Site Characteristics Influencing Back-Diffusion

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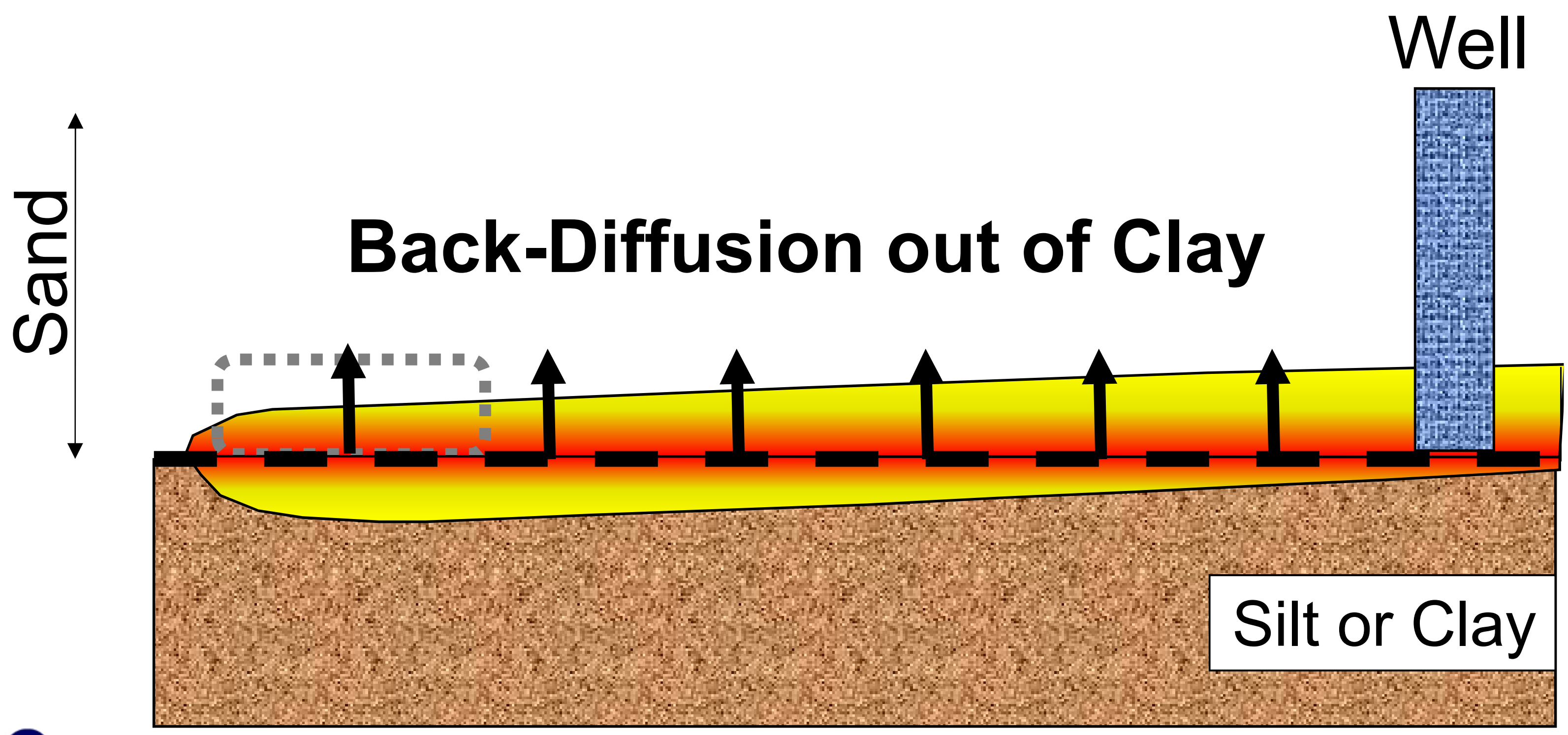

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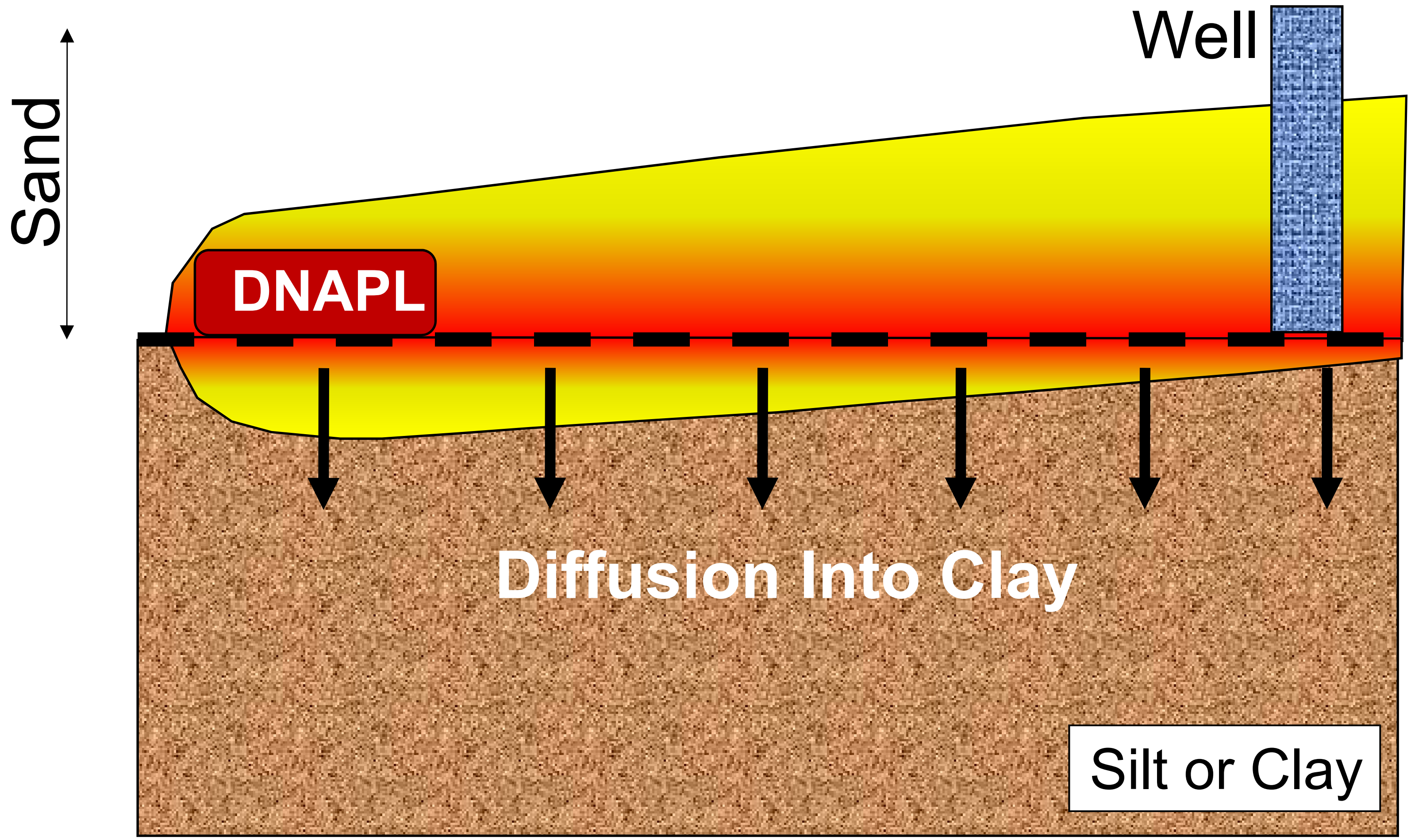
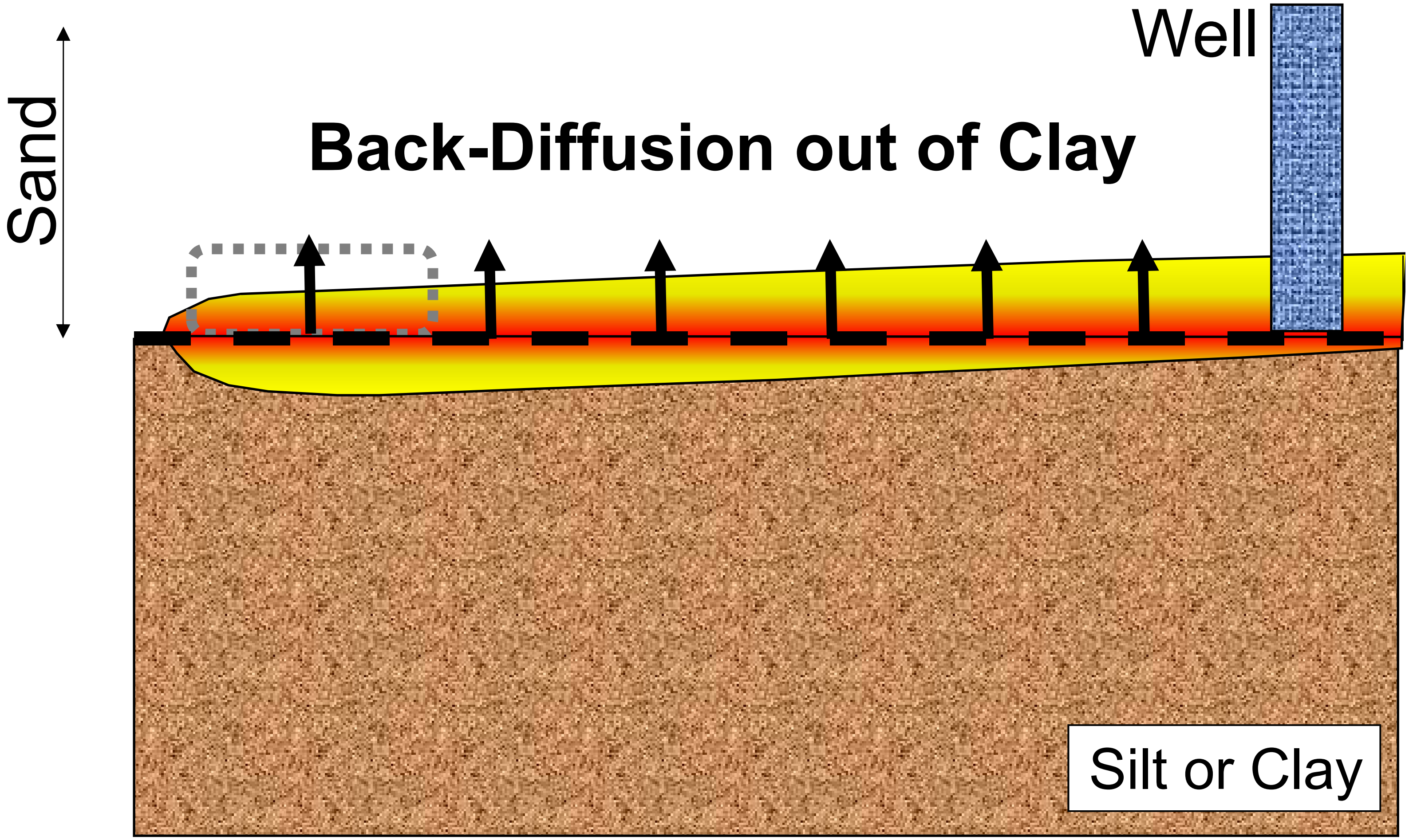
Forward Diffusion



