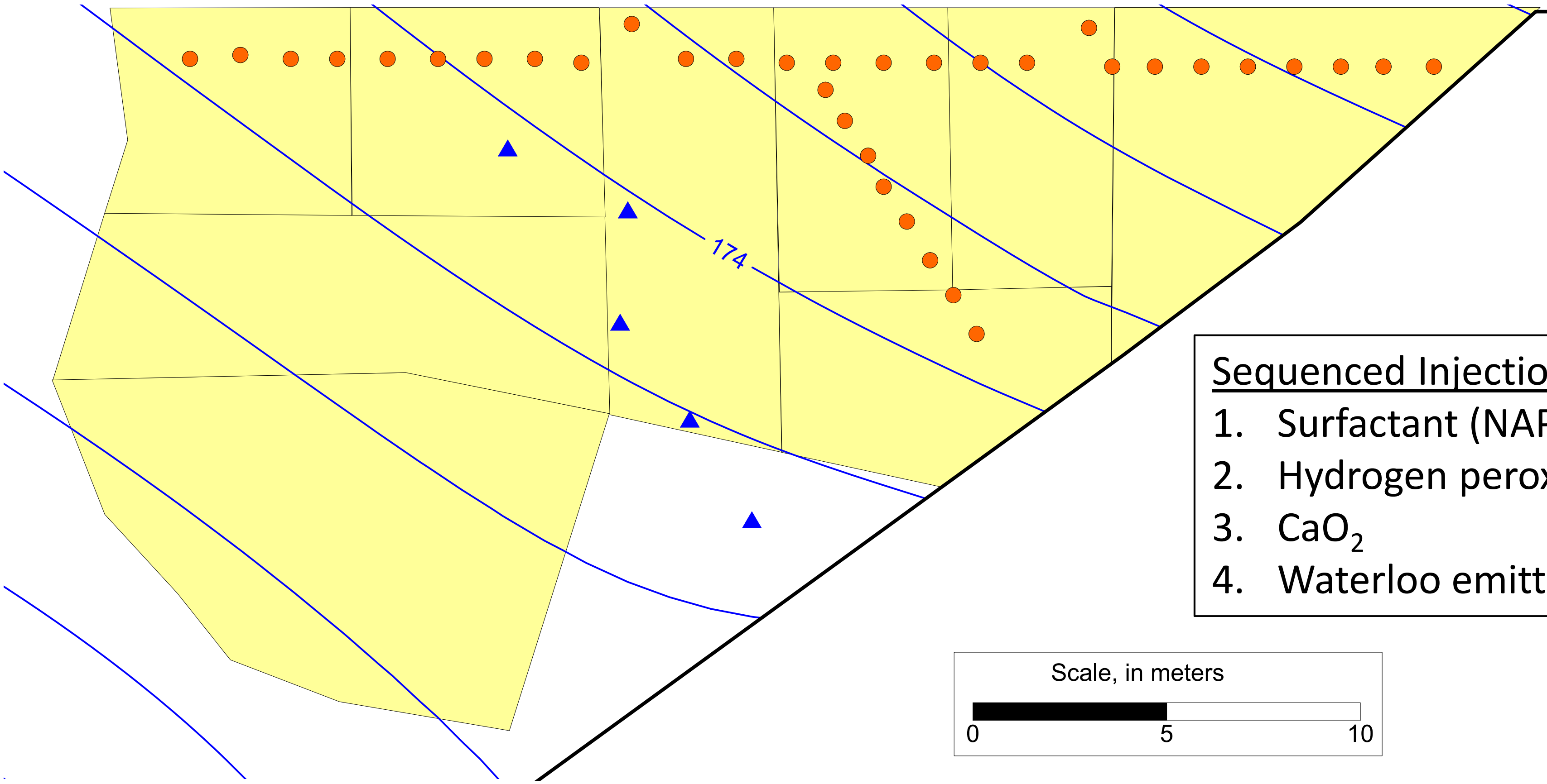
Local domain

Example Applications



Example #1: Ontario Site

Case Study #1 – Ontario Site



Sequenced Injections:

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

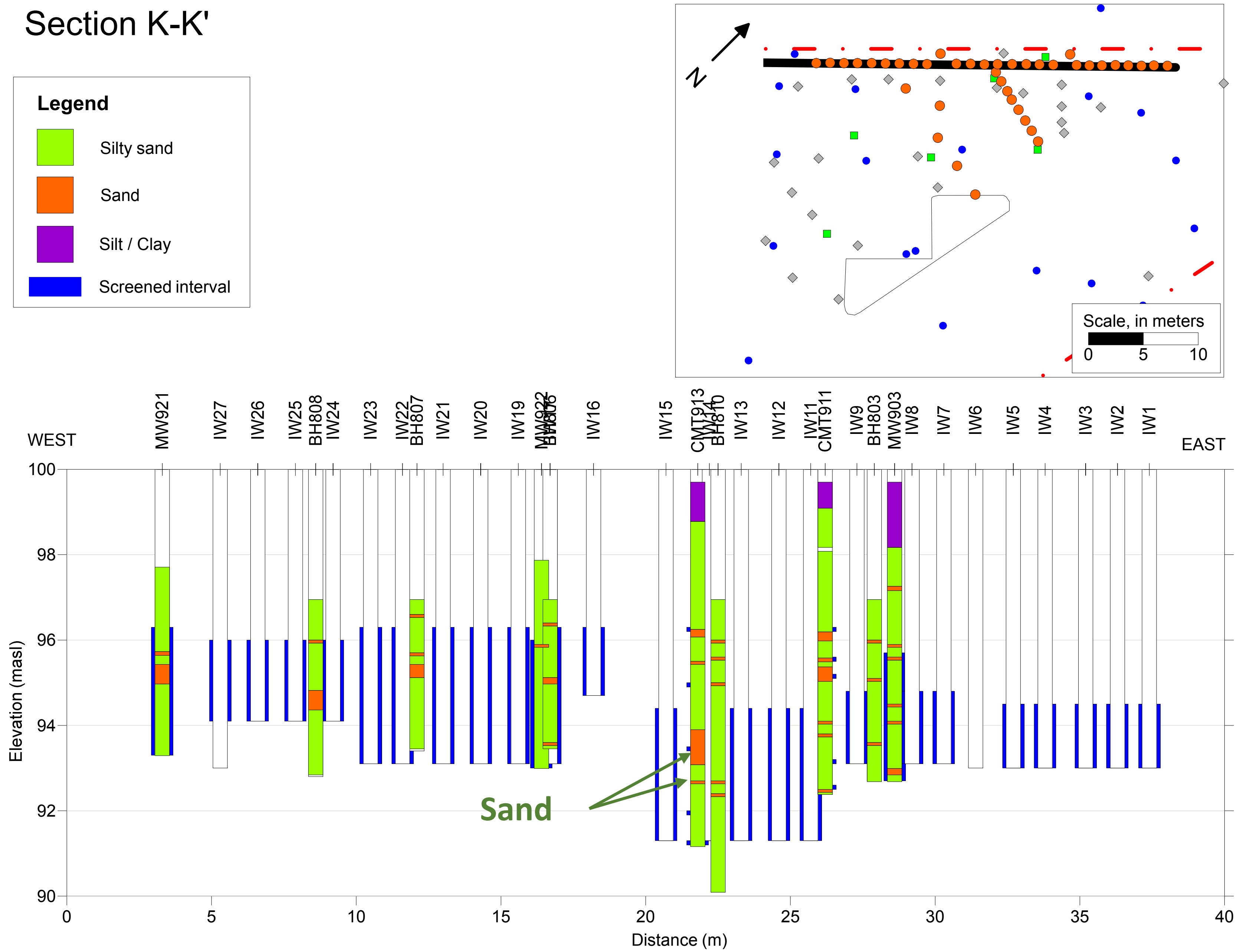
Treatment zone

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
IW13
IW12
IW11
CMT911
IW9
BH803
MW903
IW8
IW7
IW6
IW5
IW4
IW3
IW2
IW1
Elevation (masl)
100
98
96
94
92
90
Sand
0
5
10
15
20
25
30
35
40
Distance (m)

