Thank you for signing in early

The webinar will begin promptly at
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SERDP and ESTCP Webinar Series

- The webinar will begin promptly at 12:00 pm ET, 9:00 am PT
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  - Listen to the broadcast audio if your computer is equipped with speakers
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    - (669) 900-6833 or (929) 205-6099
    - Required webinar ID: 739-191-114
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REMChlor-MD Groundwater Transport and Remediation Model for Sites with Matrix Diffusion

February 7, 2019

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Welcome and Introductions

Rula A. Deeb, Ph.D.
Webinar Coordinator

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Webinar Agenda

- **Webinar Logistics** (5 minutes)
  Dr. Rula Deeb, Geosyntec Consultants
- **Overview of SERDP and ESTCP** (5 minutes)
  Dr. Andrea Leeson, SERDP and ESTCP
- **REMChlor-MD Groundwater Transport and Remediation Model for Sites with Matrix Diffusion** (60 minutes + Q&A)
  Dr. Ron Falta, Clemson University
  Dr. Chuck Newell, GSI Environmental, Inc.
  Dr. Shahla Farhat, GSI Environmental, Inc.
- **Final Q&A session**

In Case of Technical Difficulties

- Use a compatible browser (Firefox, IE or Edge)
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  - Key in Ctrl + F5 to do a hard refresh of your browser
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  - Click the arrow next to the "*Join Audio*" button
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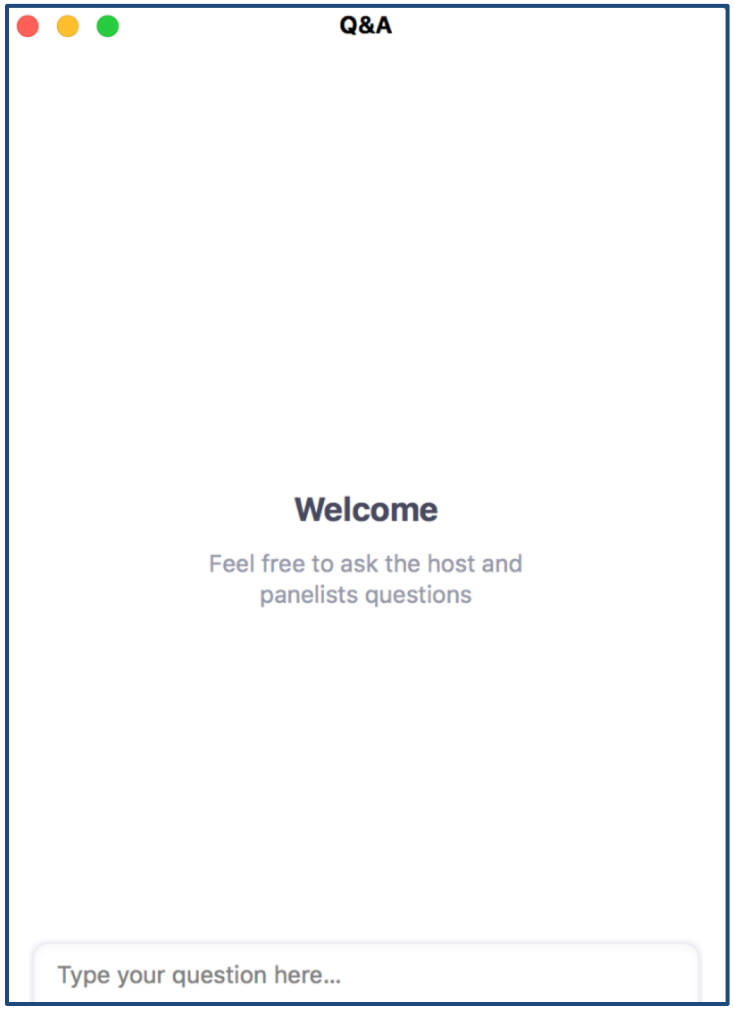
How to Ask Questions

- Find the Q&A button on your control bar and type in your question(s)
- Make sure to add your organization name at the end of your question so that we can identify you during the Q&A sessions



SERDP and ESTCP Overview

Andrea Leeson, Ph.D.
SERDP & ESTCP

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DoD's Environmental Technology Programs

Science and Technology

- Statutory program established 1991
- DoD, DOE, EPA partnership
  - Advanced technology development to address near-term needs
  - Fundamental research to impact real world environmental management

Demonstration and Validation

- Demonstrate innovative cost-effective environmental and energy technologies
  - Transition technology out of the lab
  - Establish cost and performance
  - Partner with end user and regulator
  - Technology transfer
    - Accelerate commercialization or broader adoption
    - Direct technology insertion

Environmental Drivers

Sustaining Ranges, Facilities and Operations

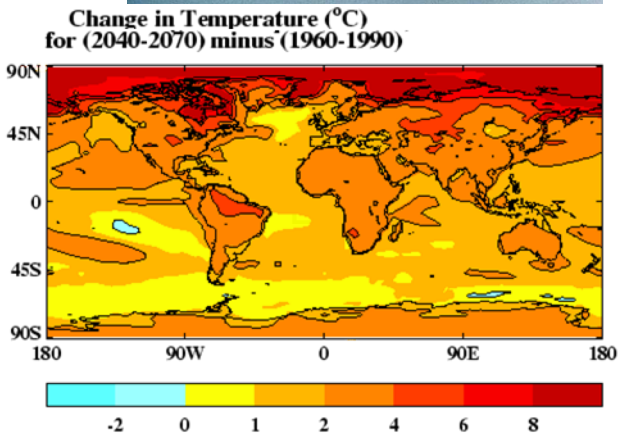
Maritime Sustainability
Threatened and Endangered Species

Toxic Air Emissions and Dust

UXO and Munitions Constituents

Noise

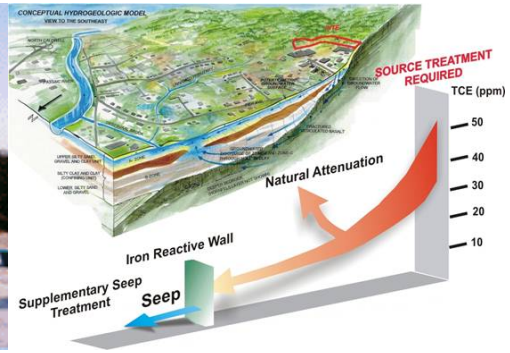
Sustainable FOB



Environmental Drivers

Reducing Current and Future Liability

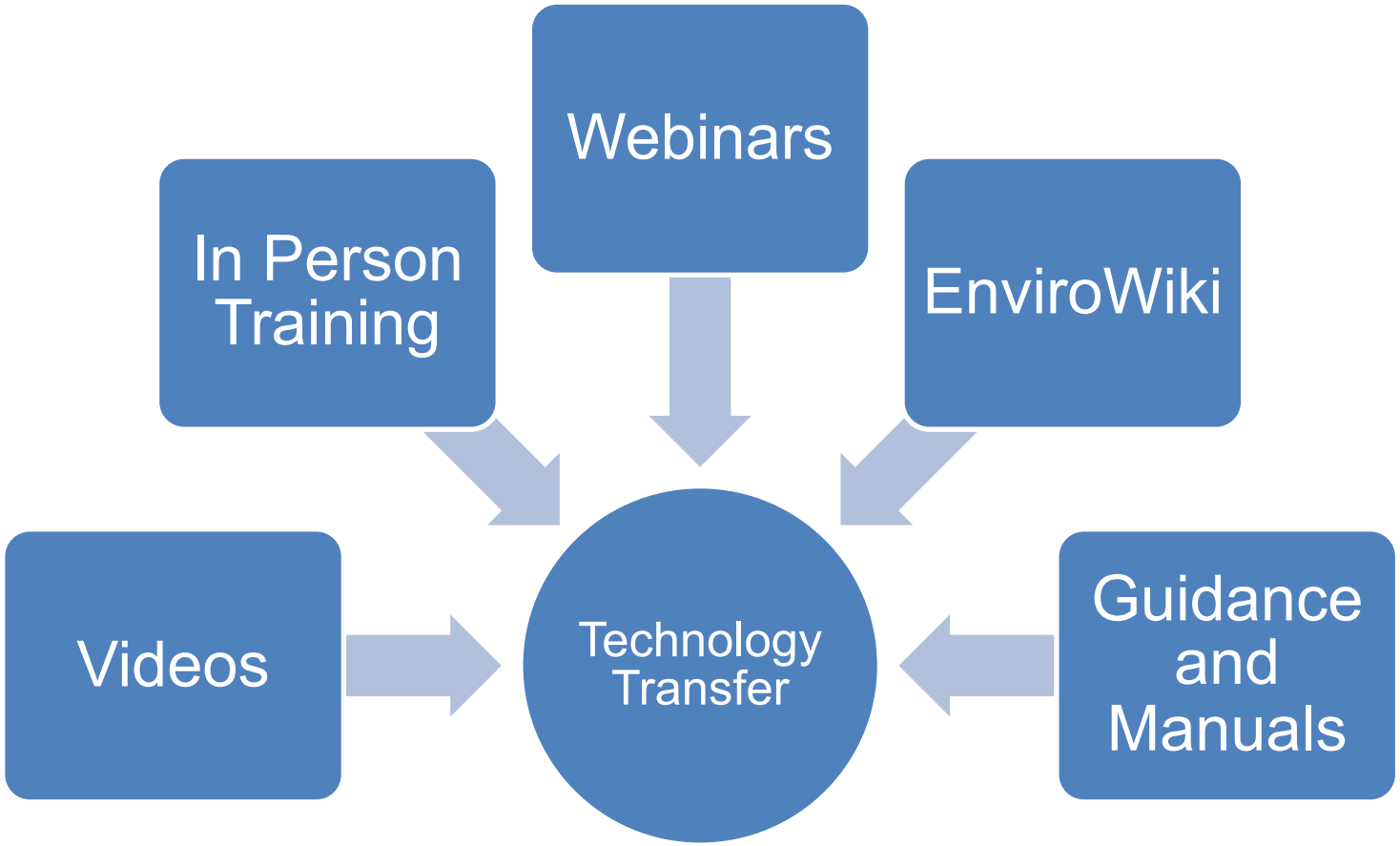
Contamination from Past Practices



- Groundwater, soils and sediments
- Large UXO liability
- Emerging contaminants

Pollution Prevention to Control Life Cycle Costs

- Elimination of pollutants and hazardous materials in manufacturing, maintenance, and operations
- Achieve compliance through pollution prevention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www.serdp-estcp.org

Webinars

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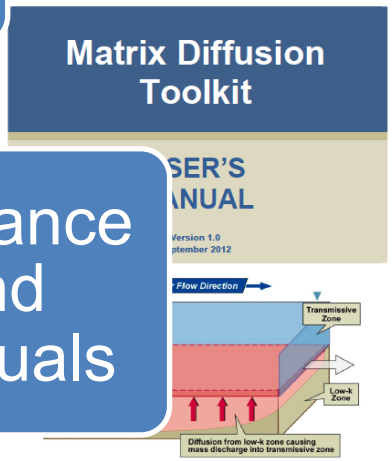

SERDP and ESTCP Webinar Series

Date	Topic
February 21, 2019	Utilization of Advanced Conservation Voltage Reduction for Energy Reduction on DoD Installations
March 14, 2019	Determining the Temporal and Spatial Scales of Non-Stationarity in Temperature and Precipitation across the Continental U.S.
March 28, 2019	Weapons Systems and Platforms: Accelerated Aging Studies
April 11, 2019	Managing Contaminated Sediments
April 25, 2019	Unexploded Ordnance Characterization and Detection on the Beach Face and in Muddy Estuarine Environments
May 9, 2019	Soil Microbial Communities: Critical Roles in Control of Non-Native Invasive Species and Restoration of Ecosystem Functions

For upcoming webinars, please visit

http://serdp-estcp.org/Tools-and-Training/Webinar-Series

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Save the Date!