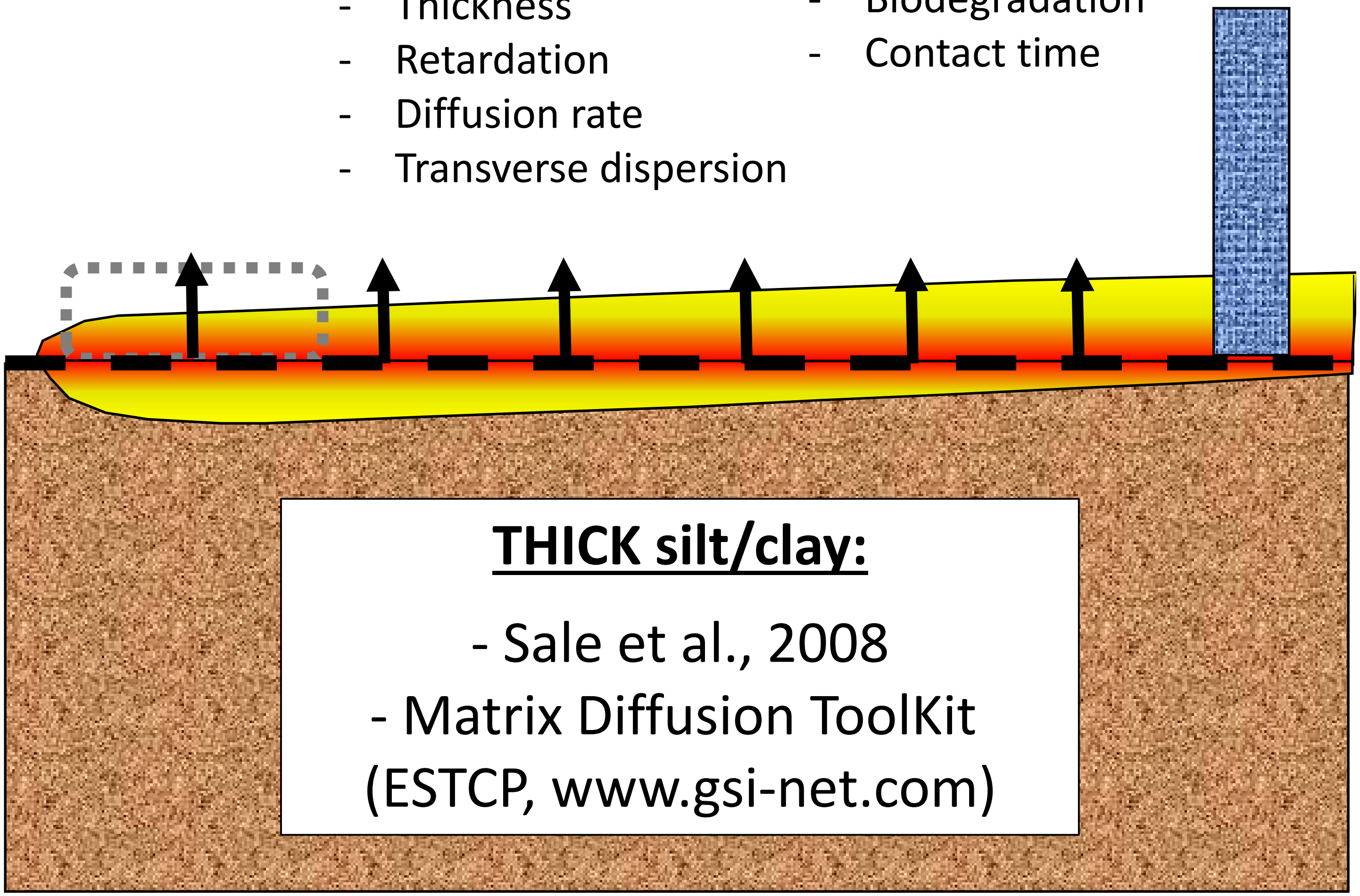
Back-Diffusion



Factors Influencing Remediation Timeframe

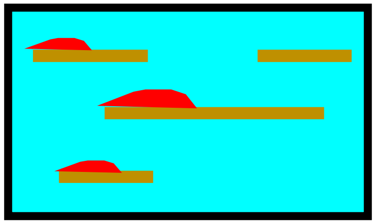
Influencing factors:

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



Modeling Challenges

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



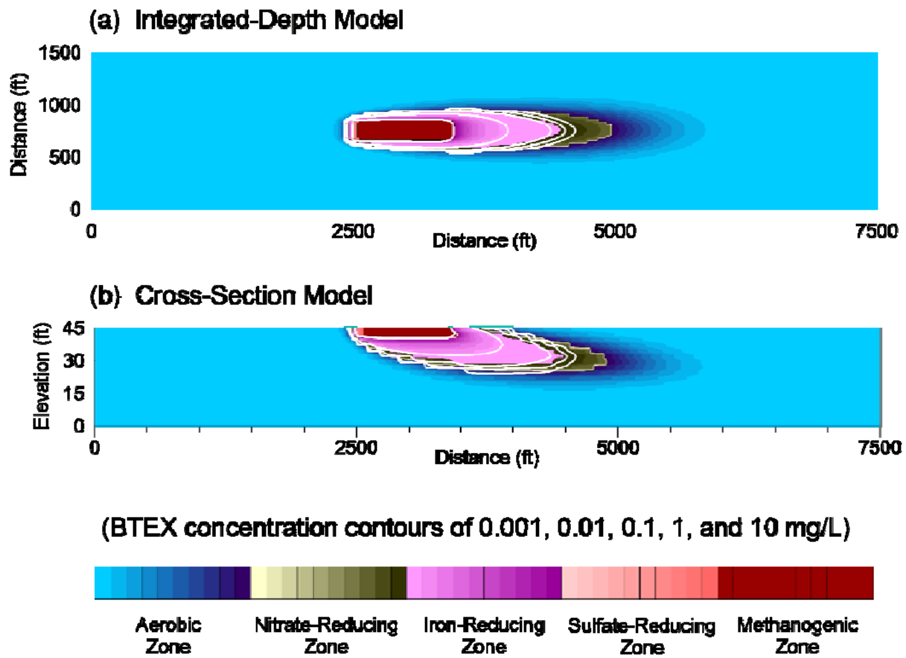
- Numerical models
  - Small grid spacing, time steps
  - Prohibitive for 3-D models
- **ISR-MT3DMS: new approach**

In-Situ Remediation (ISR-MT3DMS)

Public domain – available 2016

MT3DMS v5.3

BioRedox RCT package



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

Carey, Van Geel, and Murphy (1999)

In-Situ Remediation (ISR-MT3DMS)

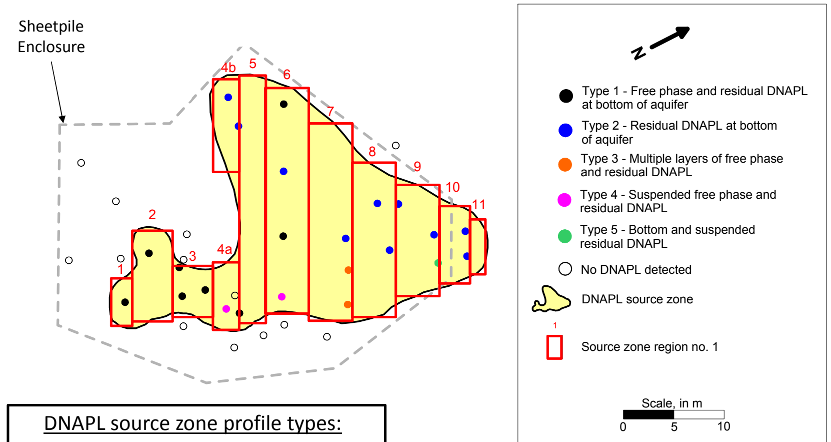
MT3DMS v5.3

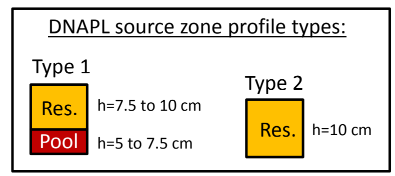
BioRedox RCT package

Contact Time Calculator

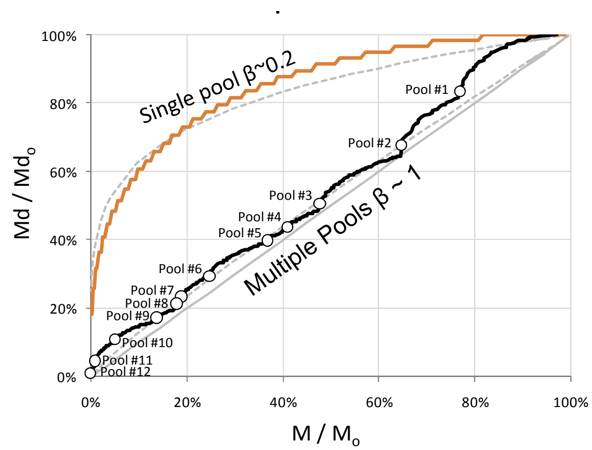
NAPL Depletion Model

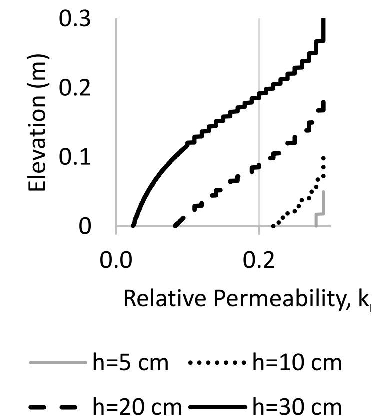
FREE (www.porewater.com)