Model Grid

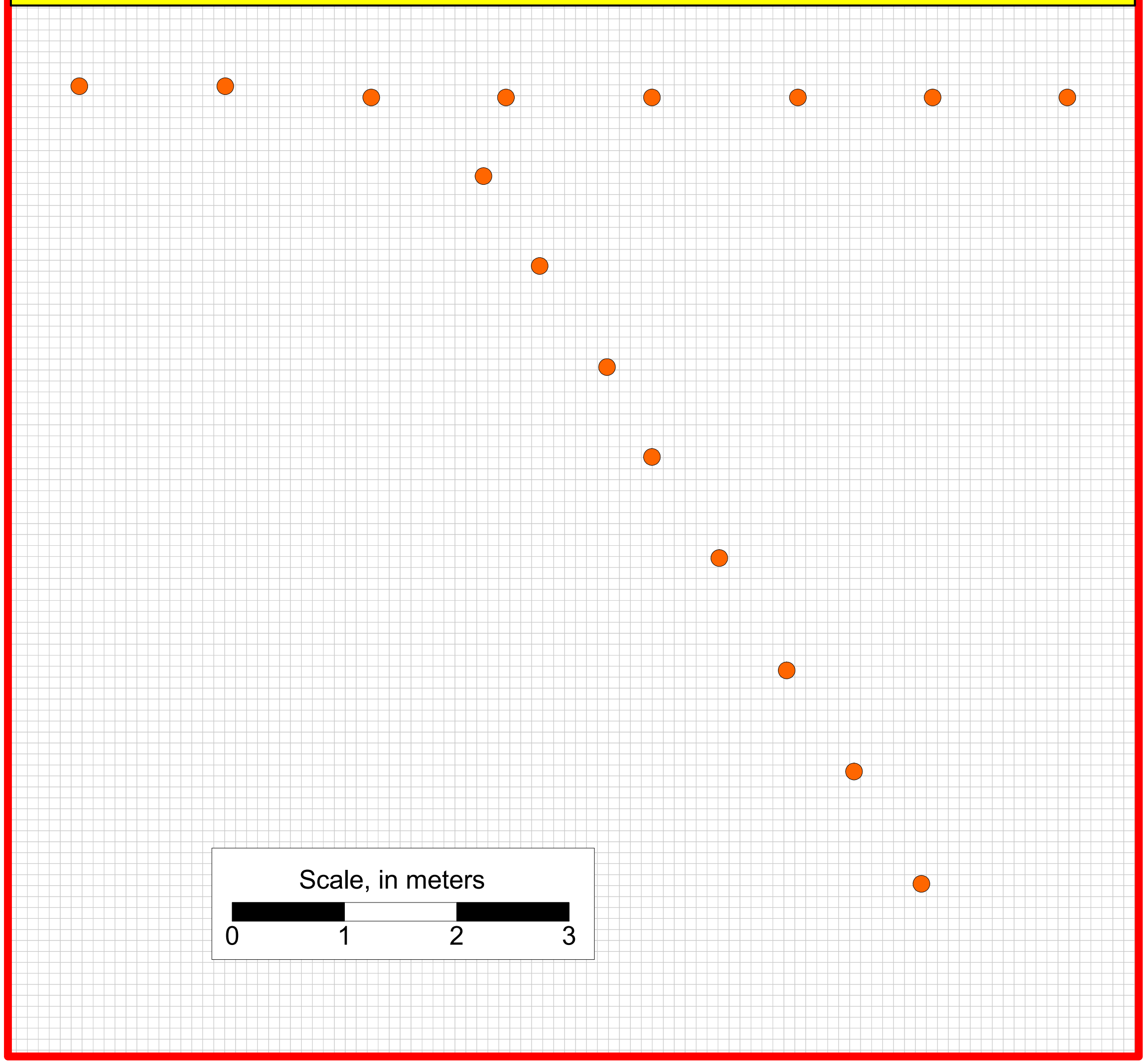
Minimum spacing = 4 inches
(Waterloo Emitter diameter)

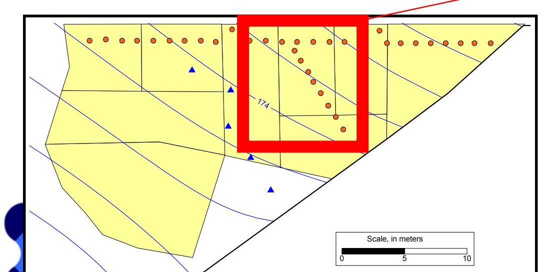
2-D: 450 columns, 280 rows

Time step = 0.05 d

Phase I – 5 solutes
(4-hour run-time)

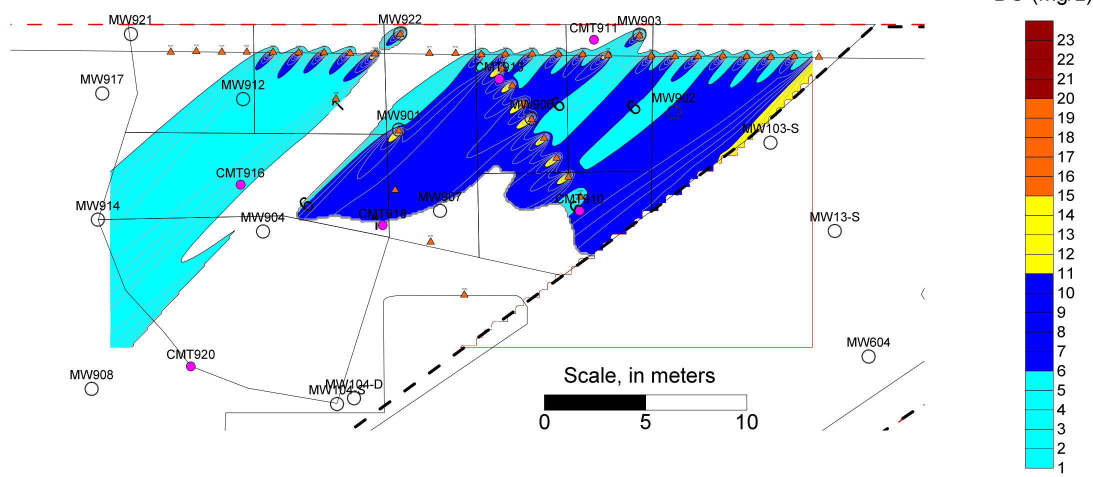
Phase I – Waterloo Emitters horizontal influence



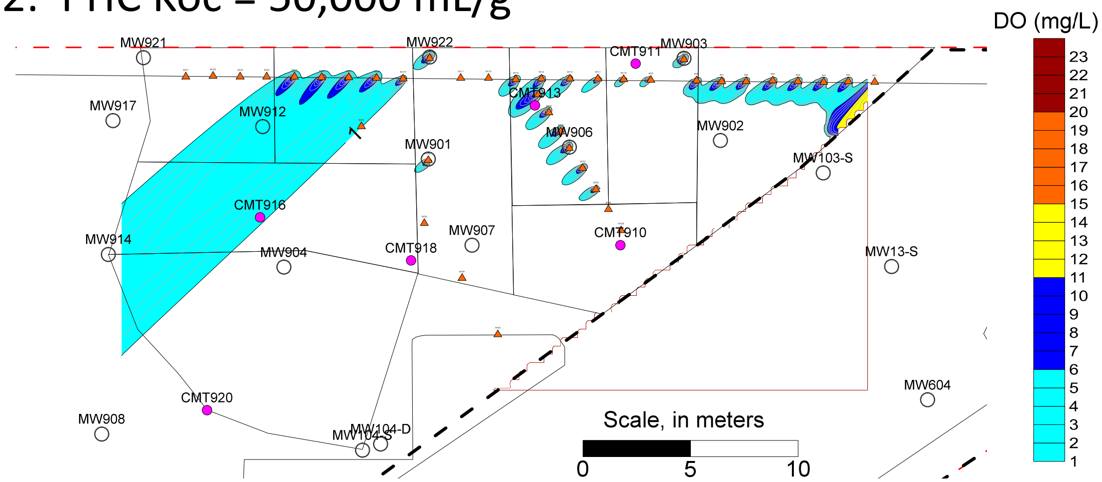


Phase I: Waterloo Emitters (t=3y)

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**

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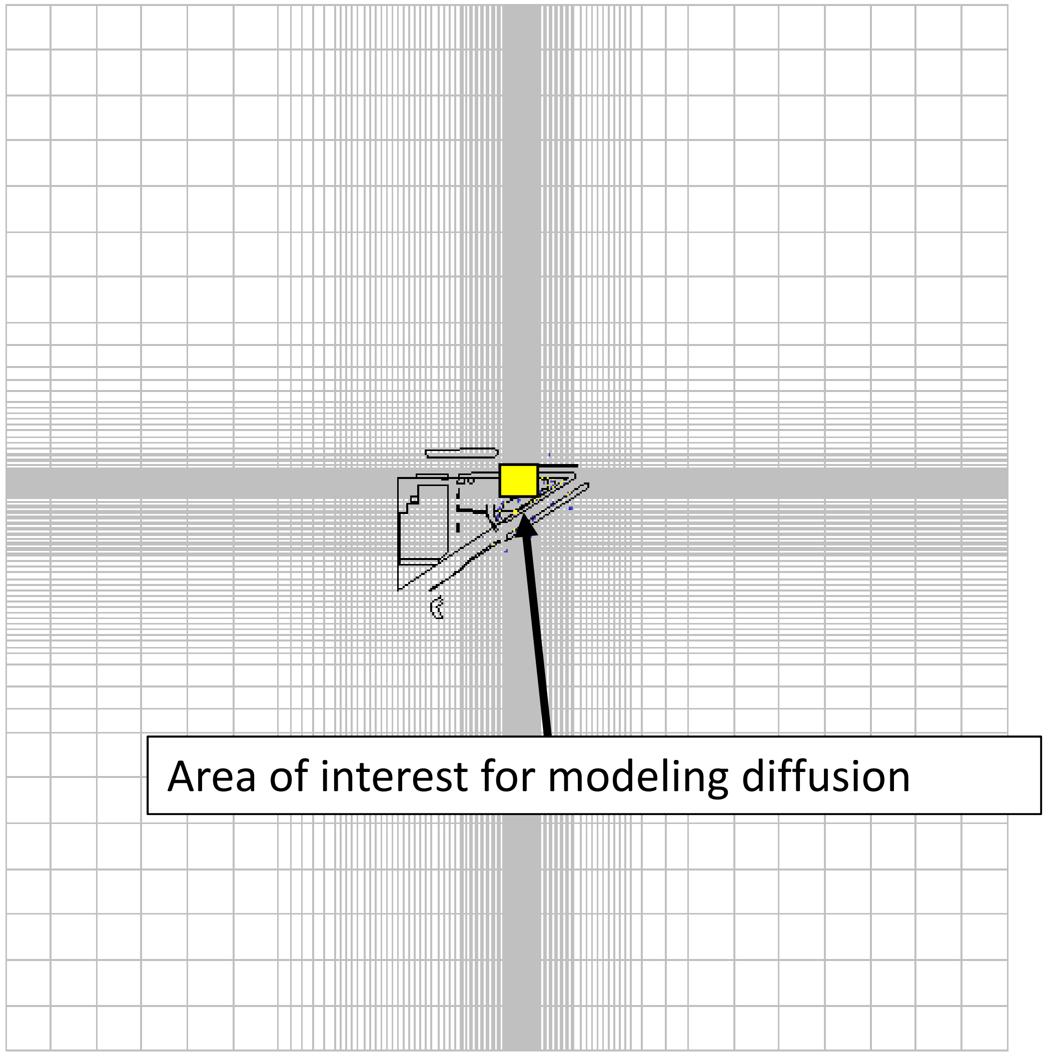
Case Study #1