SERDP • ESTCP
SYMPOSIUM

A three-day symposium showcasing the latest technologies that enhance DoD's mission through improved environmental and energy performance

December 3-5, 2019
Washington Marriott Wardman Park

Registration information available soon

REMChlor-MD Groundwater Transport and Remediation Model for Sites with Matrix Diffusion

Ron Falta, Clemson University
Chuck Newell, GSI Environmental, Inc.
Shahla Farhat, GSI Environmental, Inc.

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Background, Testing and Results

Dr. Ron Falta
Clemson University

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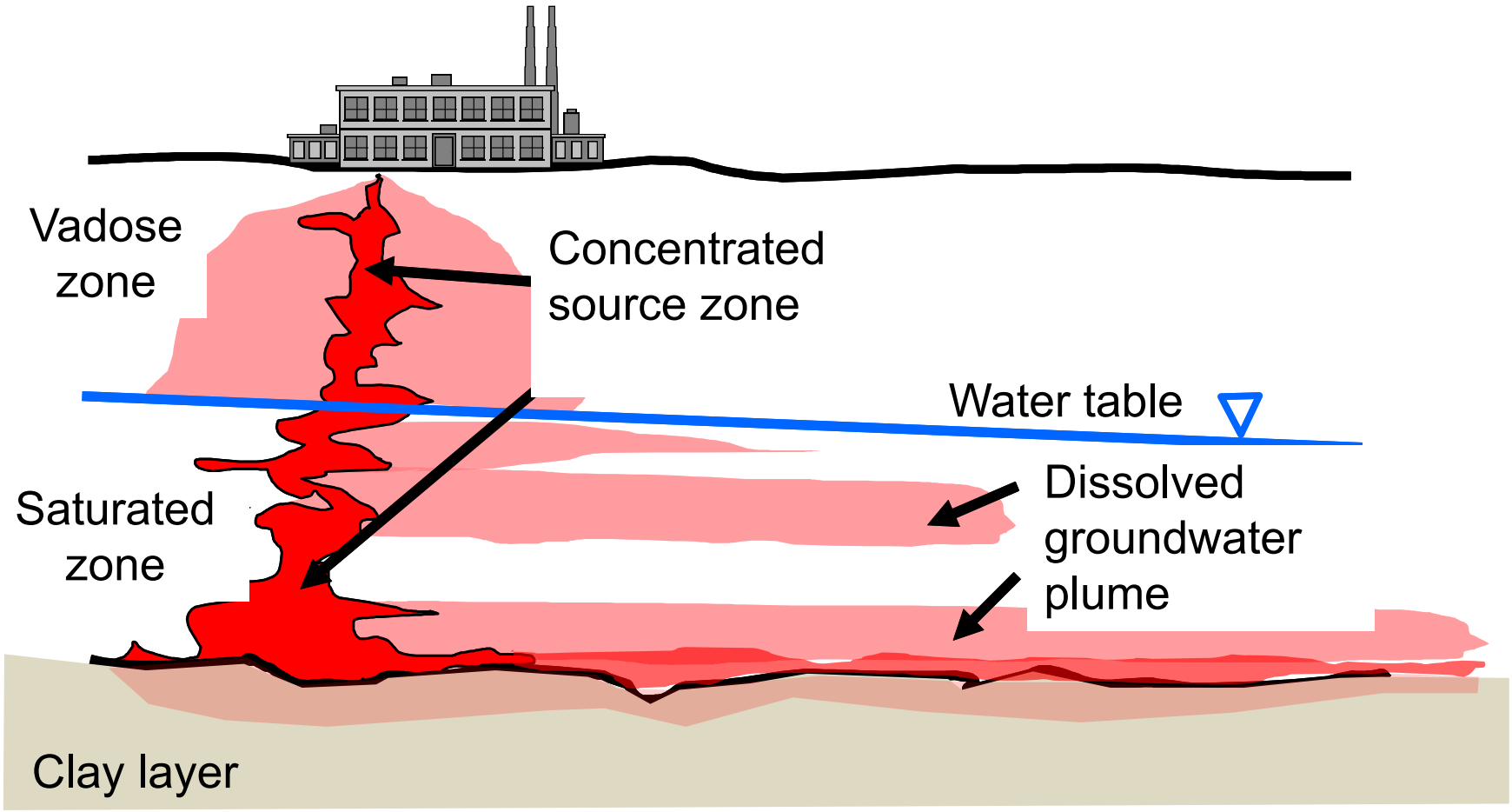
Agenda

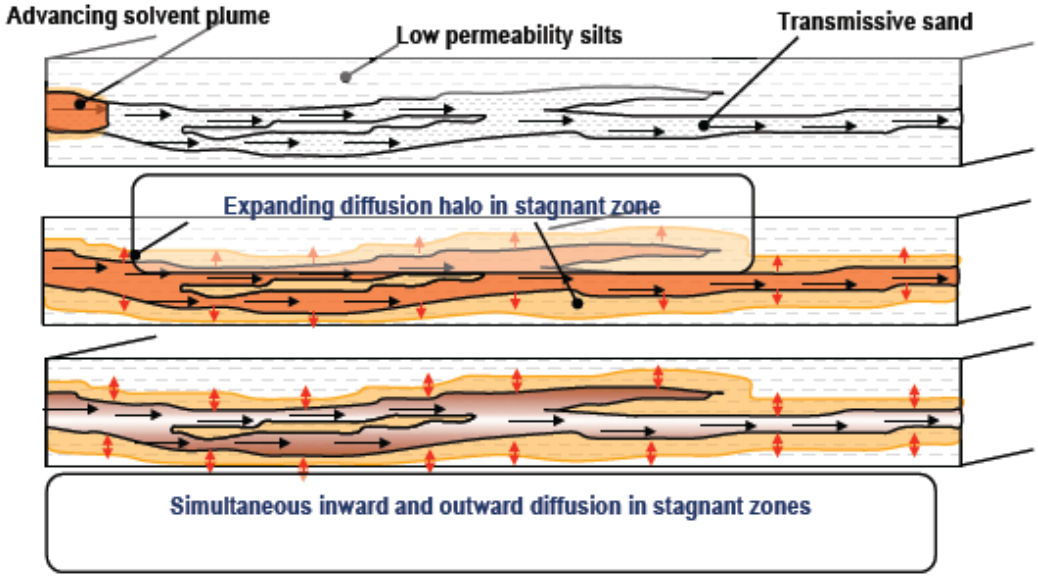
- Background
  - Introduction to matrix diffusion and modeling approaches
  - High resolution semi-analytical method used in REMChlor-MD
- Testing and results
  - Matrix diffusion in aquitards with parent-daughter reactions
  - Matrix diffusion in fractured and heterogeneous systems
- How to use REMChlor-MD
  - REMChlor-MD interface
- Summary

Typical Chlorinated Solvent Contamination



Matrix Diffusion in Low-K Zones

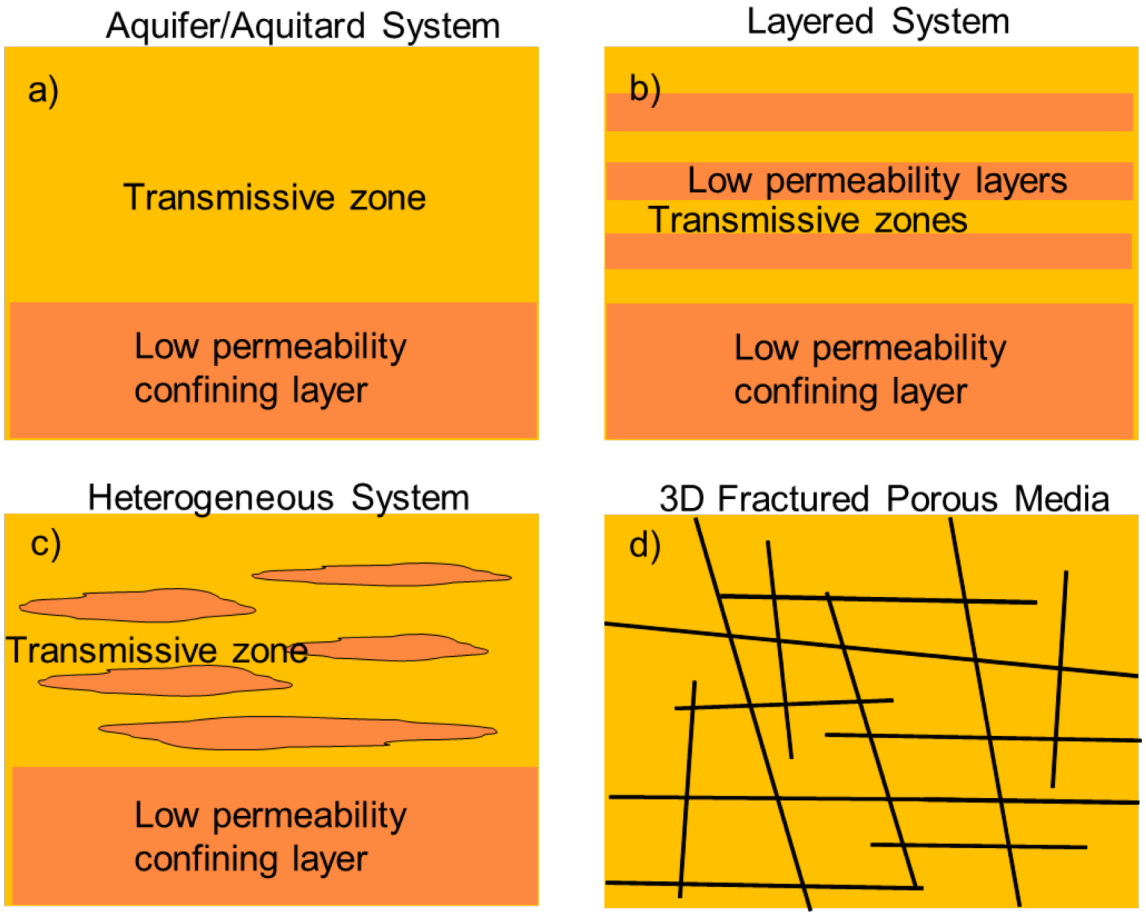
- Contaminants in the plume can diffuse into low-K zones
- After remediation, contaminants may diffuse out of the low-K zones, contaminating the groundwater again
- Back-diffusion process may last for decades to centuries*