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





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

In-Situ Remediation (ISR-MT3DMS)

MT3DMS v5.3

BioRedox RCT package

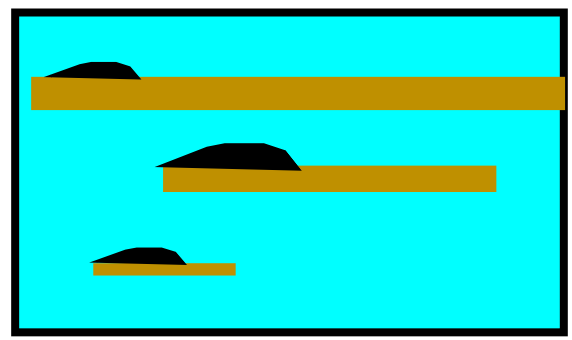
Contact Time Calculator

NAPL Depletion Model

Local Domain Approach

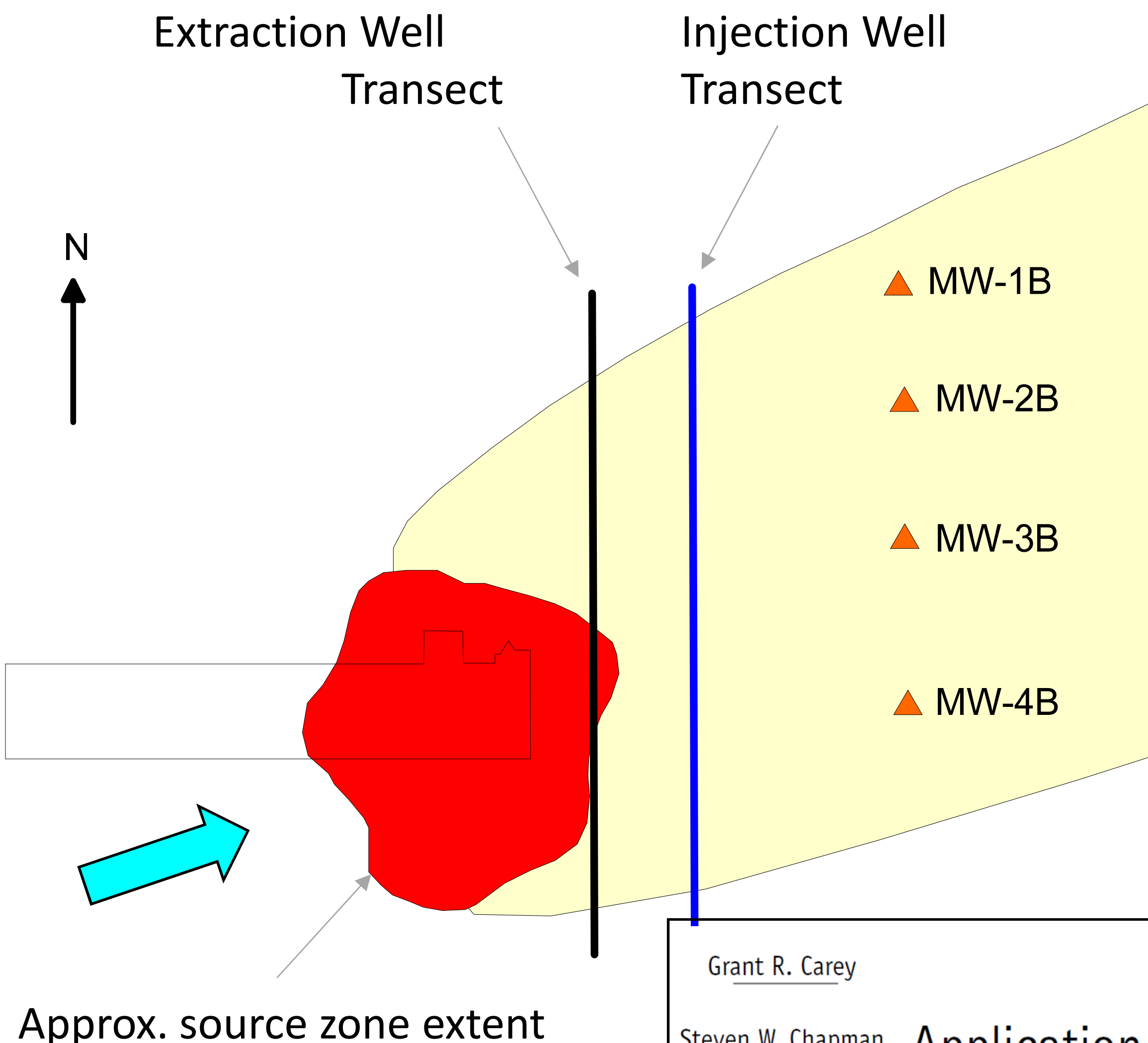
Collaborative research:

1. Dr. Brent Sleep (U. of Toronto); and
2. Dr. Beth Parker and
   Steve Chapman (U. of Guelph)



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

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

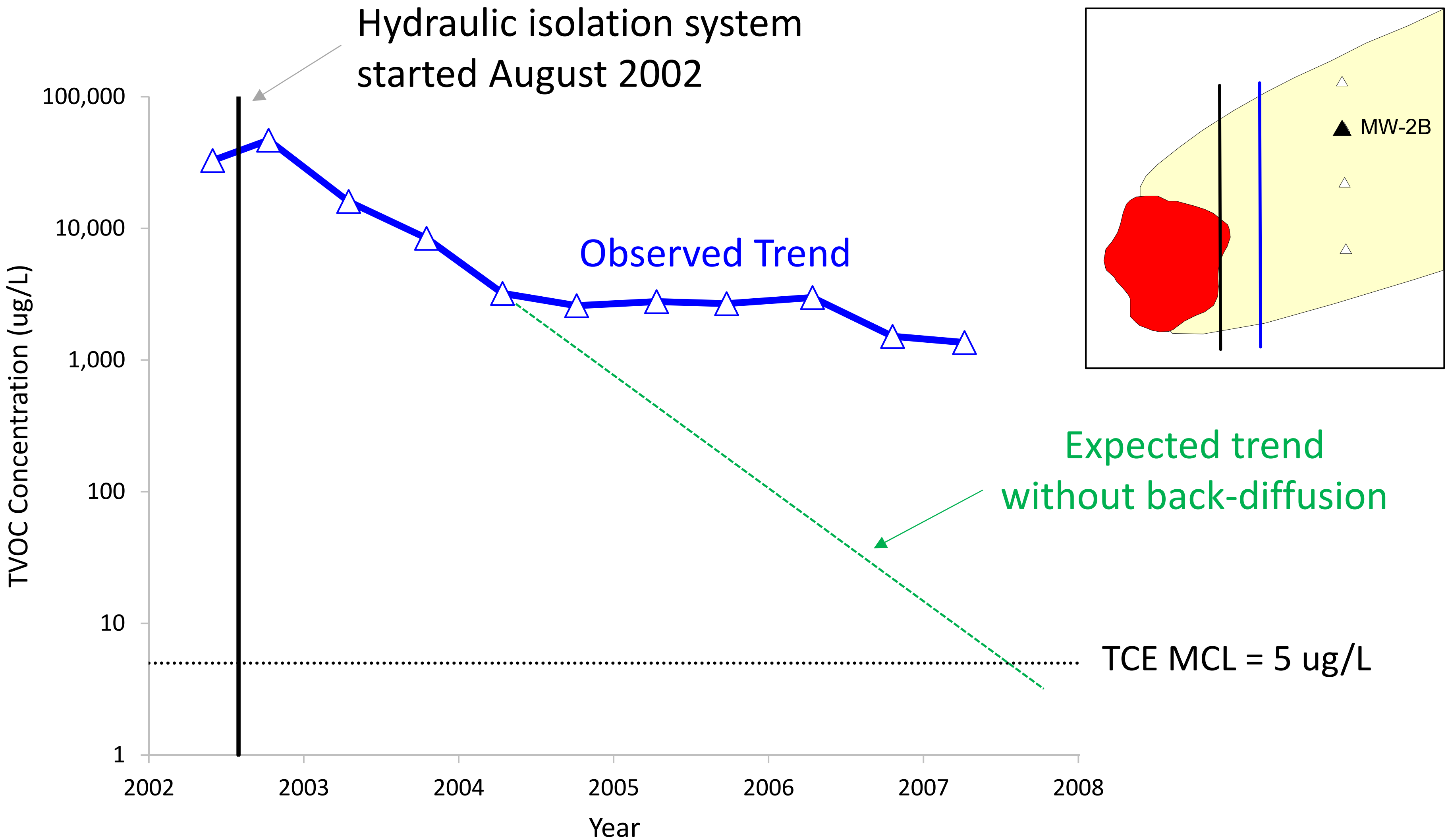
Modified from Parker et al., 2008

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

TVOC Trend After Source Containment



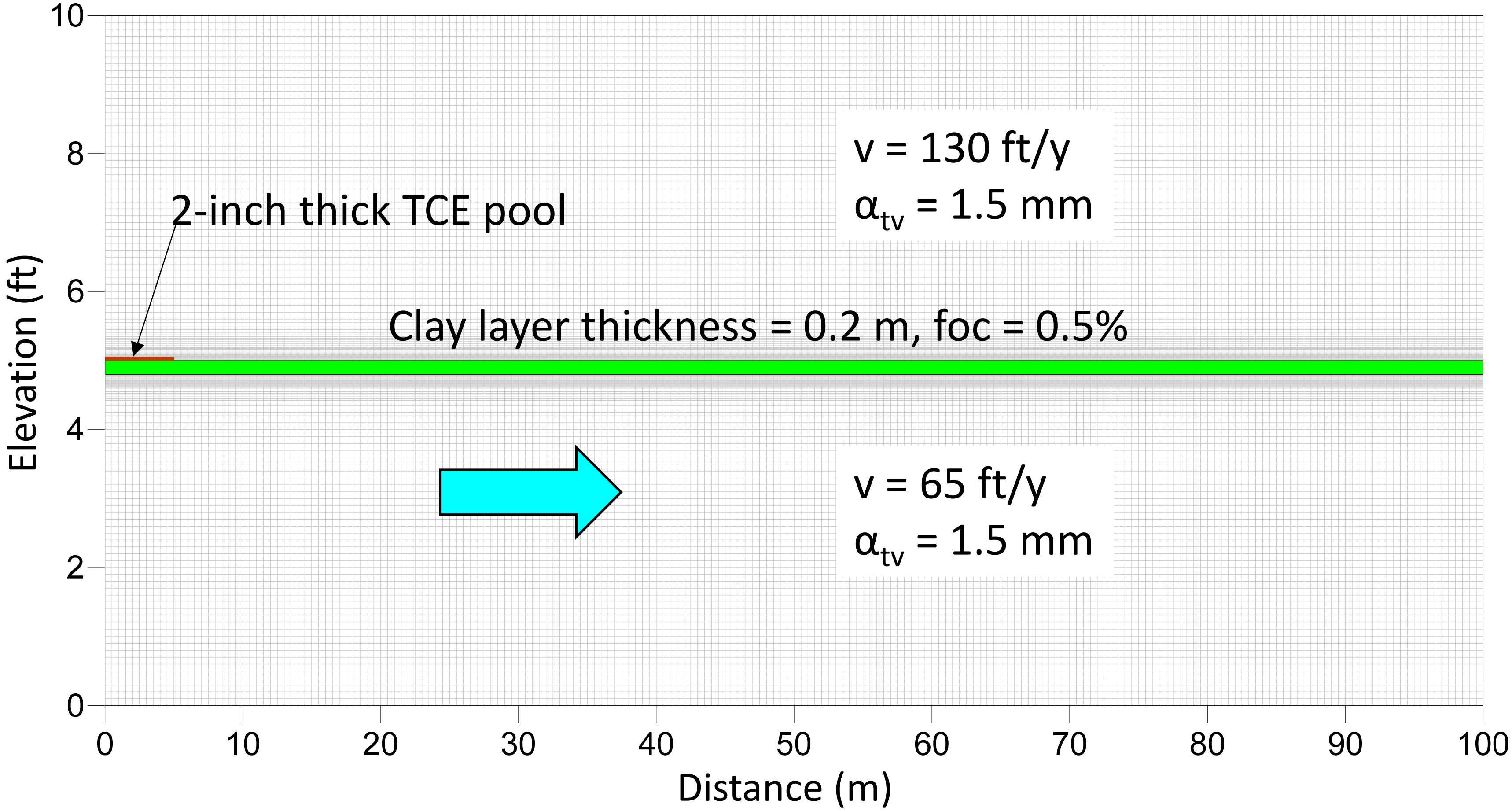
Modified from Parker et al., 2008

2-D Model Grid

200 columns, 158 rows (layers)

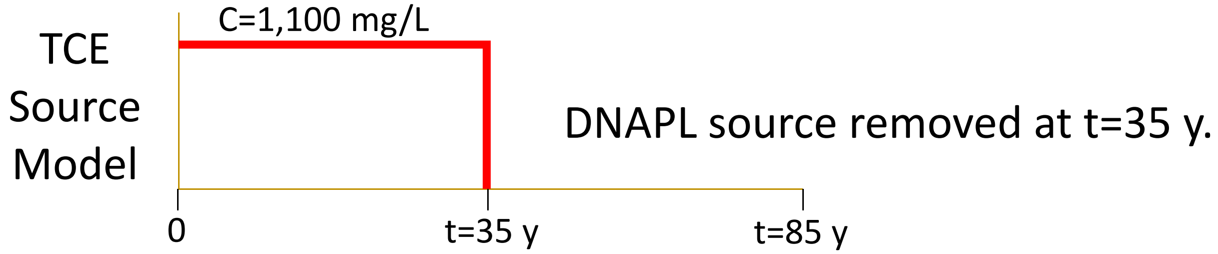
Minimum grid spacing: Δz = 1.25 cm, Δx = 0.5 m

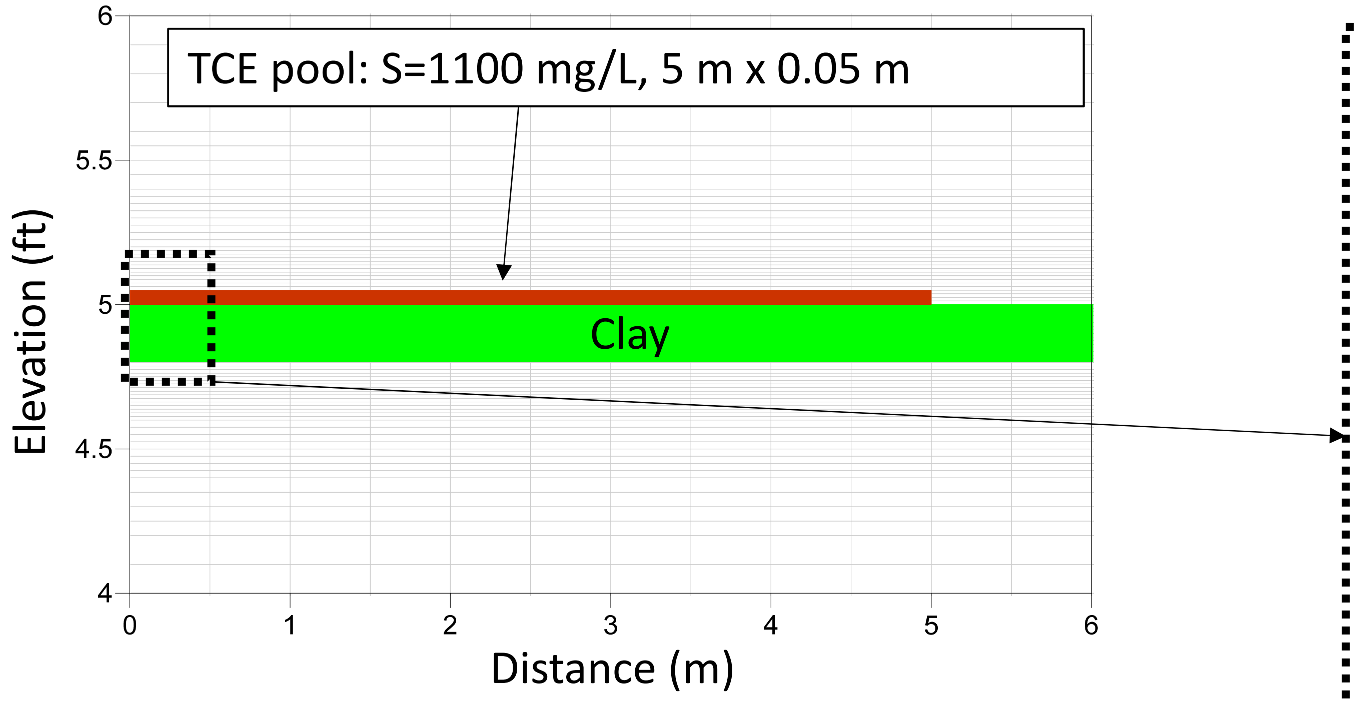
Run-time = 45 minutes for 85-y simulation (Δt = 0.24 d)

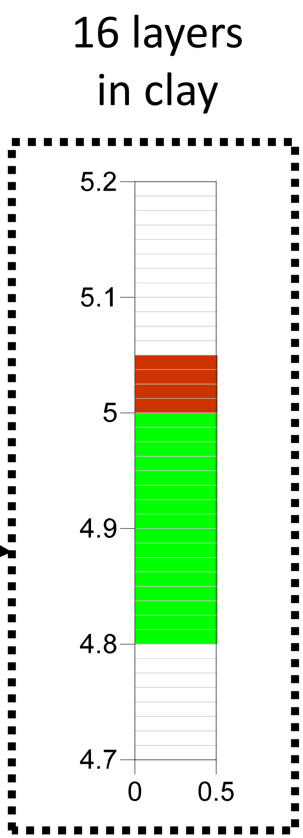


Carey et al. (2015)