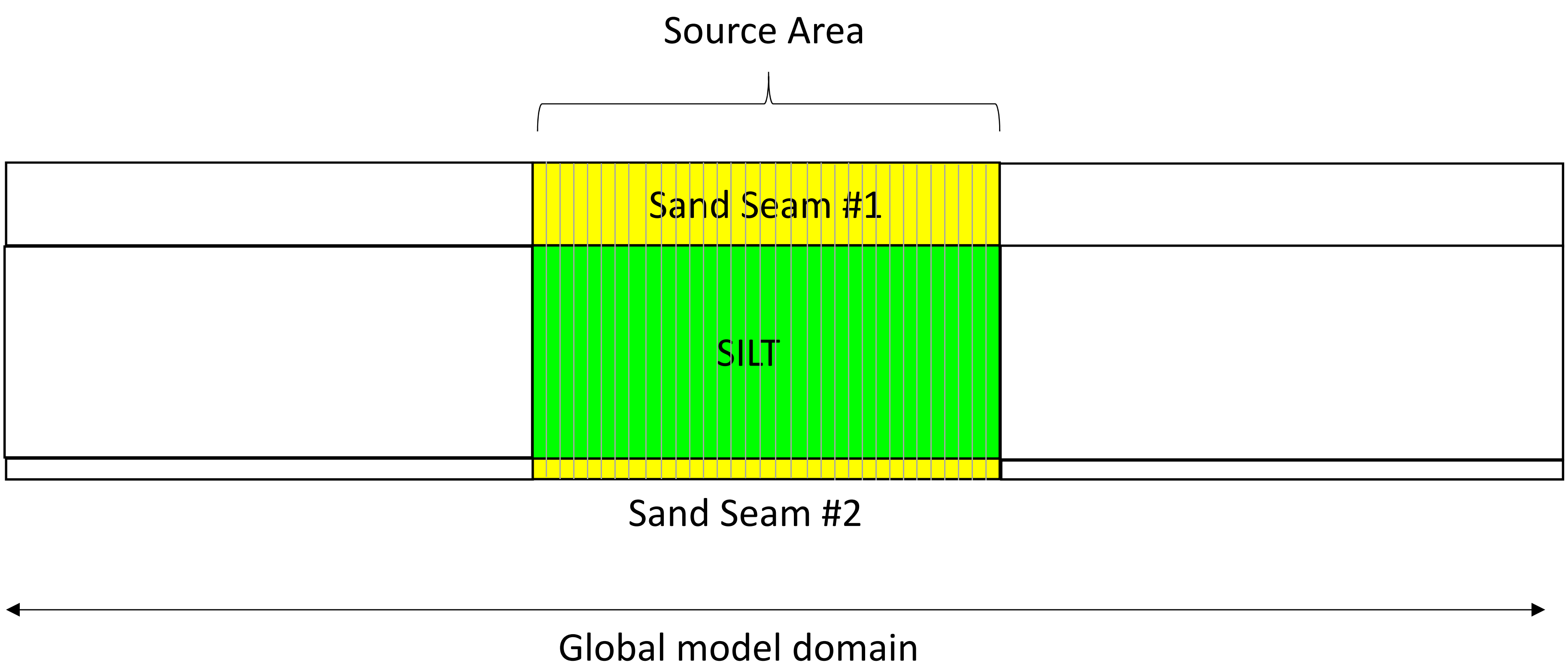
- Waterloo emitters used for passive oxygen injection, with approx. 1 meter spacing between wells
- Same wells also used for periodic active injections of oxygen-releasing compound, chemical oxidant, or surfactant (depending on the event)
- Tight spacing of passive injection wells required high resolution grid discretization to evaluate zone of influence from passive injections
- Geology is interbedded sands with tight fine-grained layers.
- Costs were prohibitive to develop a 3-D model for evaluating vertical diffusion-dominated transport in thick fine-grained layers, given tight horizontal spacing and number of species in reactive transport model.

Local Domain Approach

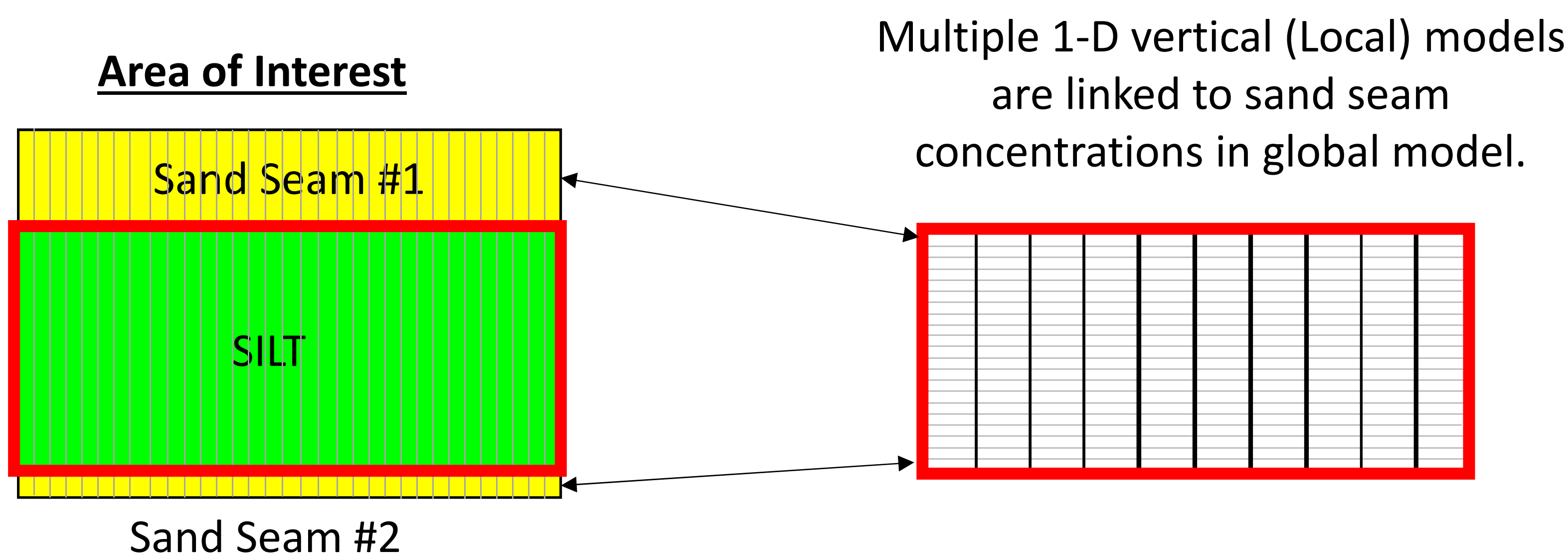
Global Model Domain



Cross-Section in Global Model (3 layers)



Local Model Domains for Silt (1-D Diffusion)