** Chapman, S.W., and B.L. Parker (2005)*
Parker, B.L., S.W. Chapman, and M.A. Guilbeault (2008)

Matrix Diffusion

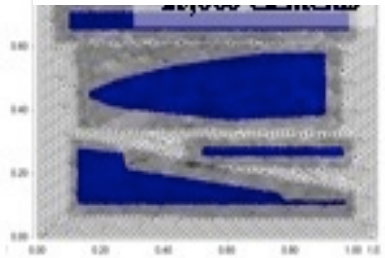
- Simulating matrix diffusion in these types of sites is difficult with current numerical models



Conventional Models of Matrix Diffusion

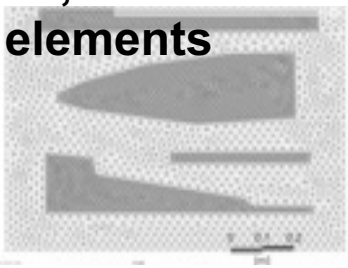
HydroGeoSphere

~25,000 elements



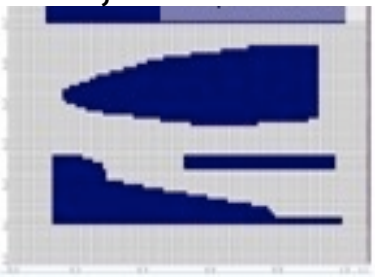
FEFLOW

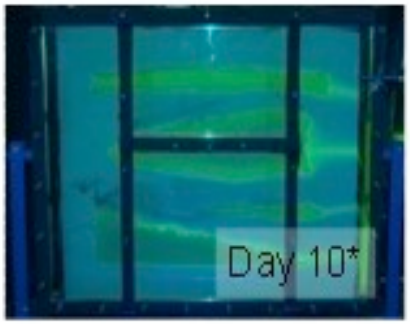
~7,500 elements

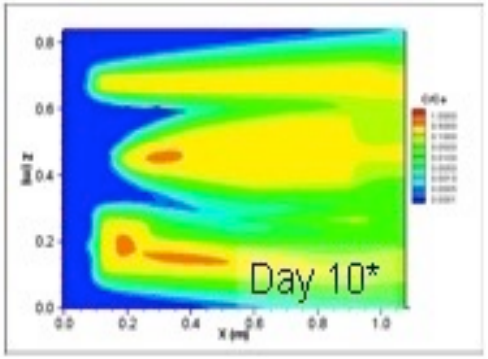


MODFLOW/MT3DMS

~10,000 nodes







Contents lists available at SciVerse ScienceDirect

Journal of Contaminant Hydrology

journal homepage: www.elsevier.com/locate/jconhyd

Testing high resolution numerical models for analysis of contaminant storage and release from low permeability zones

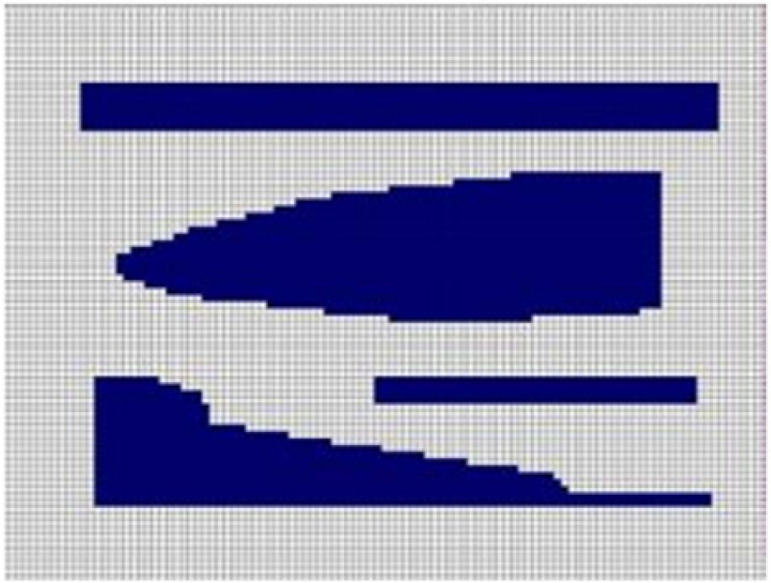
Steven W. Chapman [a,*], Beth L. Parker [a], Tom C. Sale [b], Lee Ann Doner [b,1]

[a] School of Engineering, University of Guelph, 50 Stone Road E, Guelph, ON, Canada N1G 2W1
[b] Department of Civil & Environmental Engineering, Colorado State University, Fort Collins, CO 80523, United States

Numerical Modeling: *"…requires much higher resolution than commonly practiced"* to simulate matrix diffusion

"High Resolution" Method May Be Impractical for 3D Field Simulations

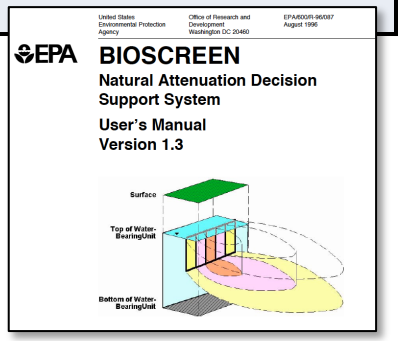
- Matrix diffusion is controlled by gradients at the millimeter to centimeter range
- Field scale gridblock sizes are on the order of tens of centimeters to several meters
- Key matrix diffusion processes occur at the sub-gridblock scale



From Chapman et al., 2012

Models May Not Account for Matrix Diffusion in the Plume

Model	Matrix Diffusion in Source?	Matrix Diffusion in Plume?
BIOSCREEN	No	No
BIOCHLOR	No	No
AT3D	No	No
REMChlor	Approximation	No

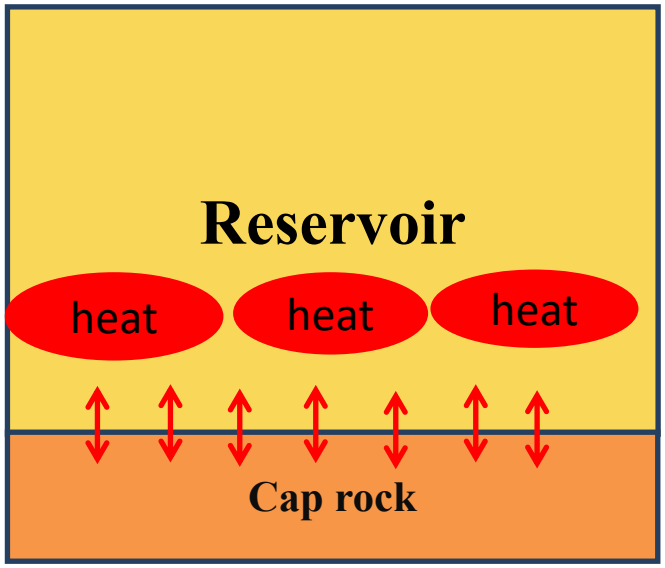


REMChlor-MD

- Free screening-level transport/remediation model
- Original REMChlor source/plume remediation framework
  - First order parent-daughter reactions
  - Simple 1-D linear flow field
- Models matrix diffusion in the plume (ESTCP ER-201426)
  - Uses semi-analytical approximations in normal numerical gridblocks
- Considers diffusion into aquitards, and in heterogeneous or fractured aquifers
- Parent and daughter compounds have independent retardation factors and reaction rates in the transmissive and non-transmissive parts of the aquifer

Semi-Analytical Method*

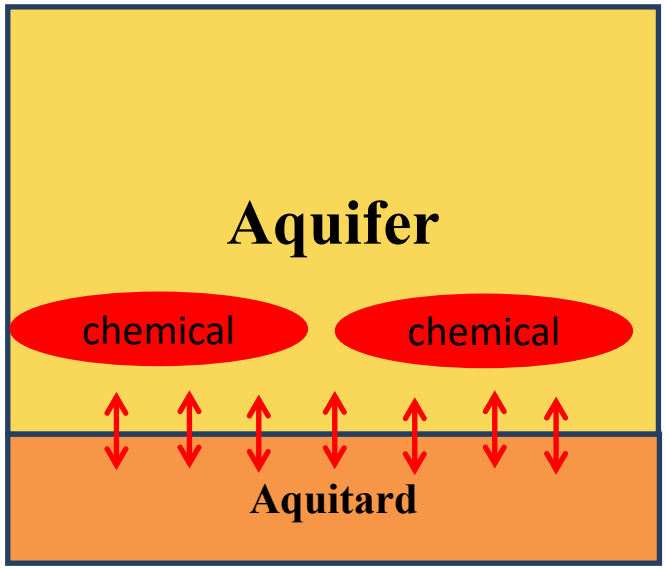
Heat Conduction



(Vinsome and Westerveld, 1980)

$$\rho C_r \frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial z^2}$$

Chemical Diffusion



$$R \frac{\partial C}{\partial t} = \tau D_w \frac{\partial^2 C}{\partial z^2} - \lambda C$$