Source Characteristics



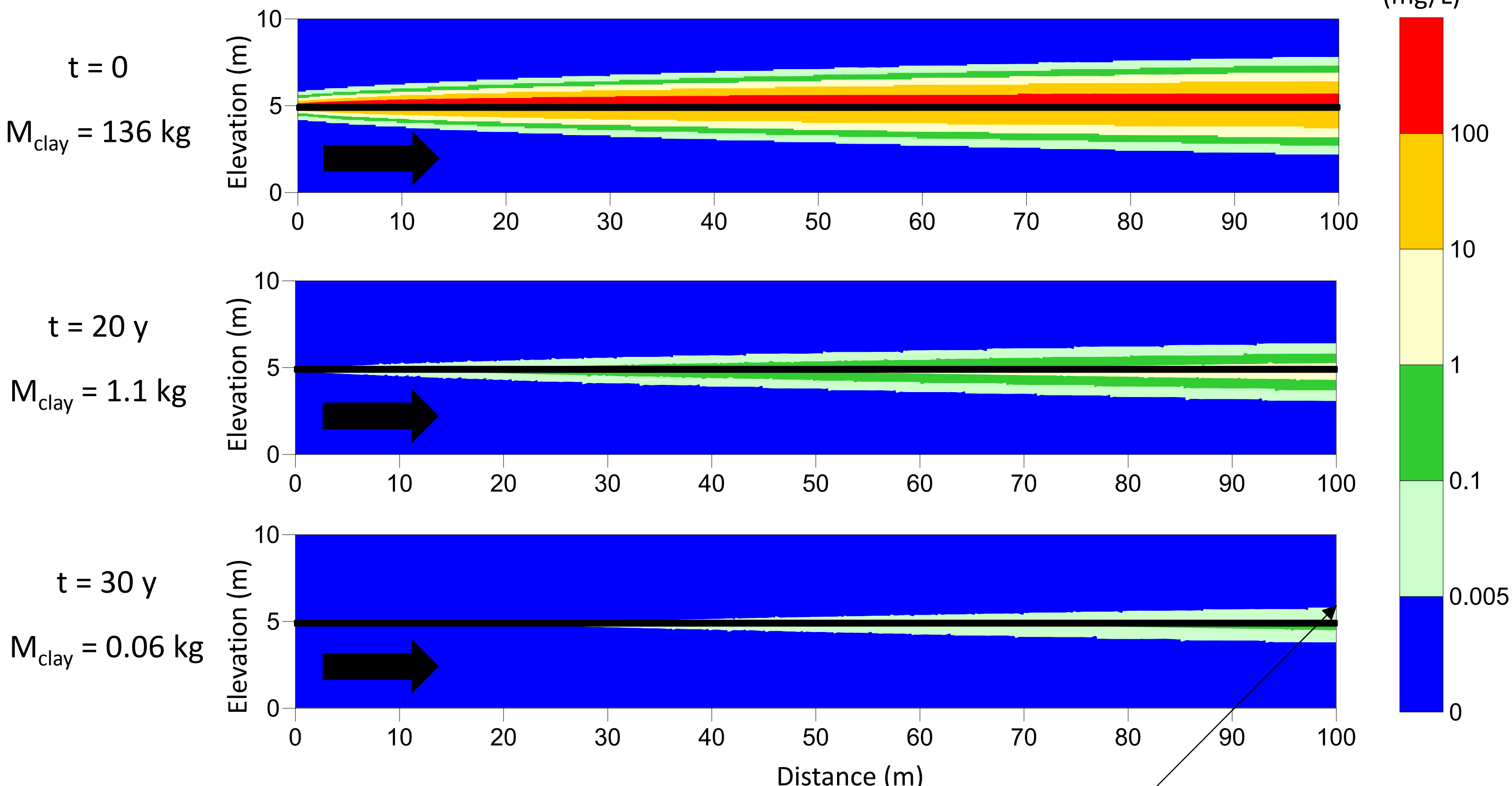




Carey et al. (2015)

Simulated TCE After Source Removal

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

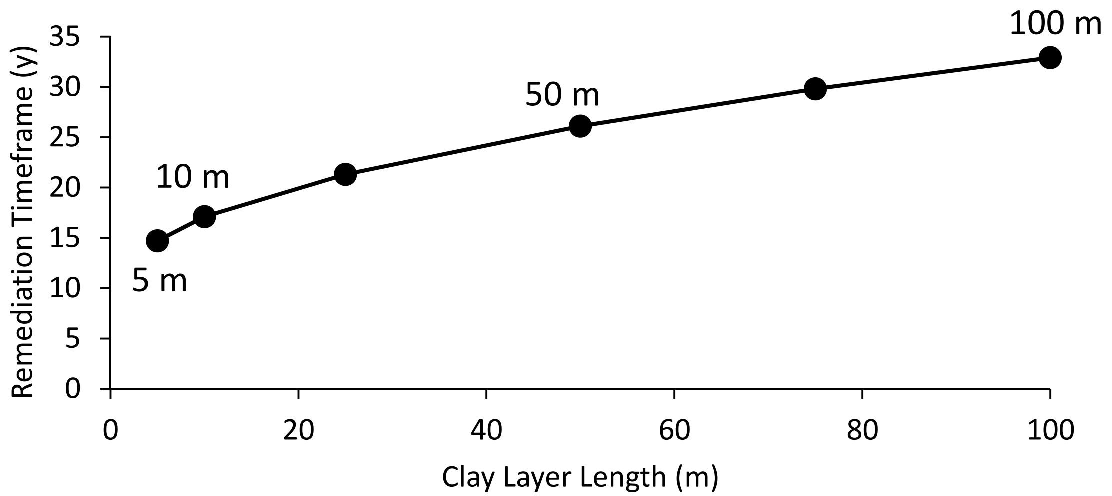


30 years after source removal:
99.96% mass depletion in clay, avg. C_{well} = 12 to 126 ug/L

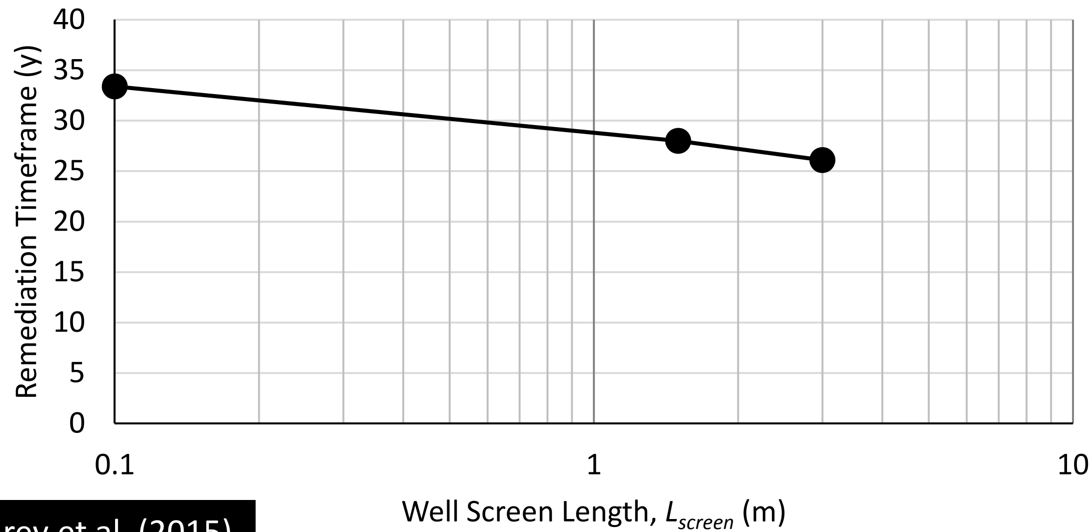
Carey et al. (2015)

Remediation Timeframe Sensitivity Analysis

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



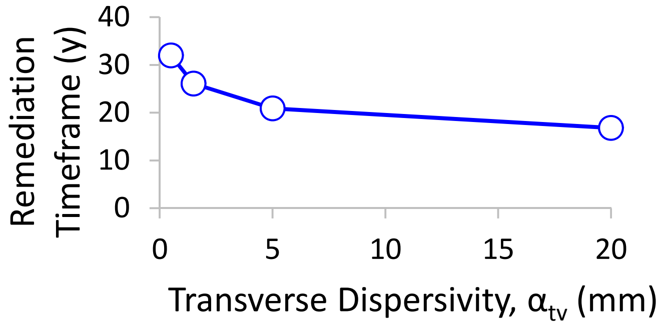
(b) RTF vs. screen length
(*x* = 50 m)



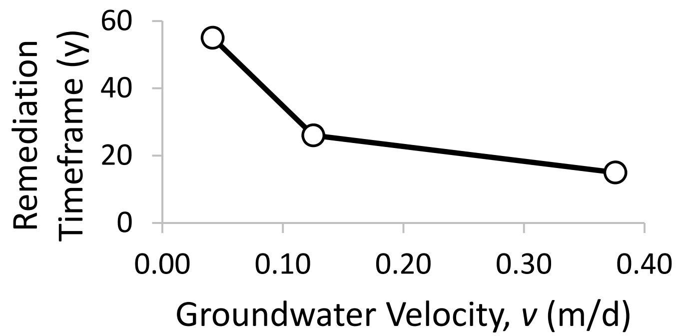
Carey et al. (2015)