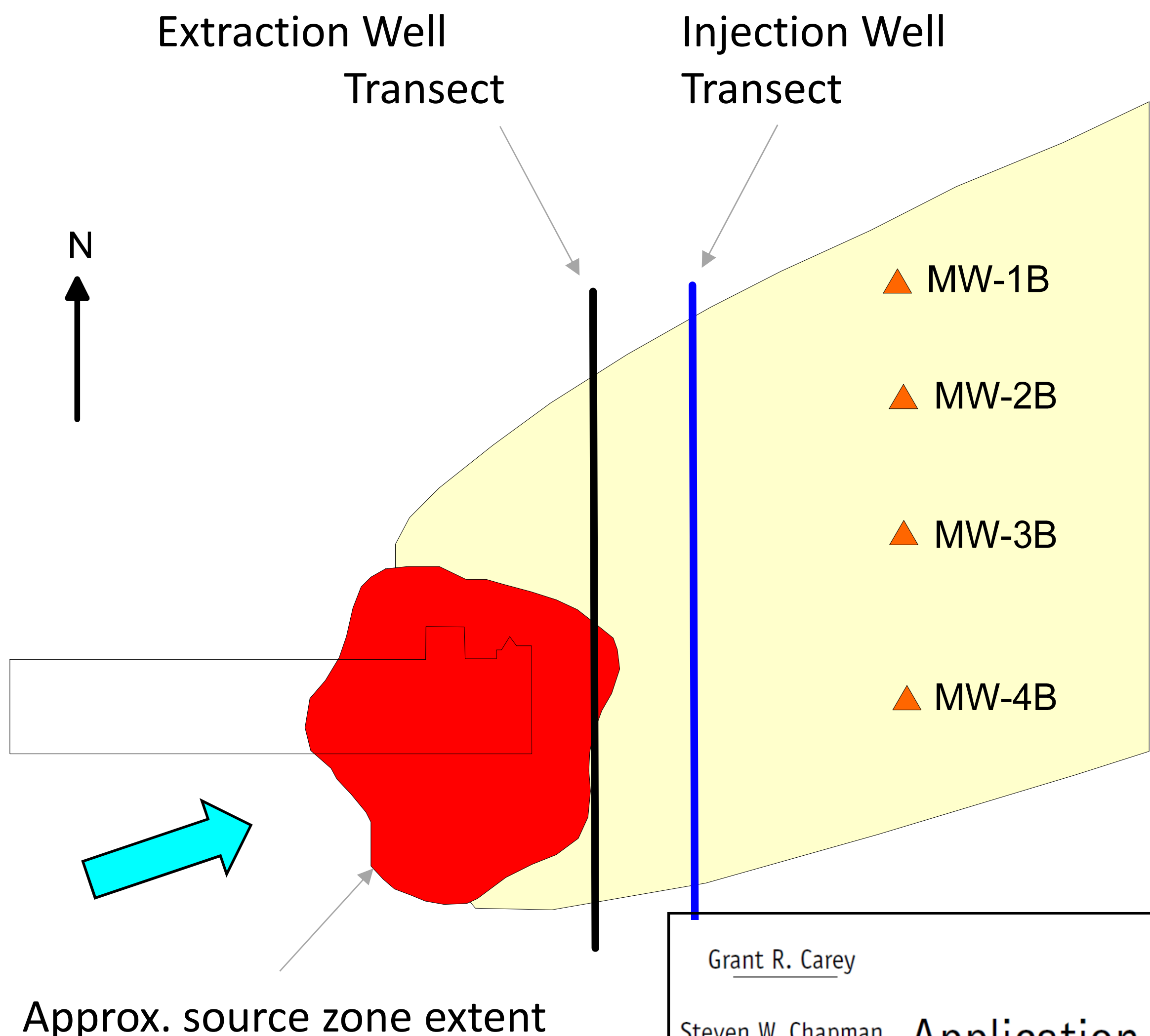
Silt layer is inactive to transport in global model.

Next Steps

- Using the local domain approach substantially reduced the size of the global model domain.
- We are currently simulating the influence of active remediation on mass in the finer-grained layers using the local domain approach.

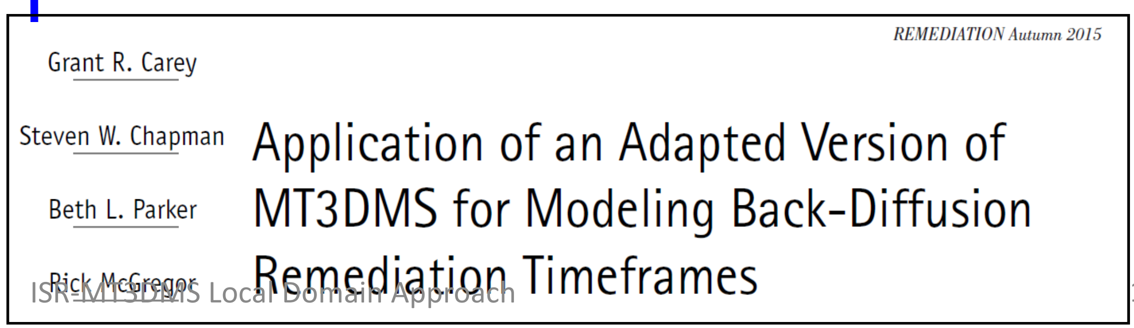
Case Study #2: Florida Site

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


REMEDIATION Autumn 2015

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

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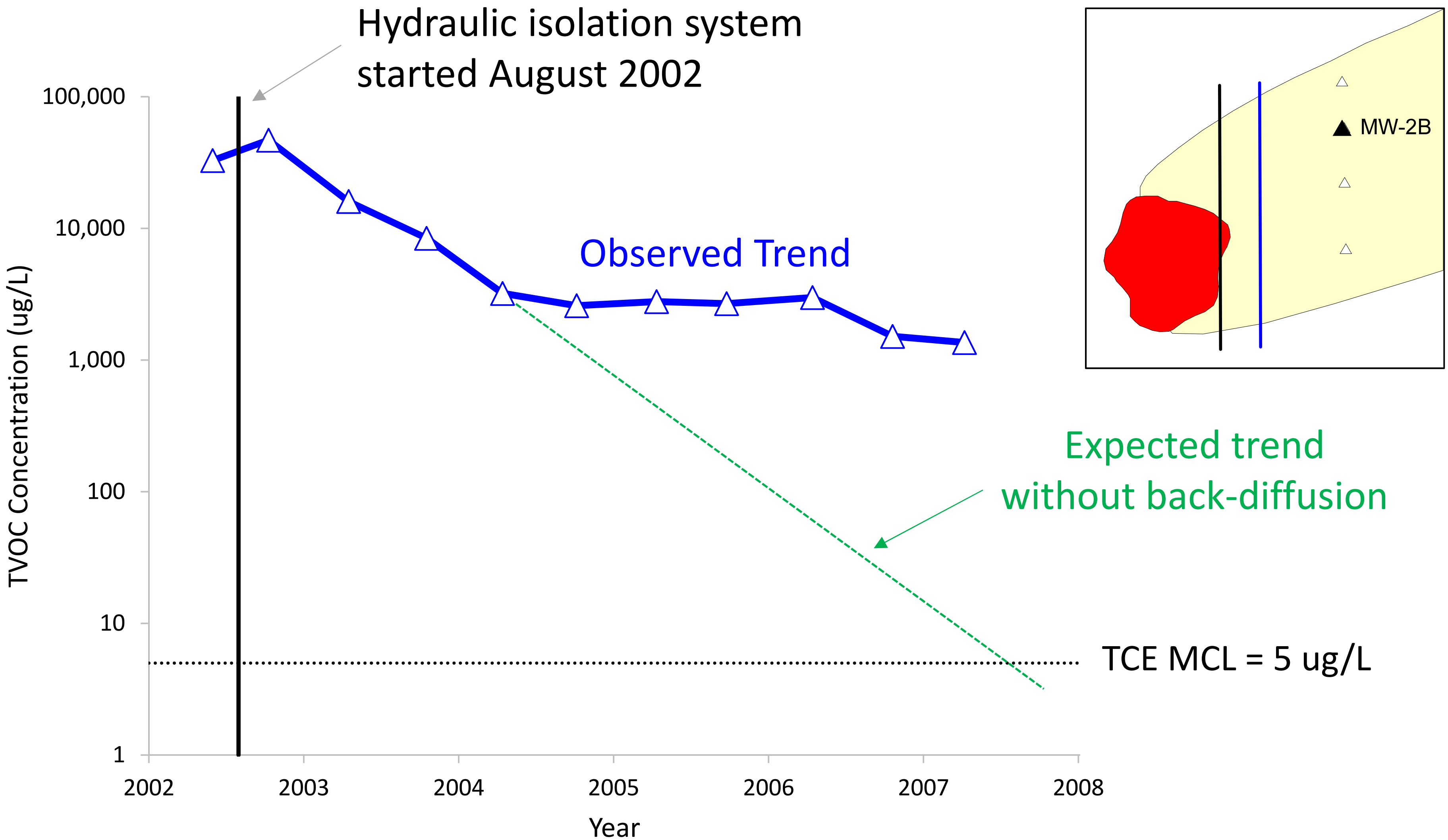
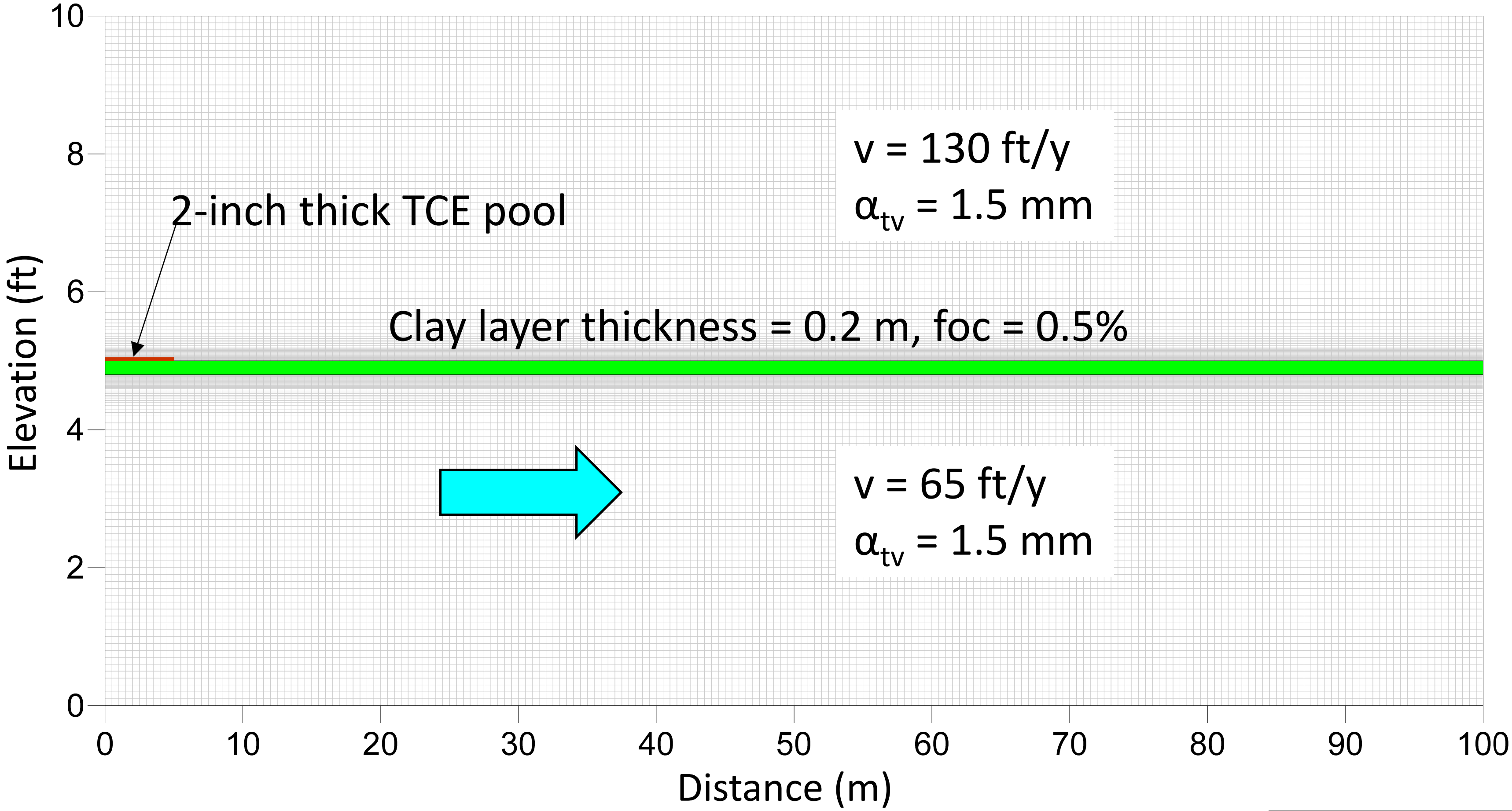
TVOC Trend After Source Containment