**Geothermal reservoir engineering method adapted to the problem of chemical diffusion with first order decay*

Semi-Analytical Method

- Similar to dual porosity
  - Much higher resolution of diffusive flux, more efficient
- Similar to MINC approaches with local 1-D grids
- The concentration of each component in low K zones in each gridblock (or in aquitard) approximated as follows:

$$C_l(z_l, t) = (C^{t+\Delta t} + pz_l + qz_l^2)e^{-z_l/d}$$

Semi-Analytical Method

- Parameters p and q are derived from differential equation for transient diffusion with decay/production and mass balance

1) The PDE is satisfied at the matrix interface

$$\frac{\partial C_m}{\partial t} = \alpha_m \left.\frac{\partial^2 C_m}{\partial z^2}\right|_{z=0} - \frac{\lambda_m}{R_m} C_m\Big|_{z=0} + \frac{\lambda_{m-1} Y_m}{R_m} C_{m-1}\Big|_{z=0}$$

2) The rate of change of mass in the low-K material is equal to the diffusive flux across the interface minus the rate of decay plus the rate of production

$$\frac{\partial}{\partial t}\int_0^L C_m\, dz = \alpha_m \left.\frac{\partial C_m}{\partial z}\right|_{z=0} - \frac{\lambda_m}{R_m}\int_0^L C_m\, dz + \frac{\lambda_{m-1} Y_m}{R_m}\int_0^L C_{m-1}\, dz$$

Semi-Analytical Method

- Trial function for C(z,t) only depends the current gridblock concentration, $C^{t+\Delta t}$
- Diffusive flux leaving each gridblock is a concentration-dependent source/sink
- Trial function is updated in each gridblock at every time-step
- Process adds almost zero additional computational effort

$$F = -\phi\tau D_w \left.\frac{\partial C}{\partial z}\right|_{z=0}$$

$$F = \phi\tau D_w \left(\left(a - \frac{1}{d} \right) C^{t+\Delta t} + b^t \right)$$

Diffusive mass flux into/out of the low-K zone

Falta and Wang, 2017; Muskus and Falta, 2018

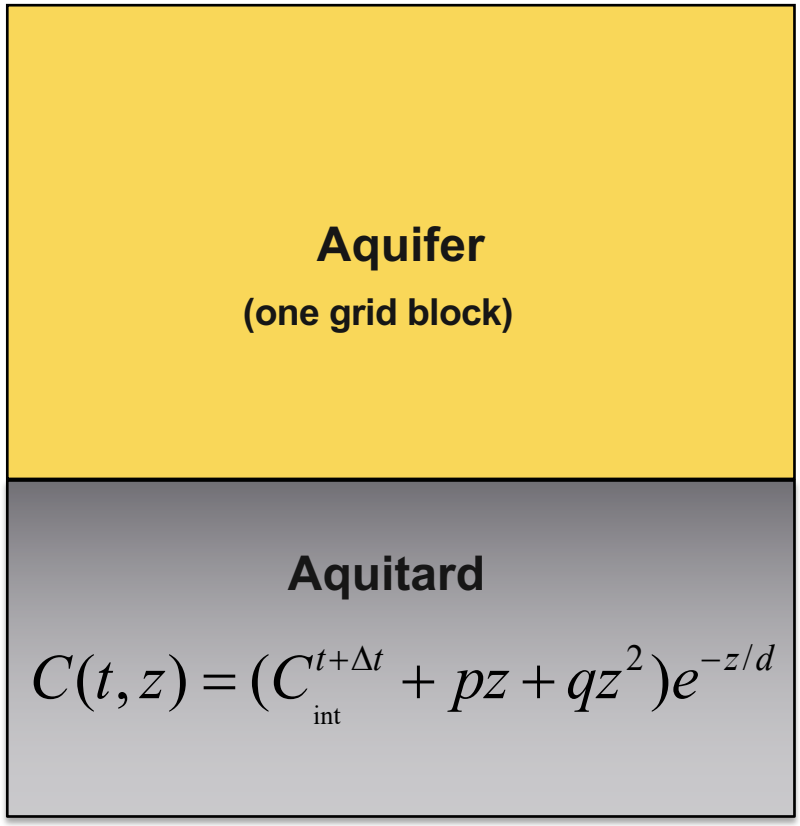
Model Parameters for Matrix Geometry

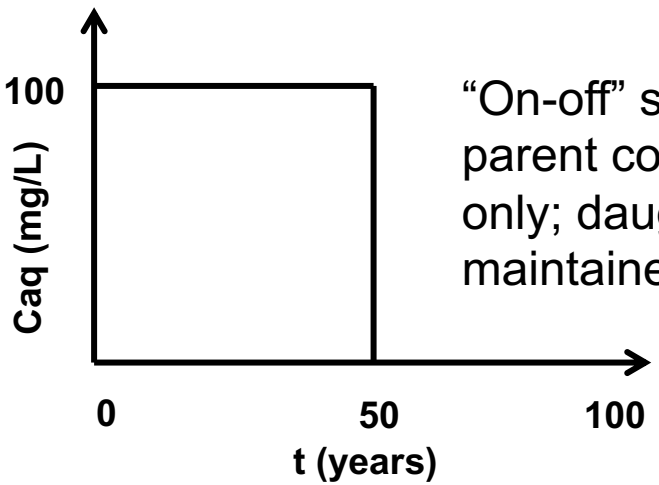
- Three geometric parameters
  - V_f = volume fraction of high permeability material in a gridblock
  - A_{md} = interfacial area between the high and low permeability zones in a gridblock of volume V_T
  - L = characteristic maximum diffusion length
- Parameters are related to each other through a volume balance on the low permeability material

$$(1-V_f)V_T = A_{md}L$$

- Only two geometrical parameters are needed for the matrix diffusion model (V_f and either A_{md} or L)

Testing Parent-Daughter Reactions in Aquitard with 10-Year Half-Life

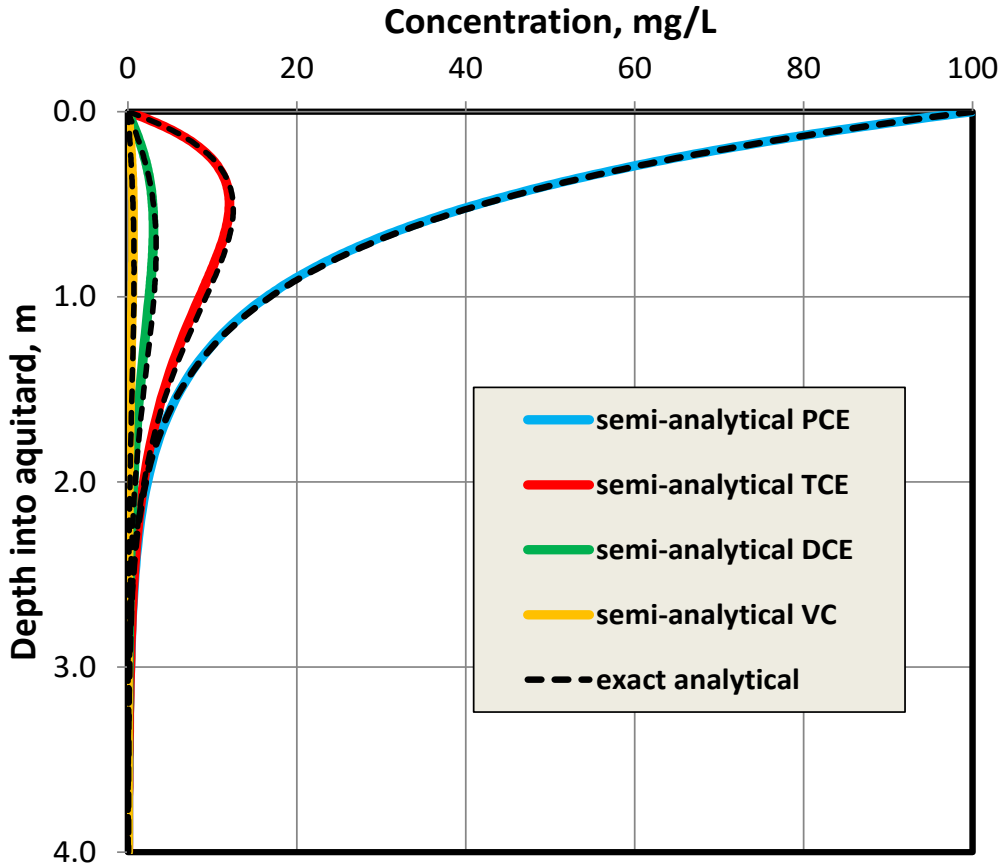




"On-off" source – parent compound only; daughters maintained at zero

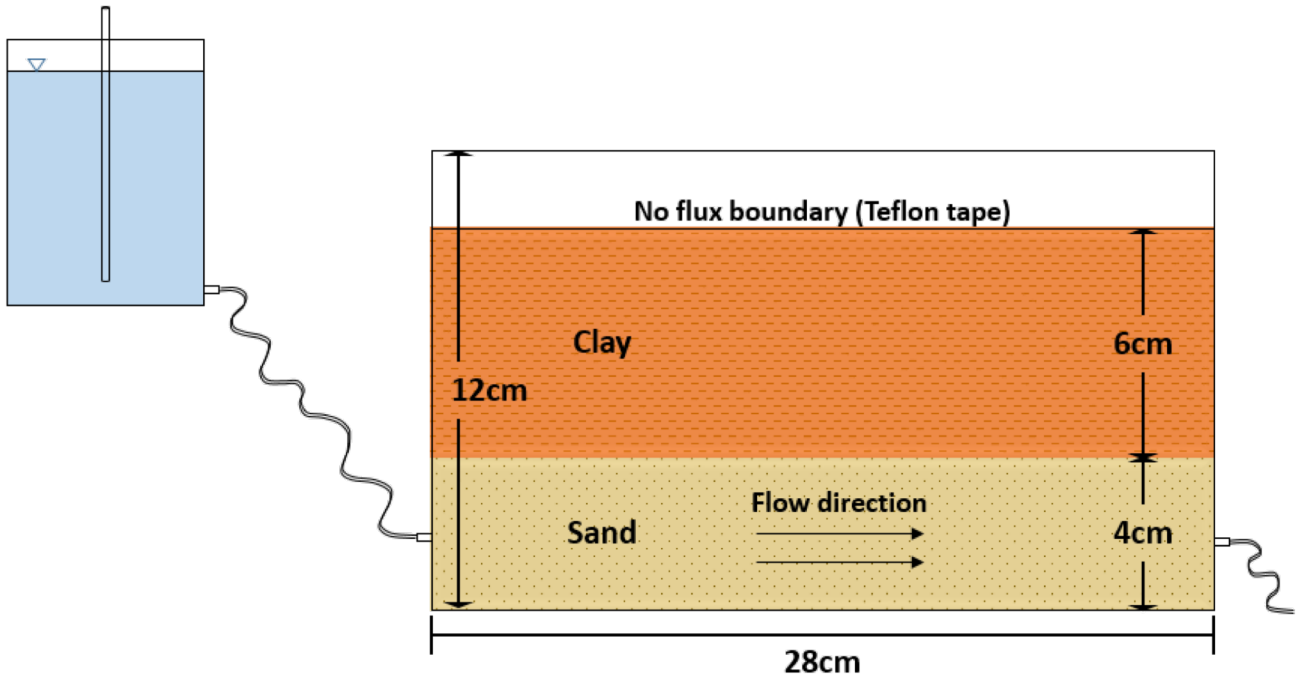
First order decay with daughter production only in low-K zone using semi-analytic method