Remediation Timeframe Sensitivity Analysis

(a) Transverse Dispersivity



(b) Groundwater Velocity

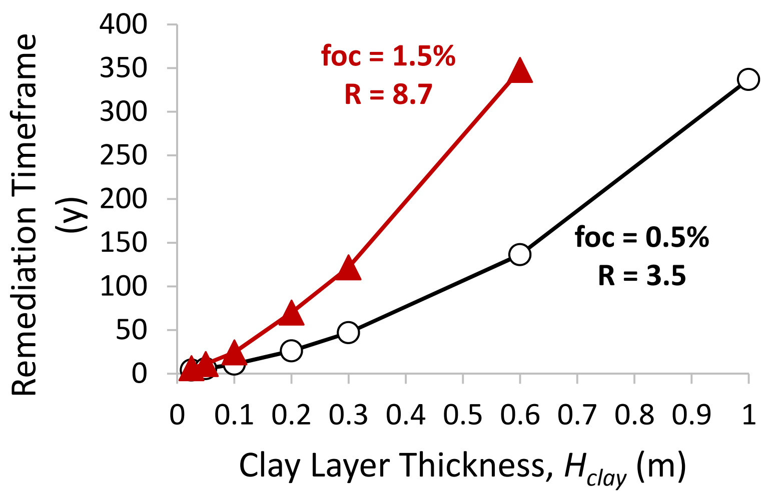


x = 50 m

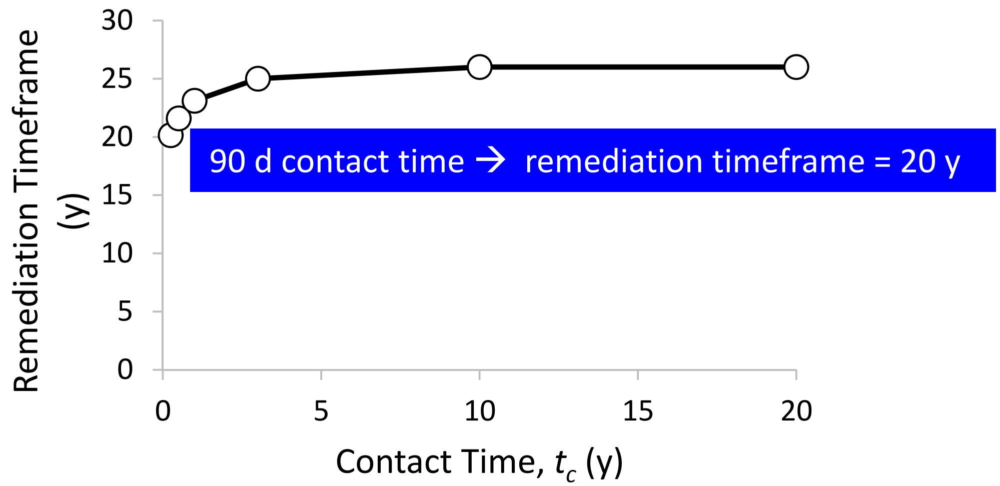
L_{screen} = 3 m

H_{clay} = 0.2 m

(c) Clay layer thickness



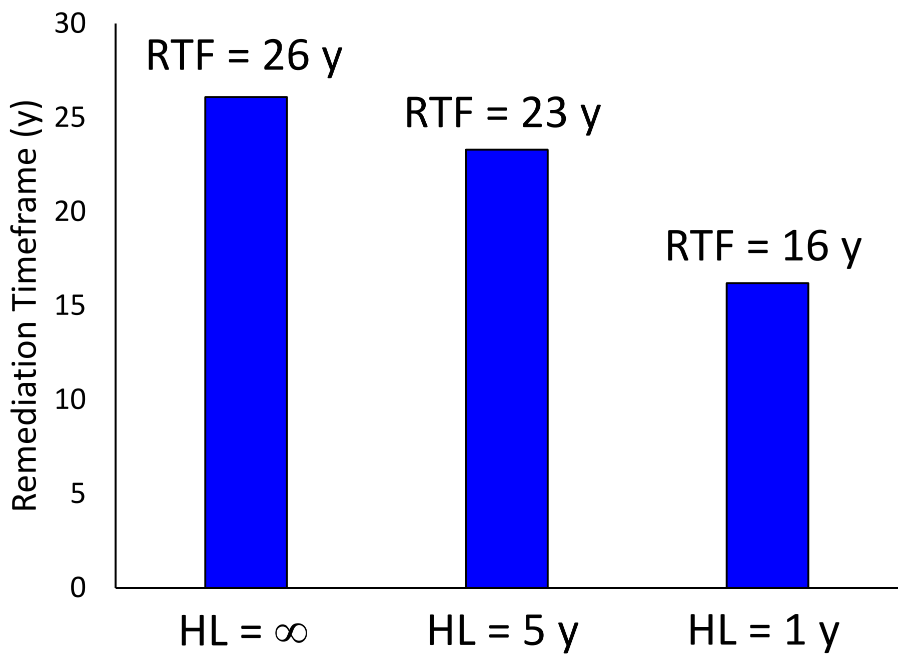
(d) Contact time (DNAPL and clay)



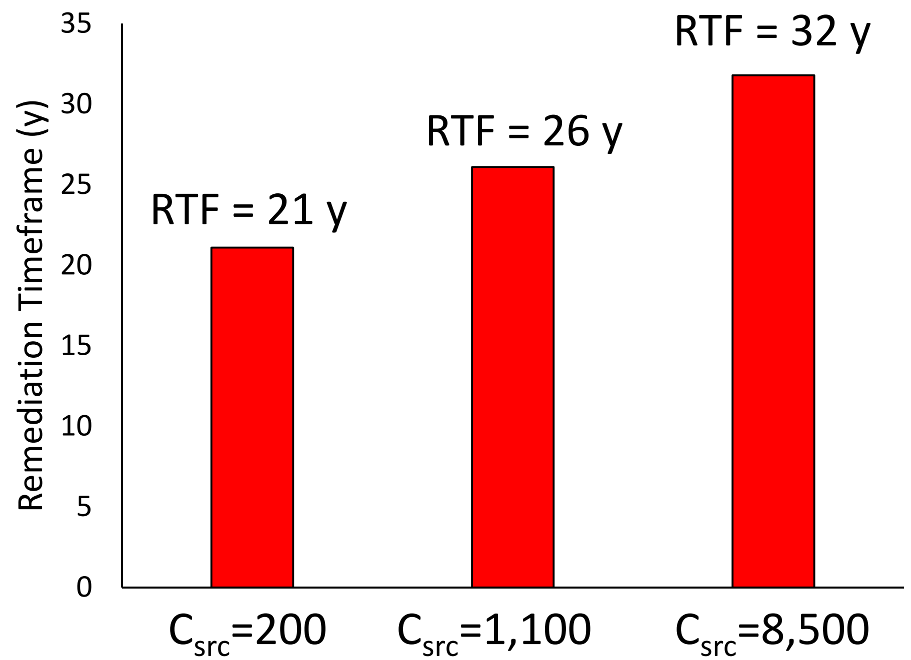
Carey et al. (2015)

Remediation Timeframe Sensitivity Analysis

a) Biodegradation Half-life in Clay Layer



b) Source Concentration (mg/L)



Note: K_d uniform

x = 50 m

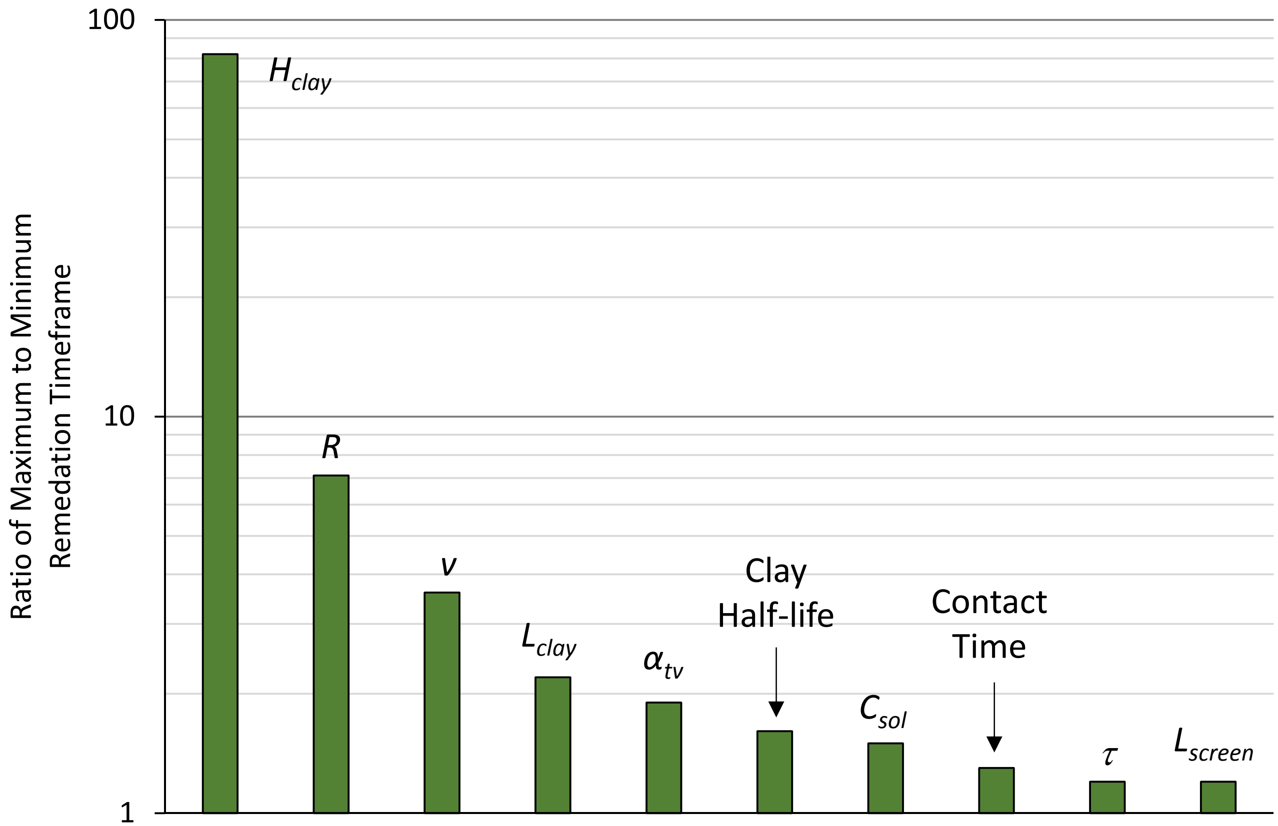
L_{screen} = 3 m

H_{clay} = 0.2 m

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

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

Florida Site Conclusions

- **Characteristics with largest influence:**
  - Low-K layer thickness
  - Retardation coefficient (f_{oc})
  - Groundwater velocity

f_{oc} is critical for:

1. Mass stored in silt/clay
2. Soil → GW concerntrations

- **Characteristics with moderate sensitivity:**
  - α_{TV}, silt/clay length, biodegradation half-life

- **Back-diffusion timeframe least sensitive to:**
  - Solubility, NAPL contact time, τ, well screen length

Questions?