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)



Carey et al. (2015)

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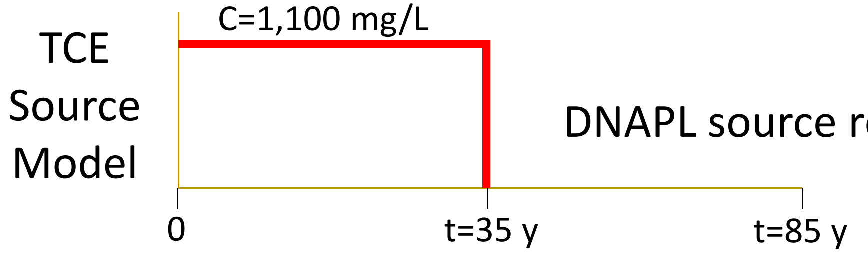
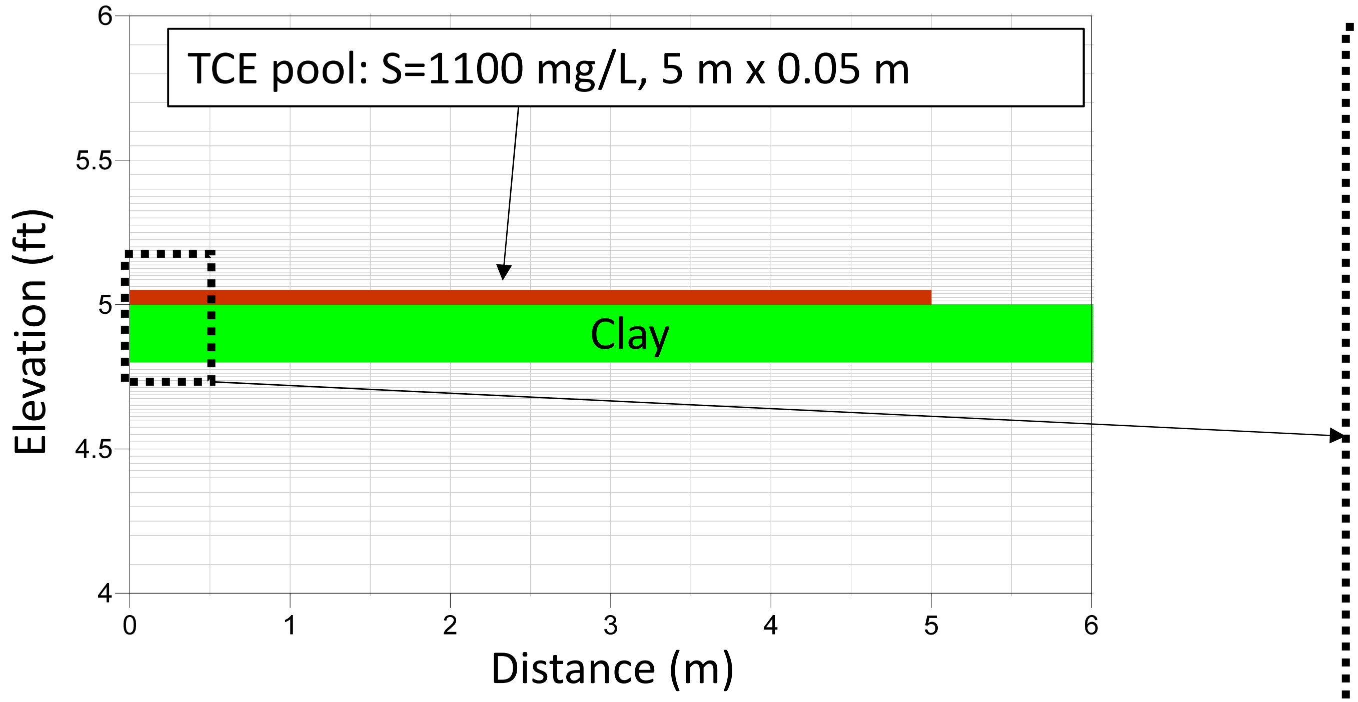
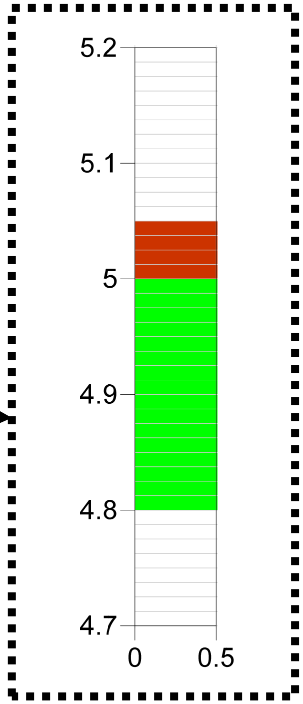
Source Characteristics



DNAPL source removed at t=35 y.



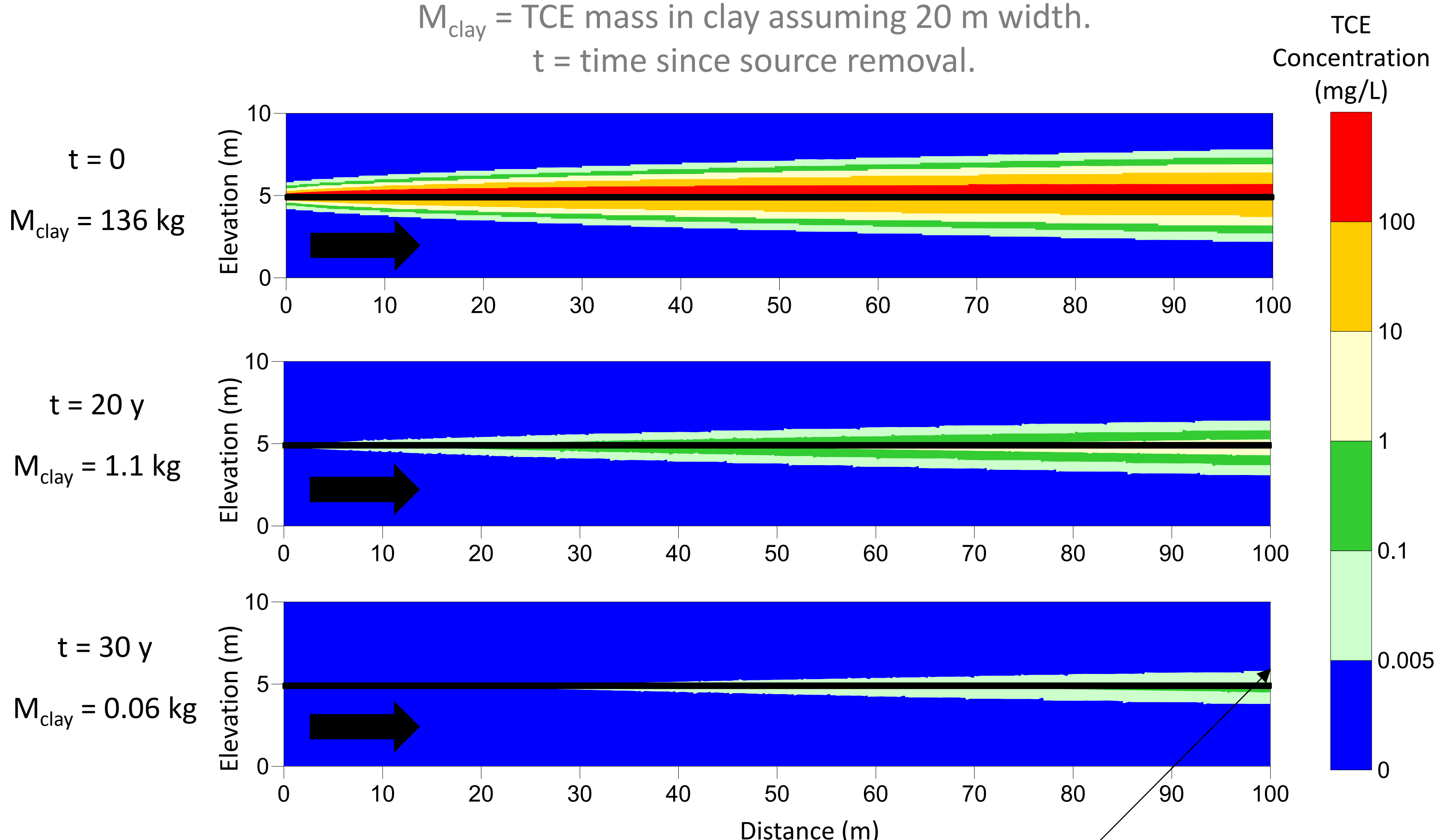
16 layers in clay



Carey et al. (2015)