Testing Parent-Daughter Reactions in Aquitard with 10-Year Half-Life



Comparison of exact analytical solution with concentration profiles in the aquitard after 50 years of diffusion and reaction

Matrix Diffusion Model Simulation of University of Florida Experiments

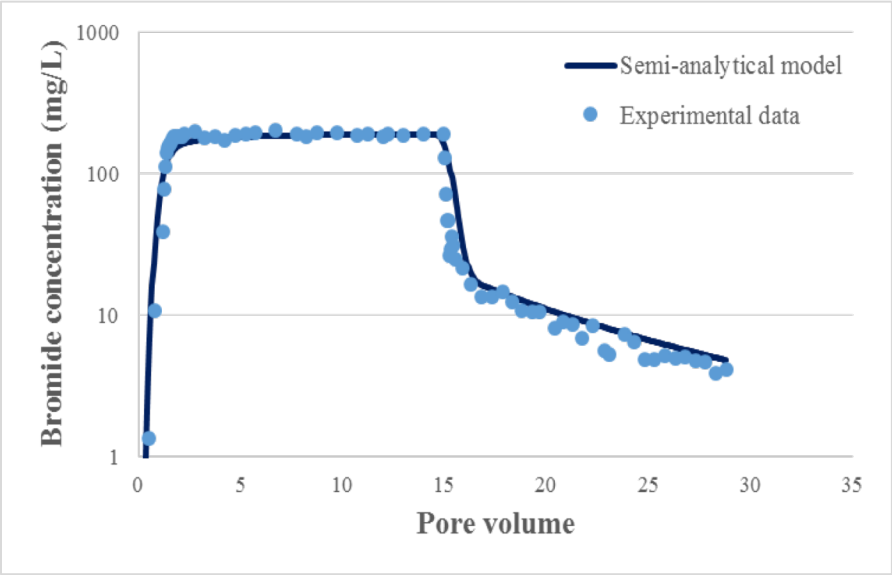


Laboratory experiment consisted of injected tracer for 5 to 15 pore volumes followed by clean water for ~ 15 pore volumes and measuring outlet concentrations. Experiment was simulated by only modeling sand in 1-D, using semi-analytical method for clay*

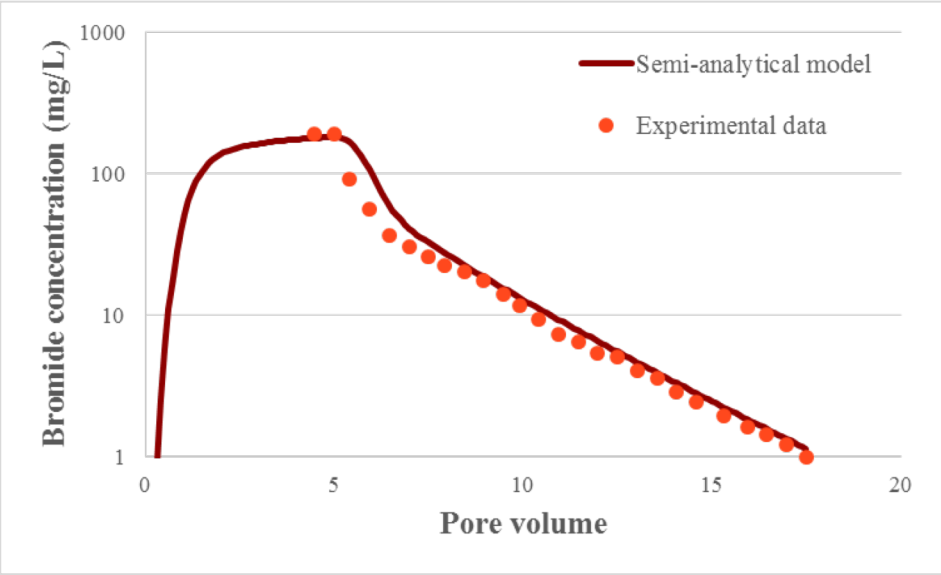
**Yang et al., 2015*

Matrix Diffusion Model Simulation of University of Florida Experiments

Experiment 1*



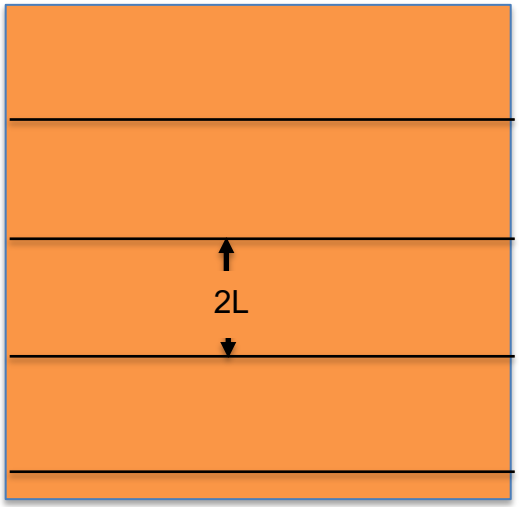
Experiment 3*



*Yang et al., 2015

Matrix Diffusion in Fractured Rock

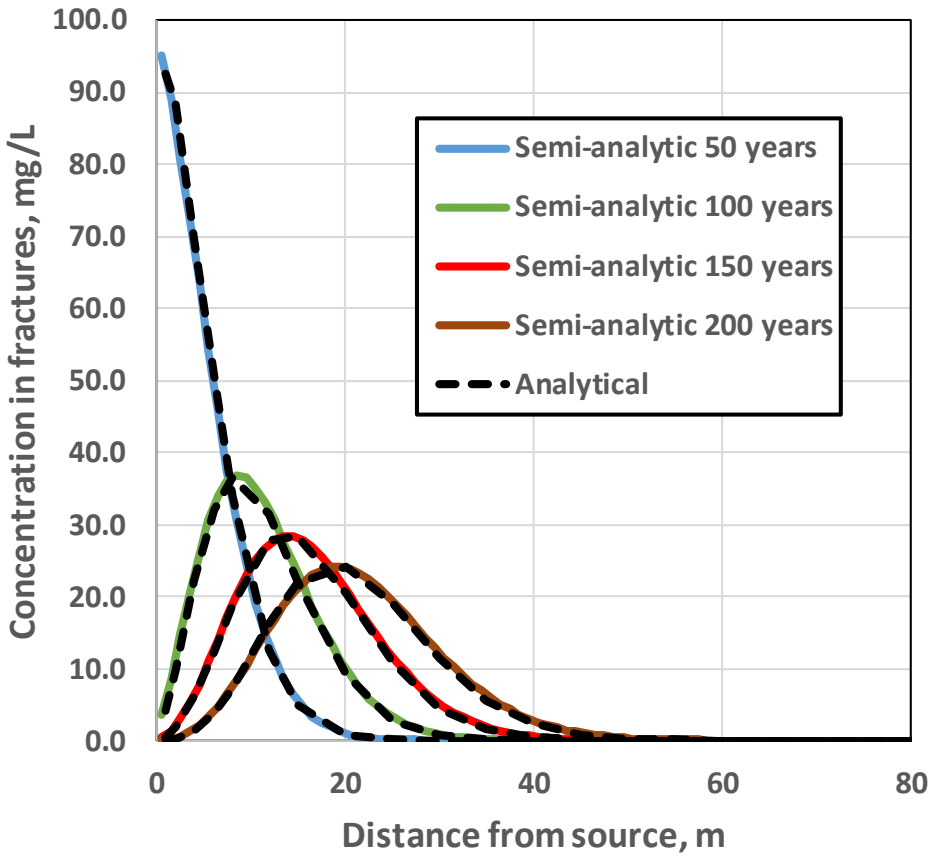
- Fractured rock = “worst case” for matrix diffusion
  - Small volume of fractures, large surface area
- Exact analytical solution called CRAFLUSH is available for the case of parallel fractures*
  - Assumes 1D advection-dispersion-retardation-decay in fracture coupled with perpendicular diffusion and decay in matrix



*Sudicky and Frind, 1982

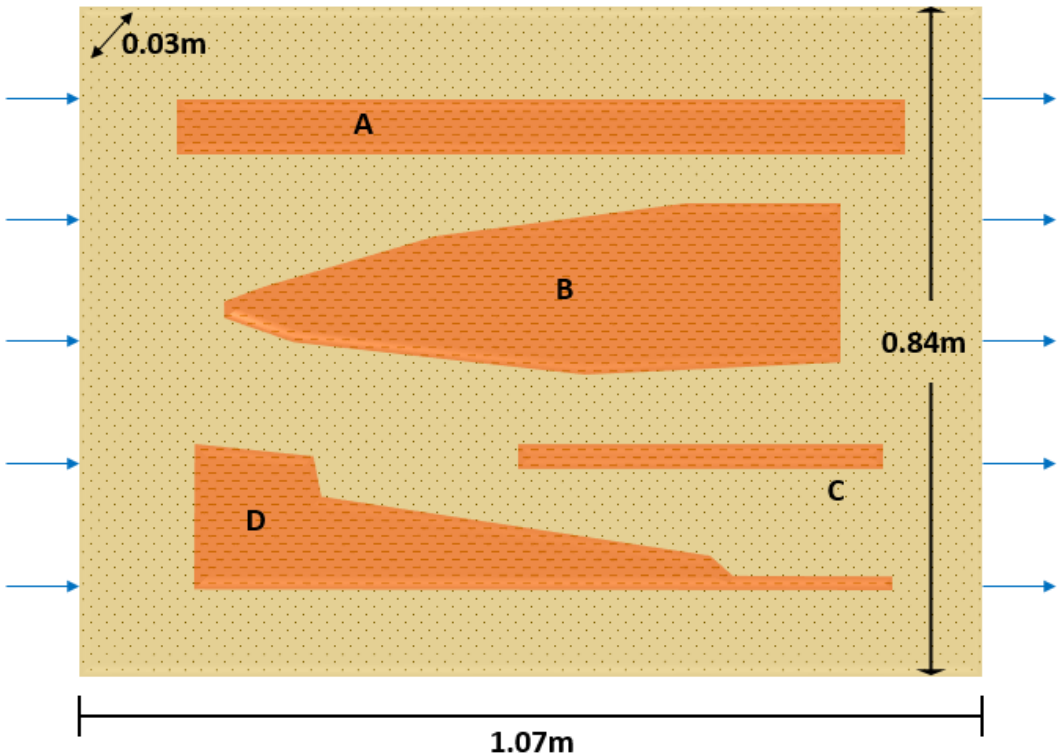
Testing Matrix Diffusion Model in Fractured Rock