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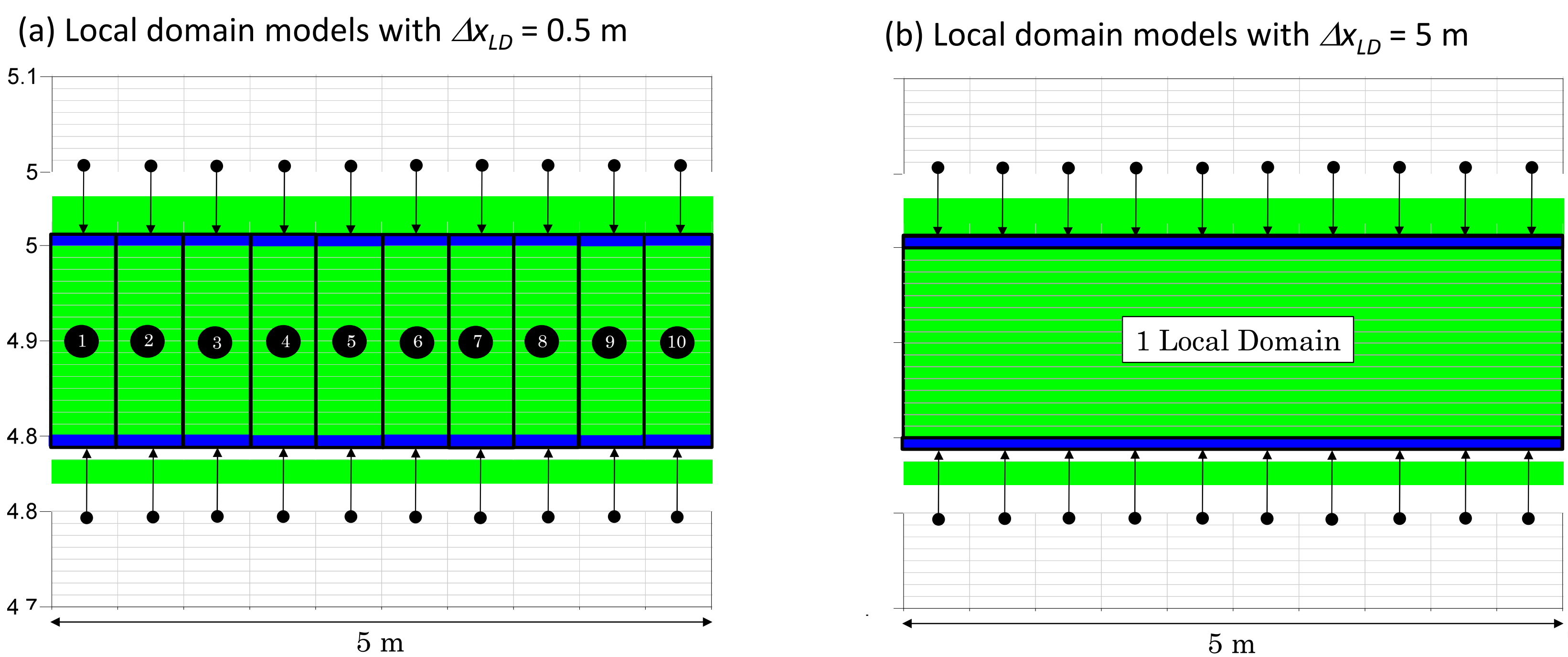
Supplemental Slides

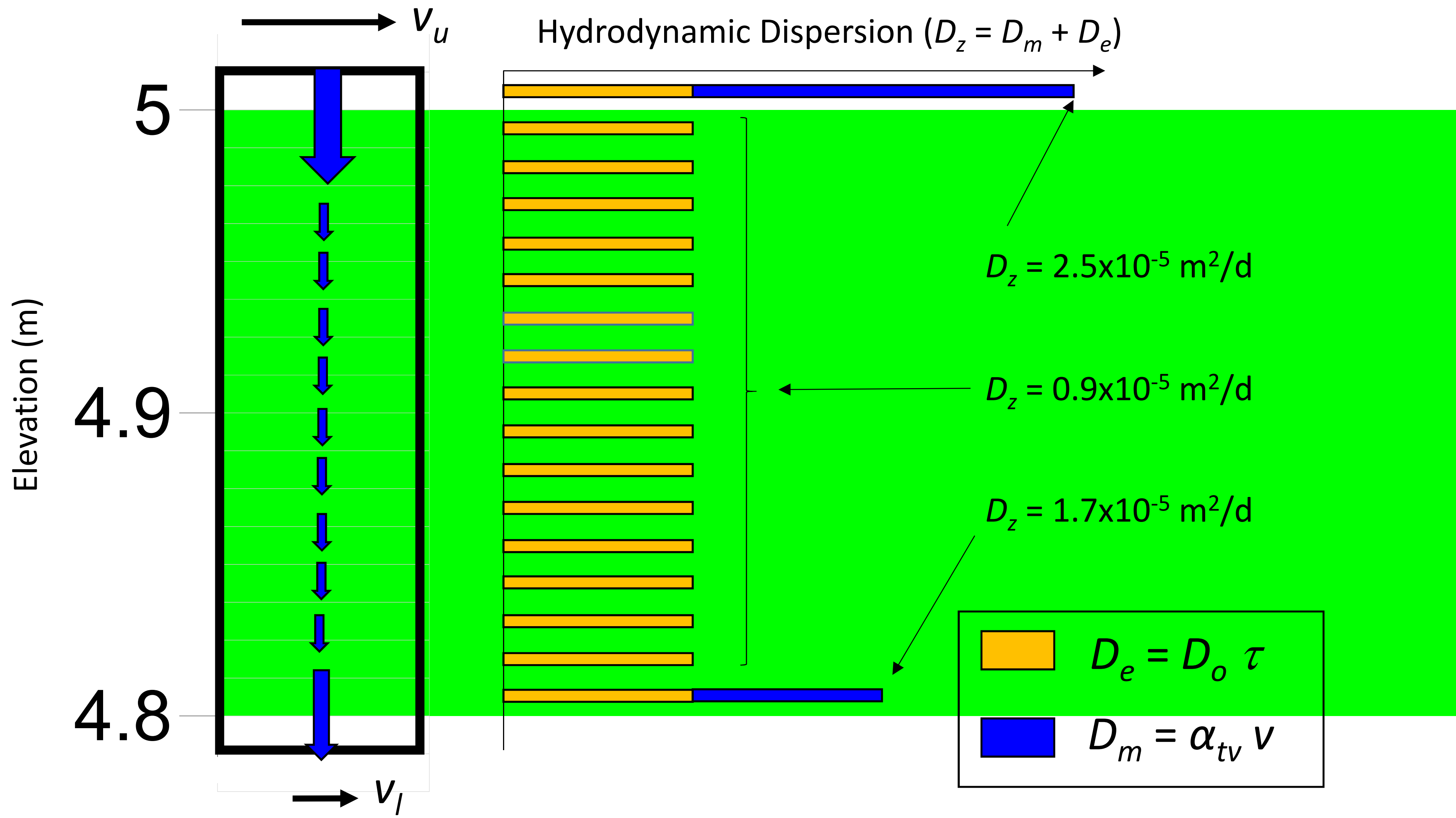
General Input Parameters	
NAPL source length, L_p (m)	5
NAPL source thickness, H_p (m)	0.05
TCE solubility, C_{sol} (mg/L)	1100
Free-water diffusion coefficient, D_o (m^2/d)	7.0E-05
Tortuosity coefficient, τ (dim.)	0.33
Effective diffusion coefficient, D_e (m^2/d)	2.3E-05

Unit-specific Input Parameters			
	Upper Sand	**Clay Layer**	**Lower Sand**
Hydraulic conductivity, K (m/d)	4.32	0.001	2.16
Horizontal hydraulic gradient, i (m/m)	0.01	0.01	0.01
Porosity, θ (m^3/m^3)	0.35	0.40	0.35
Groundwater velocity, v (m/d)	0.12	0.00003	0.06
Longitudinal dispersivity, α_x (m)	1	0.001	1
Vertical transverse dispersivity, α_{tv} (m)	0.0015	1.5E-06	0.0015
Biodegradation half-life (y)	∞	∞	∞
Fraction of organic carbon, f_{oc} (dim.)	0	0.0049	0
Dry bulk density, ρ_b (g/mL)	n/a	1.62	n/a
Organic carbon partitioning coefficient, K_{oc} (mL/g)	126	126	126
Retardation coefficient, R (dim.)	1.0	3.5	1.0

ISR-MT3DMS model input parameters.



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.