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

Carey et al. (2015)

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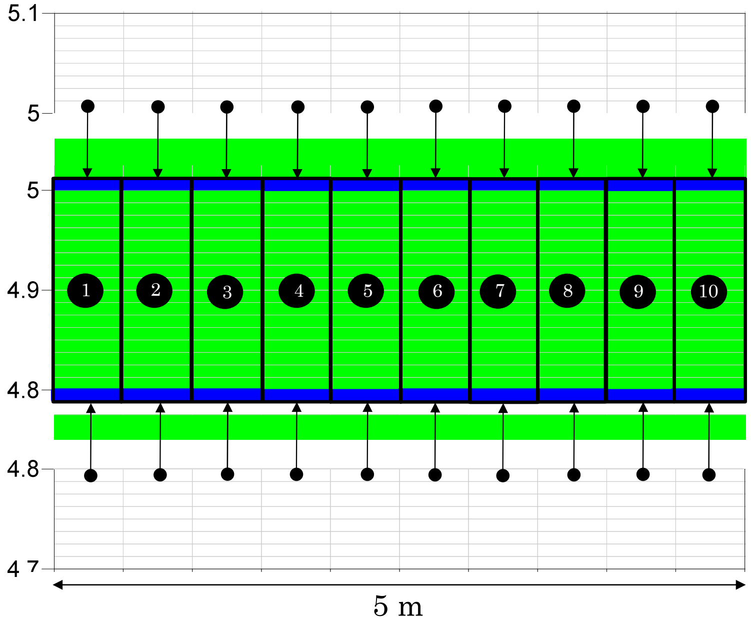
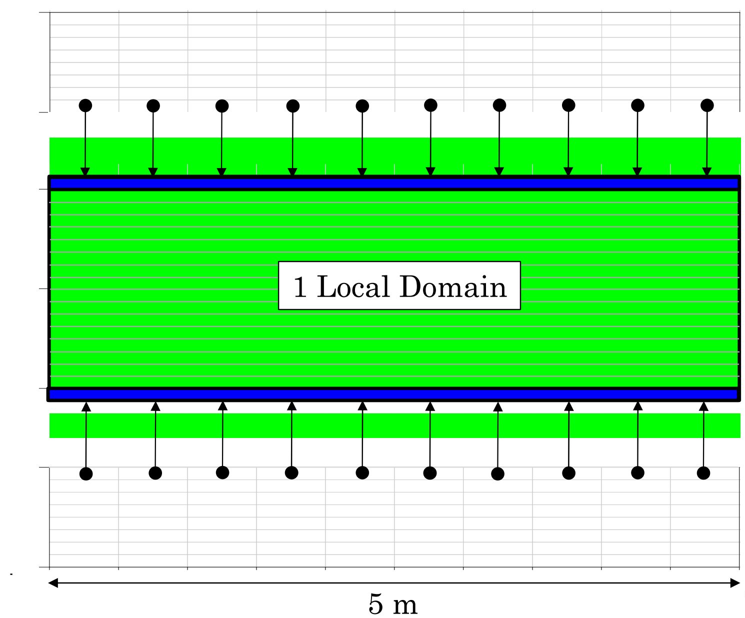
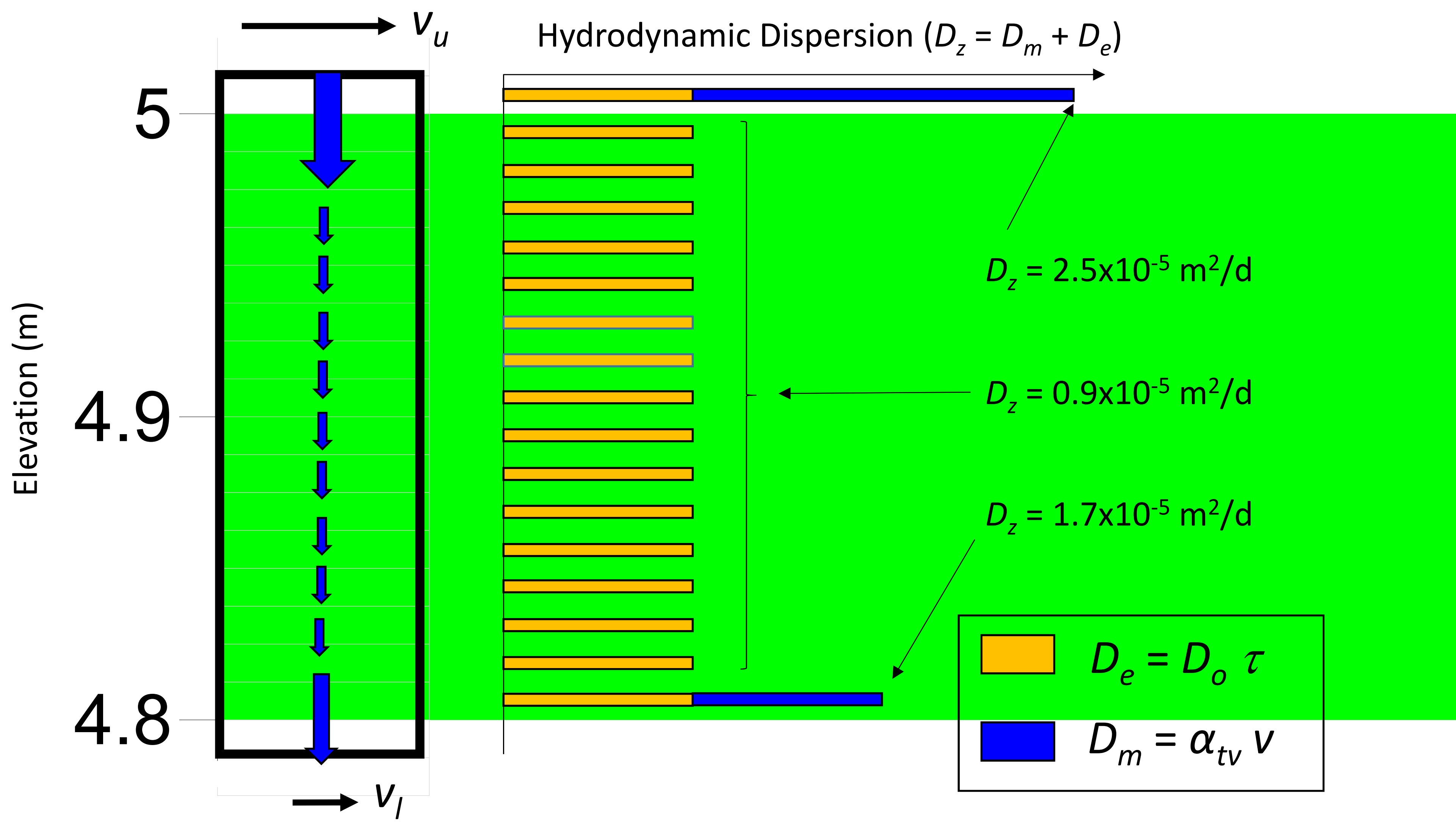
(a) Local domain models with Δx_{LD} = 0.5 m