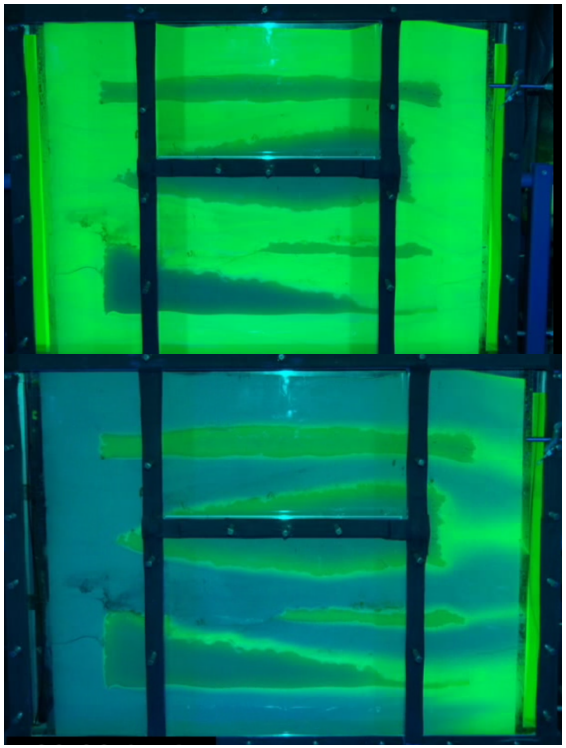
- Compare with analytical solution*
- Fracture spacing (2L) of 0.5 m
- Fracture aperture of 100 μm
- Velocity in fracture is 100 m/yr
- Introduce contaminant for 50 years at 100 mg/L, followed by clean water for 150 years
- Only simulate the flow in the 100 μm fractures using a 1-D grid, with diffusion by the semi-analytic method



*Sudicky and Frind, 1982

Matrix Diffusion Model Simulation of Colorado State Experiment



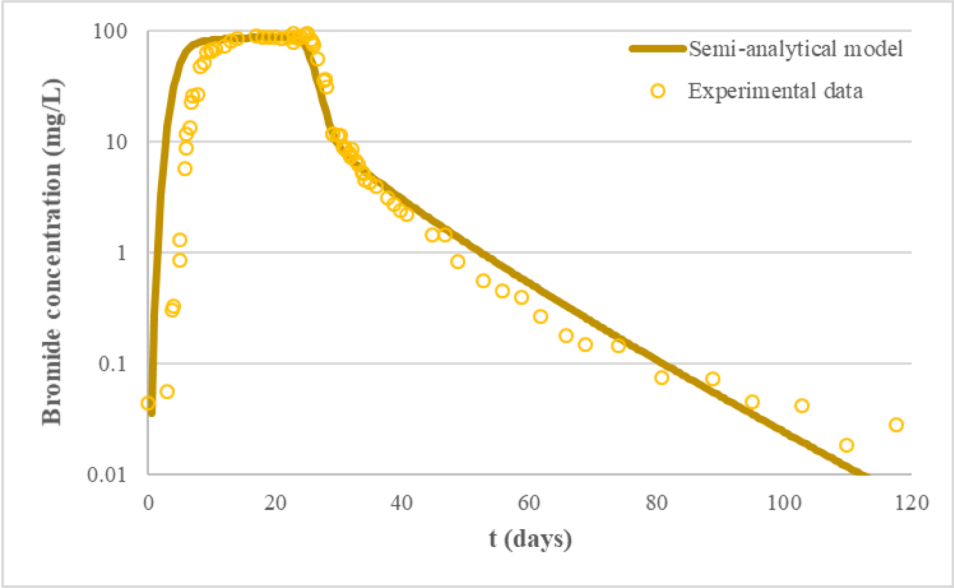


Laboratory experiment was simulated in the matrix diffusion model by only modeling sand in 1-D, using semi-analytical method for clay*

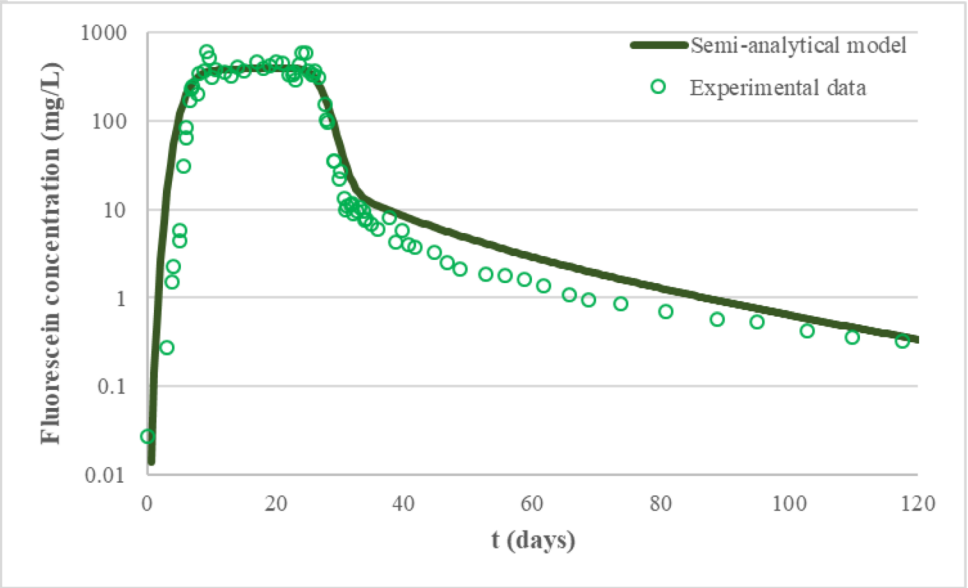
**Doner, 2008*

Matrix Diffusion Model Simulation of Colorado State Experiment

Bromide



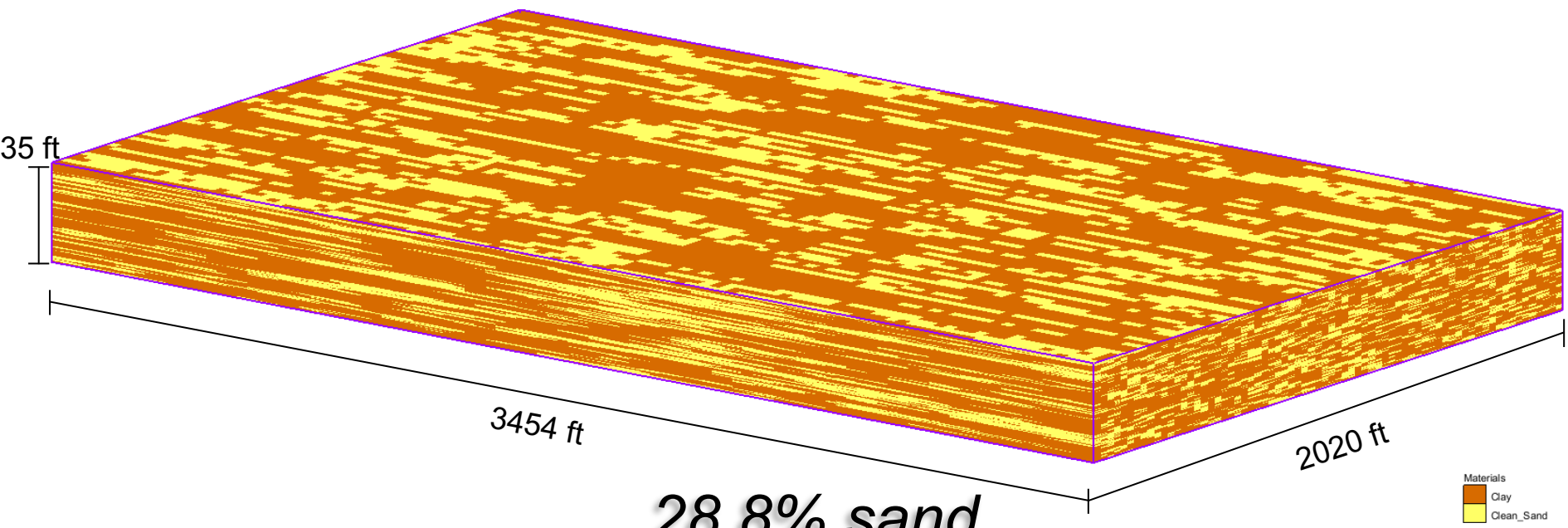
Fluorescein



*Doner, 2008

Heterogeneous Grid

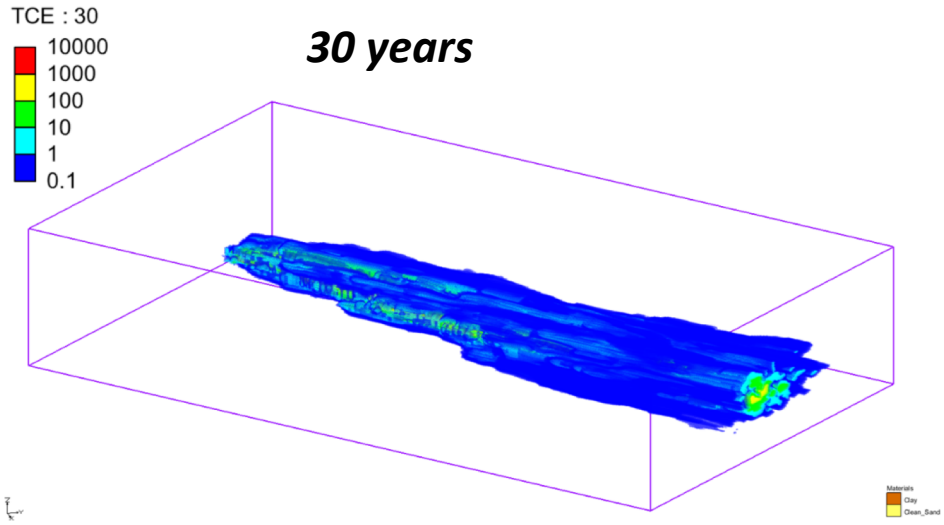
2.8 M Gridblocks, Long Correlation Length in Horizontal Direction