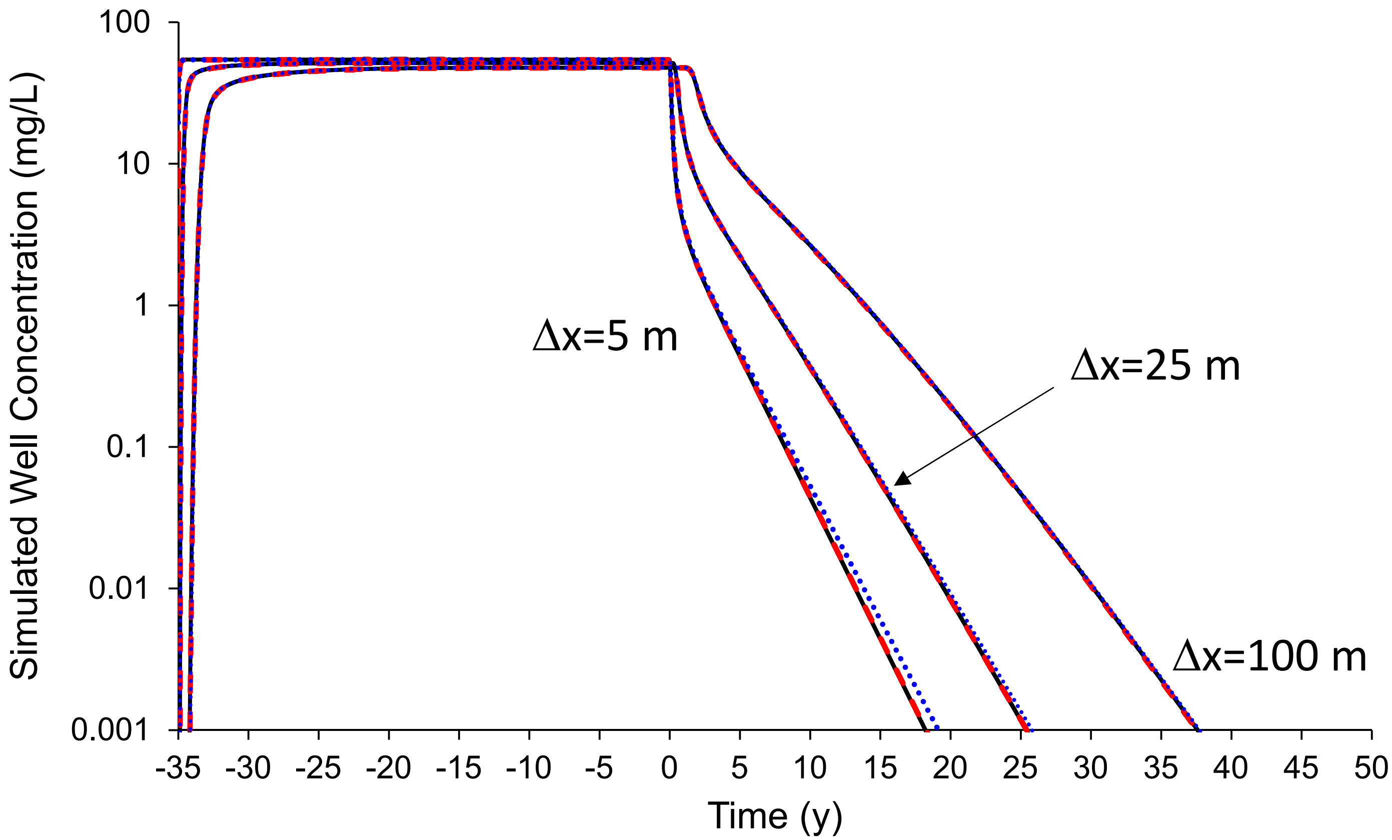


Comparison of vertical mechanical dispersion (D_m) and effective diffusion coefficient (D_e) magnitudes in each grid cell of a 1-D local domain. Vertical mechanical dispersion is shown to be significant at the top and bottom clay-sand interfaces due to the use of a three-dimensional dispersion tensor 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.

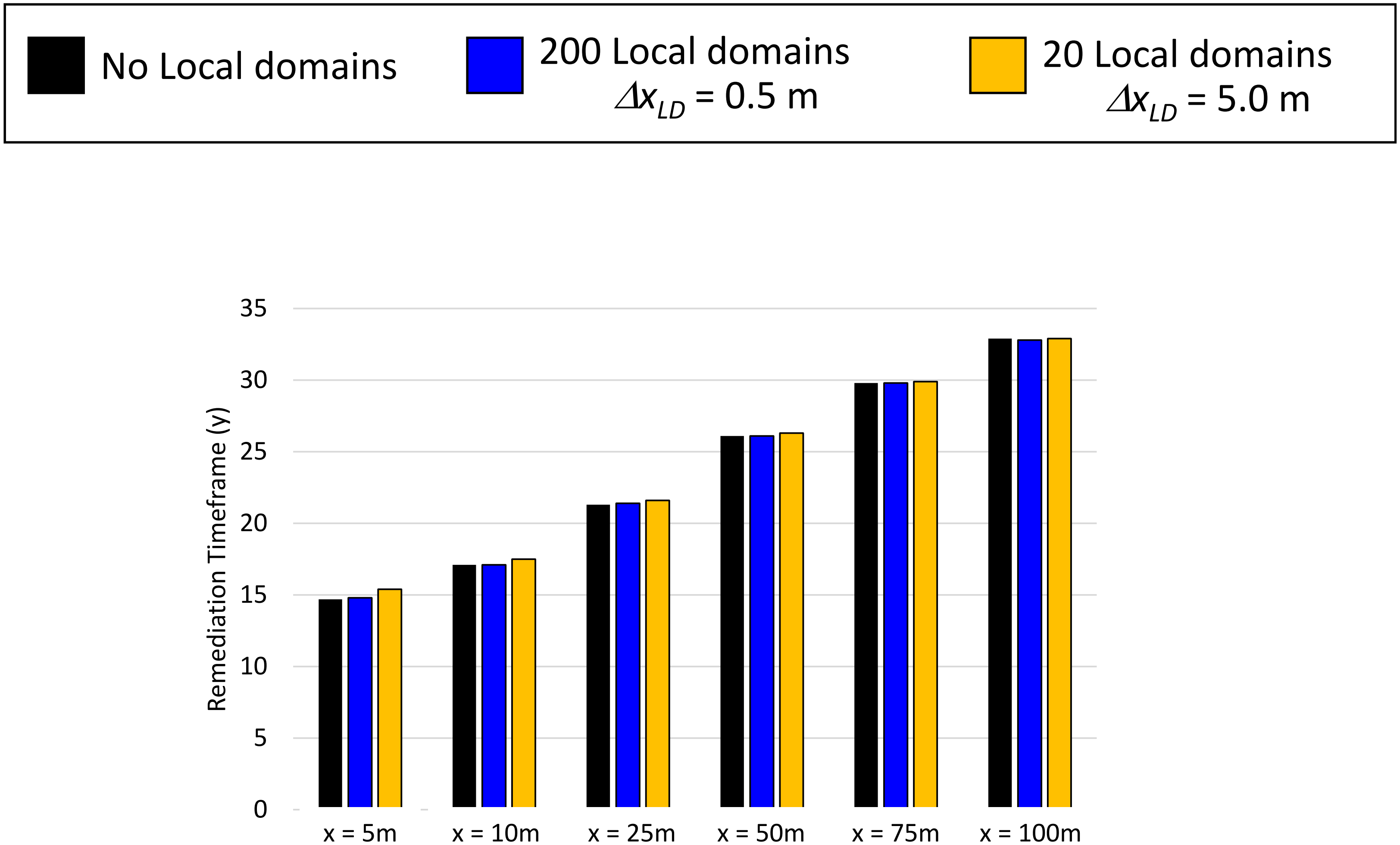
Influence of Mechanical Mixing

- 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

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



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.

Clay layer length (m):	5	10	25	50	75	100
Well screen length (m):	**3**	**3**	**3**	**3**	**3**	**3**
Input Parameter Description	**Remediation Timeframe (y)**					
α_{tv} = 0.5 mm	16.9	20.0	25.7	32.0	36.9	40.9
α_{tv} = 1.5 mm (base case)	14.7	17.1	21.3	26.1	29.8	32.9
α_{tv} = 5 mm	12.7	14.5	17.5	20.9	23.5	25.8
α_{tv} = 20 mm	11.3	12.5	14.5	16.8	18.6	20.2
τ = 0.25	17.5	20.0	24.6	29.6	33.5	36.7
τ = 0.33 (base case)	14.7	17.1	21.3	26.1	29.8	32.9
τ = 0.40	13.2	15.4	19.4	24.0	27.6	30.6
R = 1	4.4	5.2	6.7	8.7	10.4	11.9
R = 3.5 (base case)	14.7	17.1	21.3	26.1	29.8	32.9
R = 8.7	36.1	41.7	51.6	62.0	69.9	76.3
Contact time = 90 d	10.9	12.9	16.4	20.2	23.1	25.6
Contact time = 180 d	11.9	13.9	17.6	21.6	24.7	27.3
Contact time = 1y	12.9	15.1	18.9	23.1	26.3	29.0
Contact time = 3y	14.2	16.5	20.5	25.0	28.5	31.4
Contact time = 10y	14.7	17.0	21.3	26.0	29.6	32.7
Contact time = 20y	14.7	17.0	21.3	26.0	29.7	32.8
Contact time = 35y (base case)	14.7	17.1	21.3	26.1	29.8	32.9
Contact time = 50y	14.8	17.1	21.4	26.1	29.8	32.9
v_U = 0.04 m/d	26.0	31.2	41.9	54.5	64.7	73.4
v_U = 0.12 m/d (base case)	14.7	17.1	21.3	26.1	29.8	32.9
v_U = 0.36 m.d	10.0	11.3	13.3	15.3	16.8	18.0
H_{clay} = 0.025 m	1.4	1.8	2.7	4.1	5.4	6.6
H_{clay} = 0.05 m	2.3	2.8	4.1	5.8	7.3	8.7
H_{clay} = 0.1 m	5.2	6.2	8.3	10.9	13.1	15.0
H_{clay} = 0.2 m (base case)	14.7	17.1	21.3	26.1	29.8	32.9
H_{clay} = 0.3 m	28.8	32.8	39.7	46.9	52.3	56.6
H_{clay} = 0.6 m	92.1	103.5	120.4	136.2	147.4	156.3
H_{clay} = 1.0 m	204.4	231.4	301.4	337.0	356.2	372.6
C_{sol} = 200 mg/L	11	13.1	16.9	21.1	24.4	27.2
C_{sol} = 1,100 mg/L (base case)	14.7	17.1	21.3	26.1	29.8	32.9
C_{sol} = 8,500 mg/L	19.2	21.8	26.6	31.8	36	39.3
Clay half-life = infinity (no degradation)	14.7	17.1	21.3	26.1	29.8	32.9
Clay half-life = 5 y	13.4	15.5	19.2	23.3	26.4	29
Clay half-life = 1 y	9.9	11.3	13.7	16.2	18.2	19.8

Sensitivity analysis results. The simulated remediation timeframe corresponds to the time for the concentration in a monitoring well at the downgradient edge of the clay layer to decline below the MCL.

2-D Model: Horizontal Wells

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