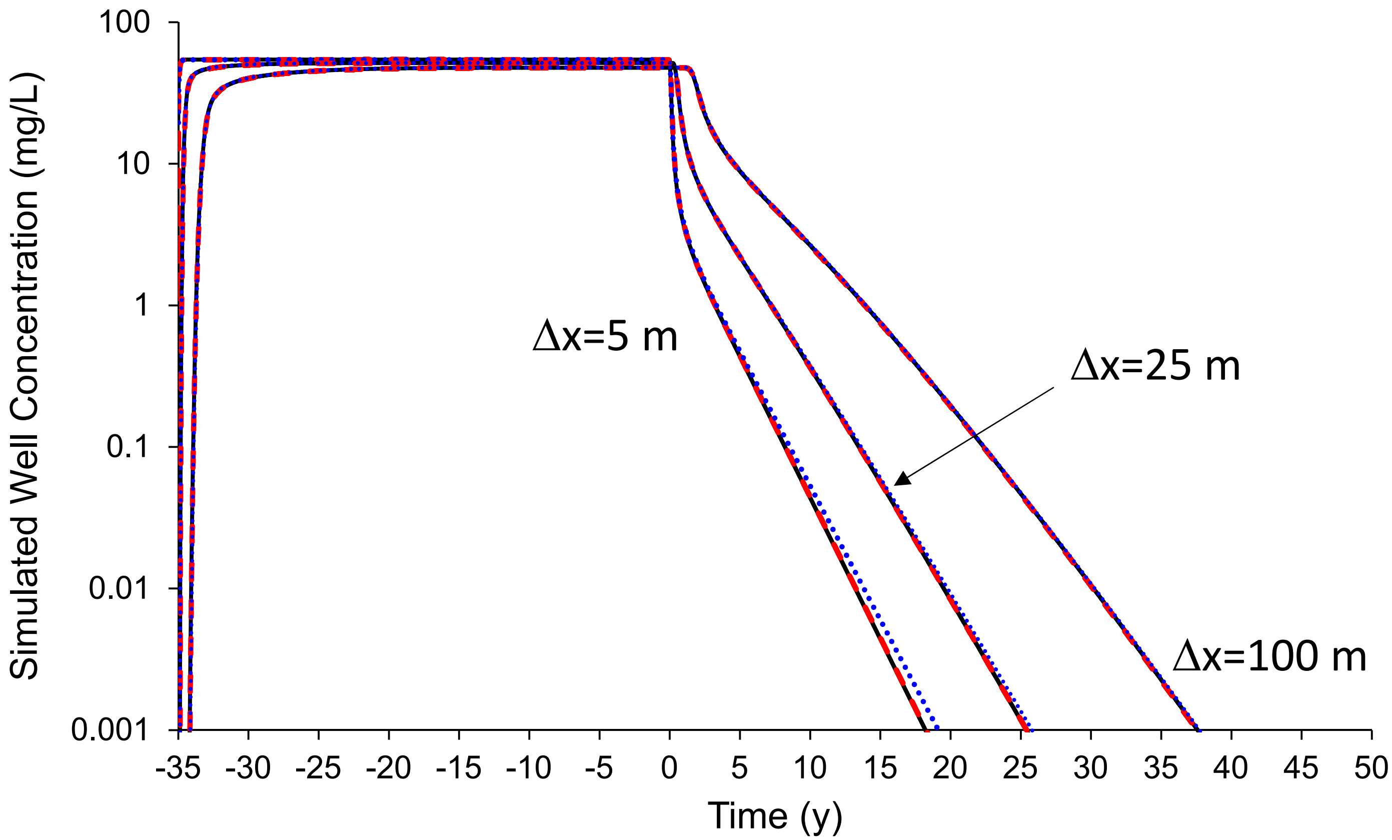
(b) Local domain models with Δx_{LD} = 5 m



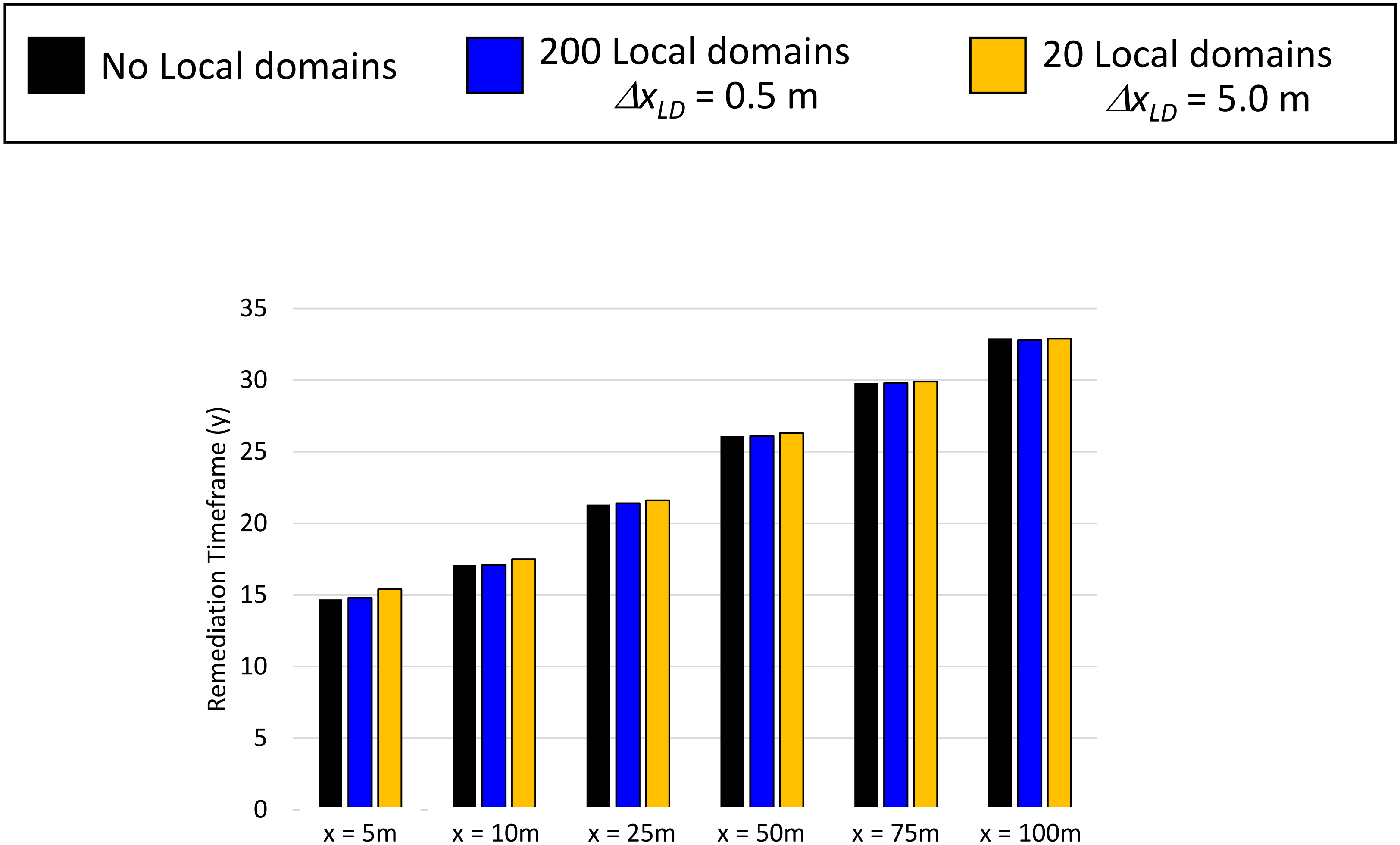
Conceptual illustration of local domains for two cases: (a) global and local domains have the same horizontal spacing; and (b) local domain has a larger horizontal spacing than the global domain grid.



Comparison of vertical mechanical dispersion (D_m) and effective diffusion coefficient (D_e) magnitudes in each grid cell of a 1-D local domain. Vertical mechanical dispersion is shown to be significant at the top and bottom clay-sand interfaces due to the use of a three-dimensional dispersion tensor and horizontal velocity components at each clay-sand interface. Application of a 1-D diffusion model will result in underestimation of the mass flux between the transmissive zone and clay layer.



Simulated monitoring well concentrations at x=5, 25, and 100 m. Solid lines represent the global domain model, dashed lines represent the local domain model with local grid Δx=0.5 m, and dotted lines represent the local domain model with local grid Δx=5.0 m.



Simulated remediation timeframe for three model cases: (a) no local domains are used; (b) 200 local domains are used with horizontal spacing of 0.5 m; and (c) 20 local domains are used with horizontal spacing of 5.0 m. Based on monitoring well with L_{screen}=3 m.

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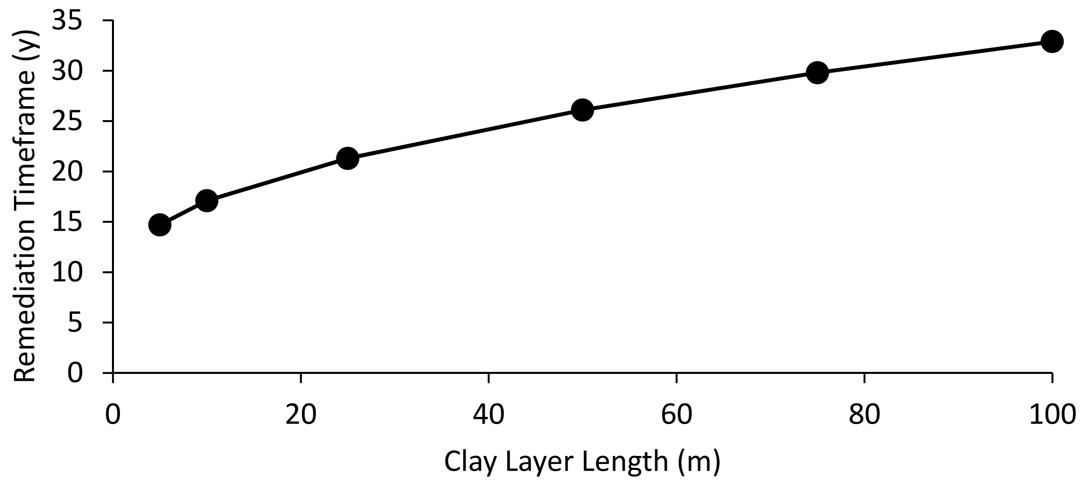
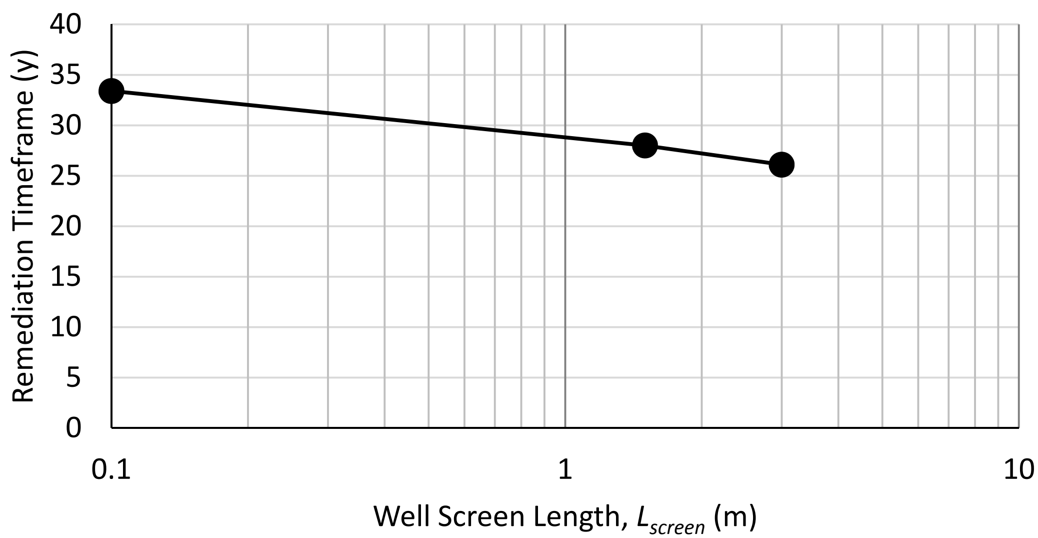
(a) Remediation timeframe versus clay layer length (L_{screen}=3 m)