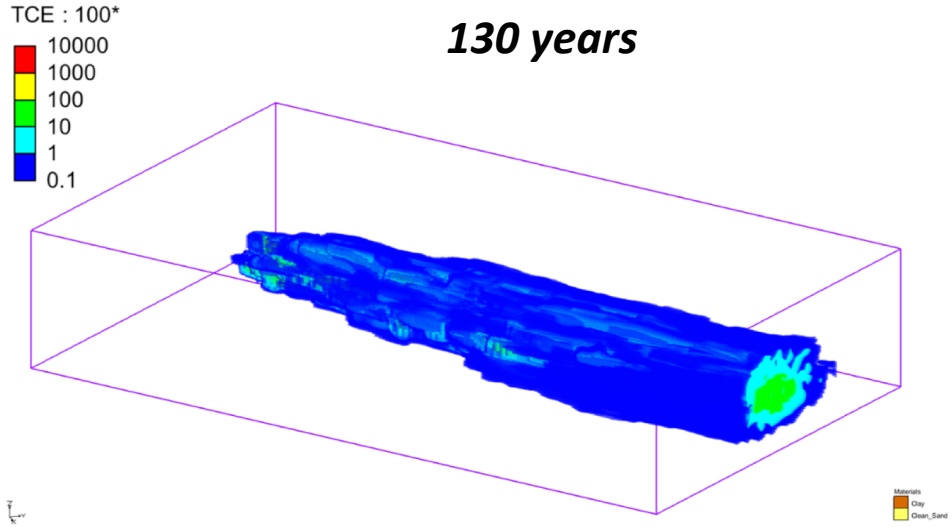


28.8% sand

Fine Grid Numerical Simulation (MT3DMS)

Localized TCE DNAPL source removal after 30 yrs





MT3DMS transport simulation models matrix diffusion into the clay lenses directly, using 400 model layers in the vertical dimension. The simulation takes several days to run. Transport is dominated by advection in the heterogeneous flow field, and by matrix diffusion

Coarse Grid Simulation (REMChlor-MD)

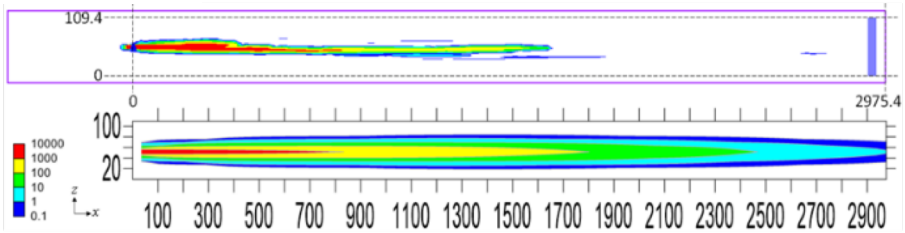
Localized TCE DNAPL source removal after 30 yrs

- Modeled using a homogeneous grid with only 7,128 gridblocks, 18 layers in vertical direction
- Macro-scale dispersion simulated with dispersivities
- Matrix diffusion simulated using the semi-analytical method
- Matrix diffusion parameters, V_f, L, and A_{md} estimated by sampling grid (like boreholes)
- Model runs in 13 seconds compared to several days for fine grid MT3DMS simulation