(b) Remediation timeframe versus well screen length (x = 50 m)



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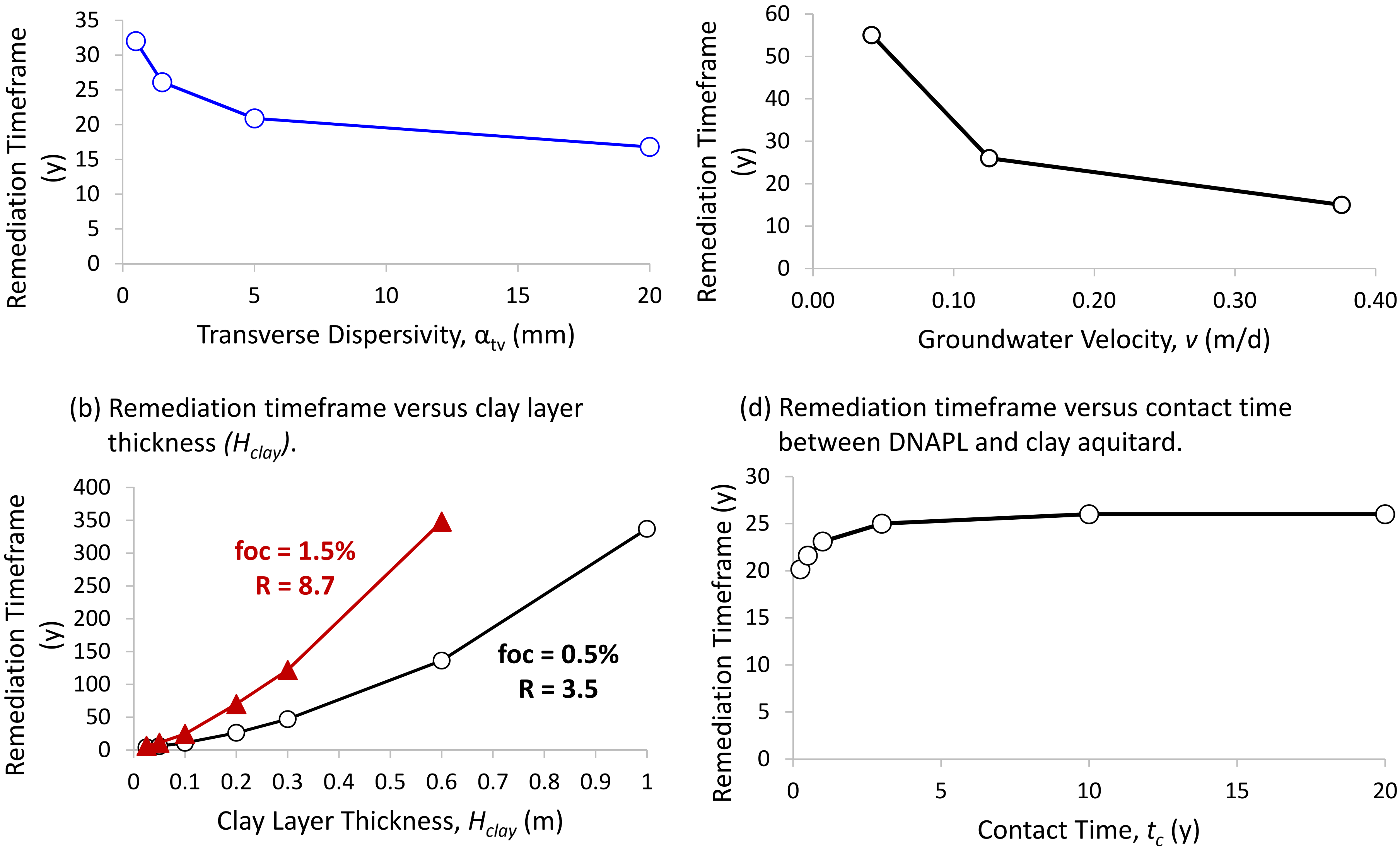
(a) Remediation timeframe versus α_{tv}.

(c) Remediation timeframe versus v.

(b) Remediation timeframe versus clay layer thickness (H_{clay}).

(d) Remediation timeframe versus contact time between DNAPL and clay aquitard.



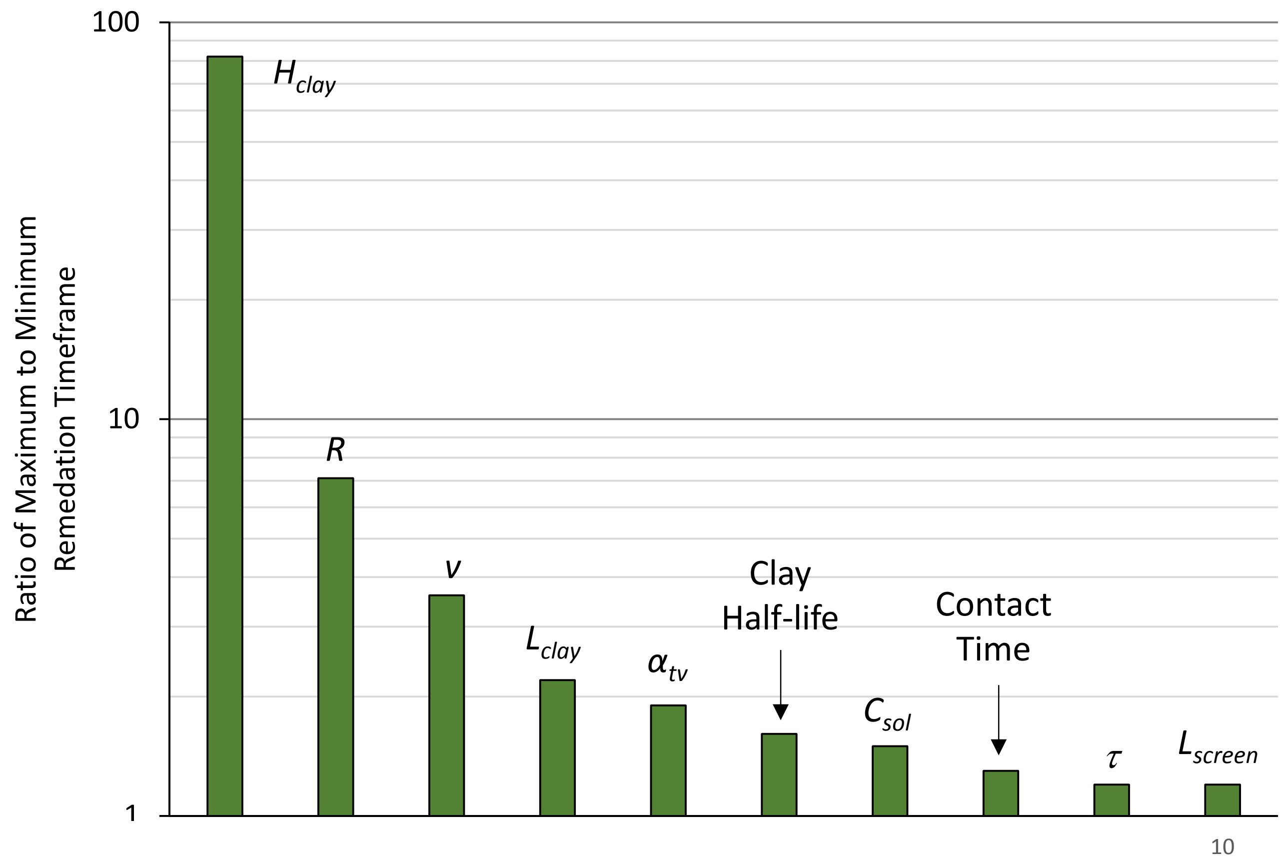


Exhibit 14 – Comparison of relative sensitivity of remediation timeframe to various input parameters, based on the ratio of maximum to minimum timeframe for each set of modeled parameter adjustments. H_{clay} is the clay layer thickness, R is the retardation coefficient, v is groundwater velocity, L_{clay} is the length of the clay layer, C_{sol} is solubility, τ is the tortuosity coefficient, and L_{screen} is the monitoring well screen length. Based on clay layer length of 50 m and well screen length of 3 m unless except for L_{clay} and L_{screen} parameter adjustments.