Comparison of MT3DMS and REMChlor-MD Results

Side View

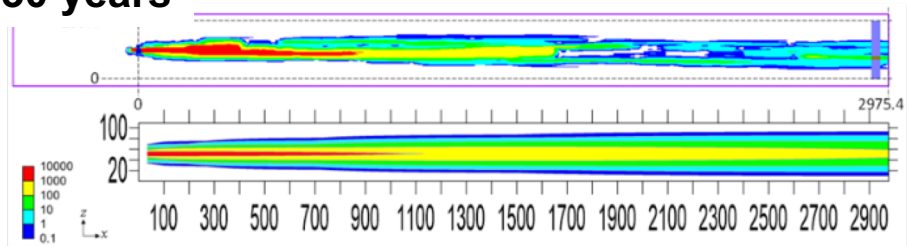
10 years



MT3DMS

REMChlor-MD

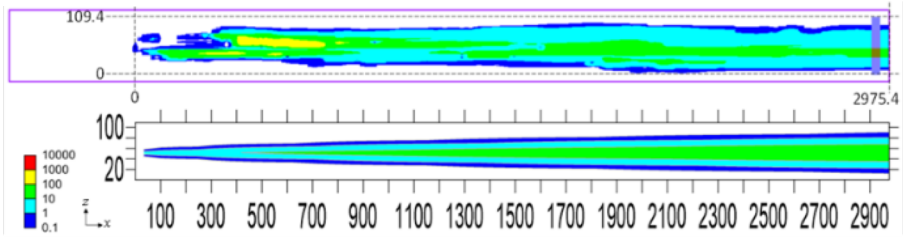
30 years



MT3DMS

REMChlor-MD

130 years



MT3DMS

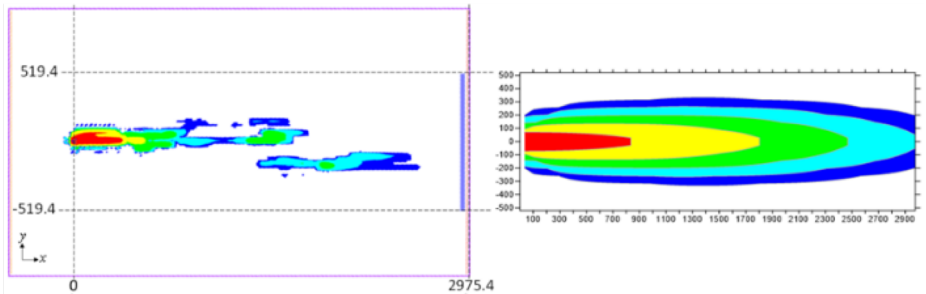
REMChlor-MD

Comparison of MT3DMS and REMChlor-MD Results

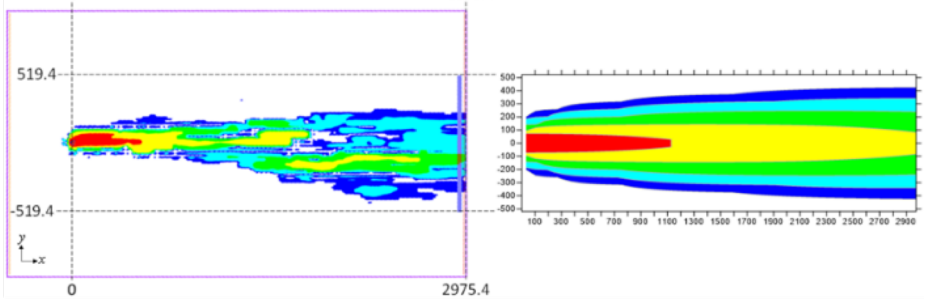
Top View

MT3DMS | REMChlor-MD

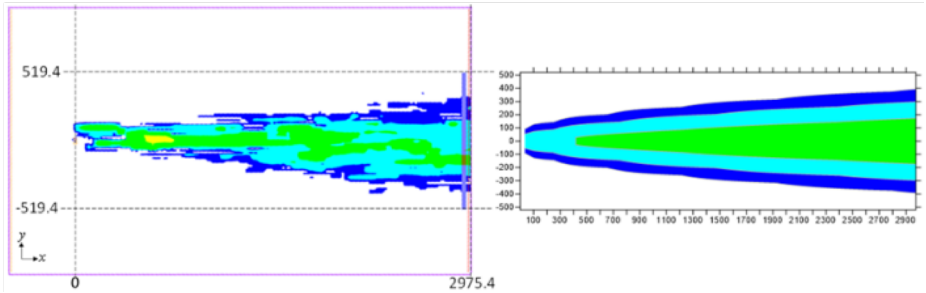
10 years



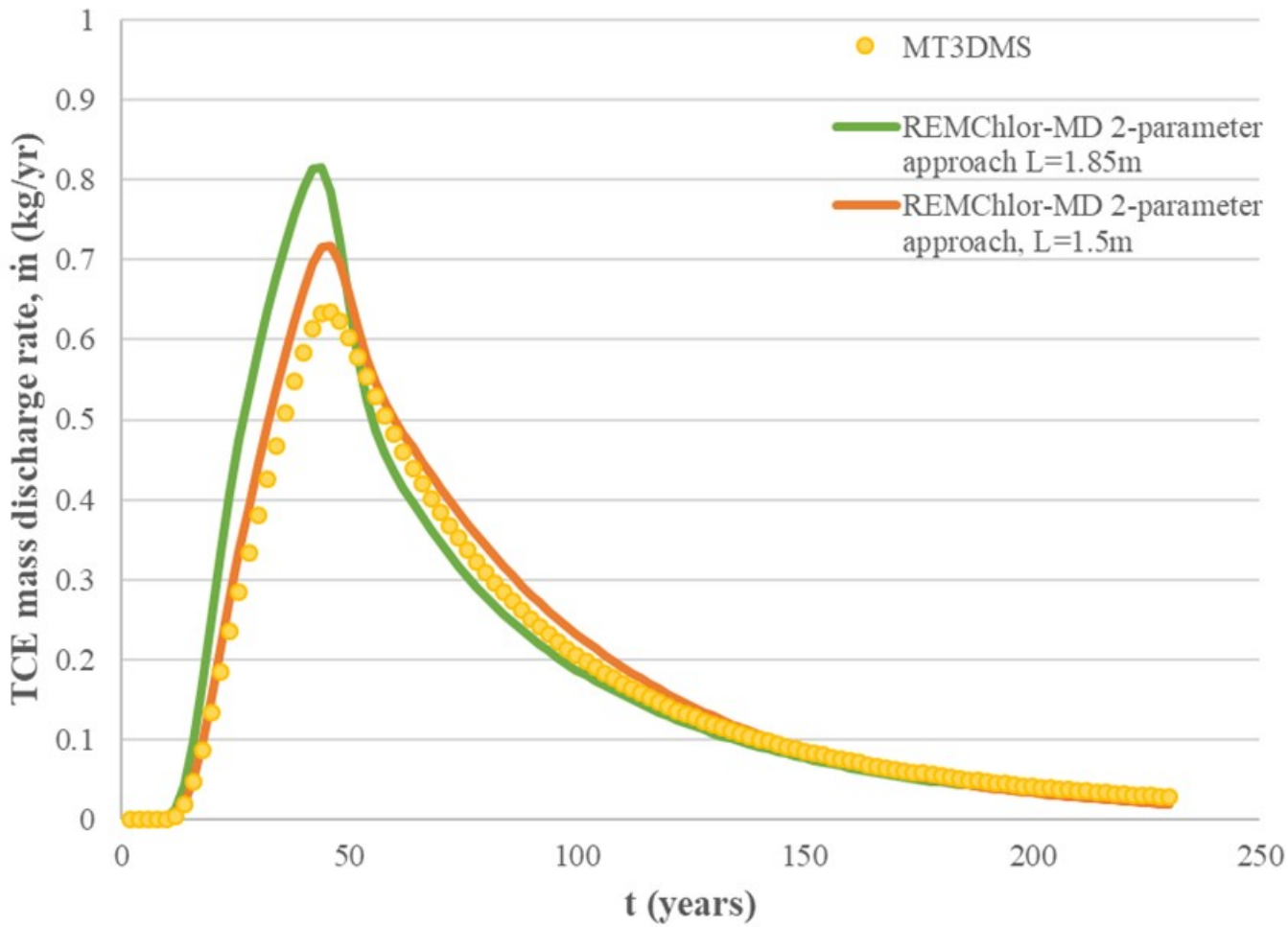
30 years



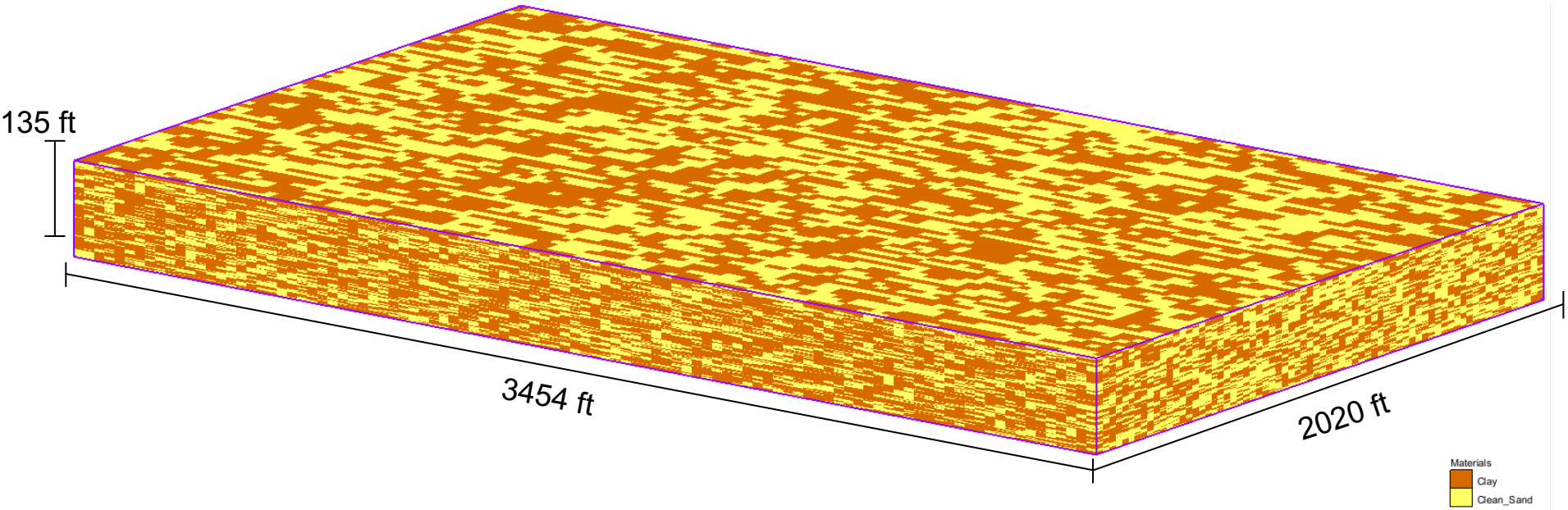
130 years



Comparison of Mass Discharge at Downstream Face (x=3000 ft)



Second Heterogeneous Grid with More Random Heterogeneity

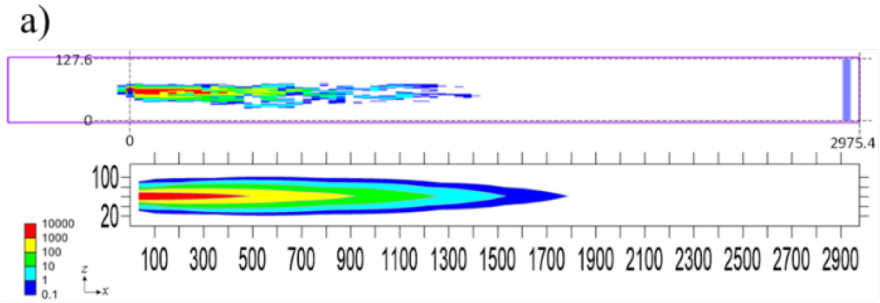


35.1% sand

Comparison of MT3DMS and REMChlor-MD

Side View

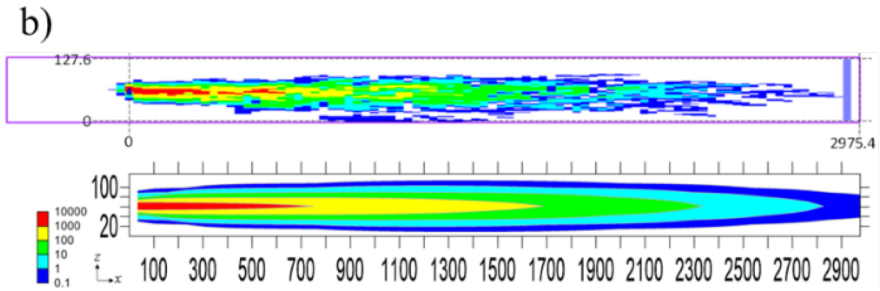
10 years



MT3DMS

REMChlor-MD

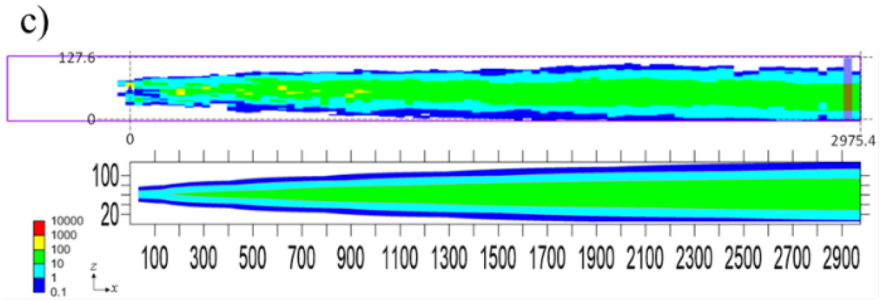
30 years



MT3DMS

REMChlor-MD

130 years



MT3DMS

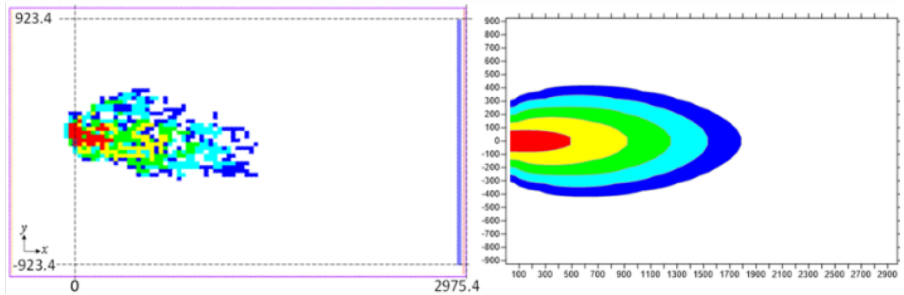
REMChlor-MD

Comparison of MT3DMS and REMChlor-MD

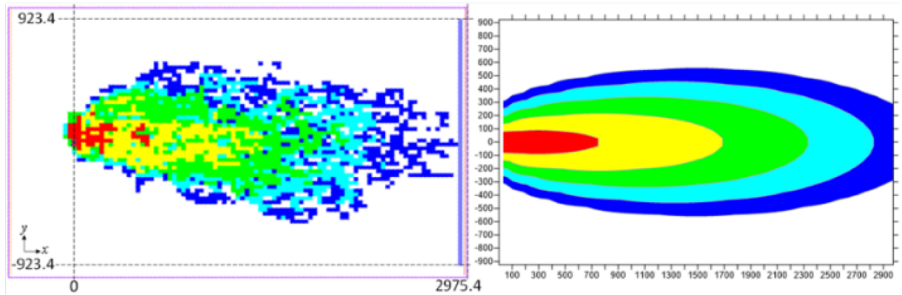
Top View

MT3DMS | REMChlor-MD

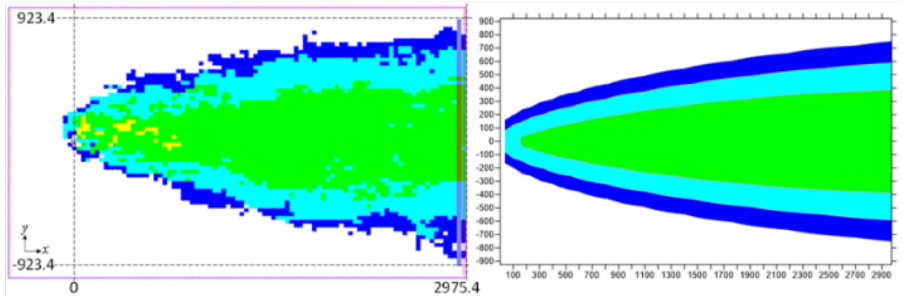
10 years



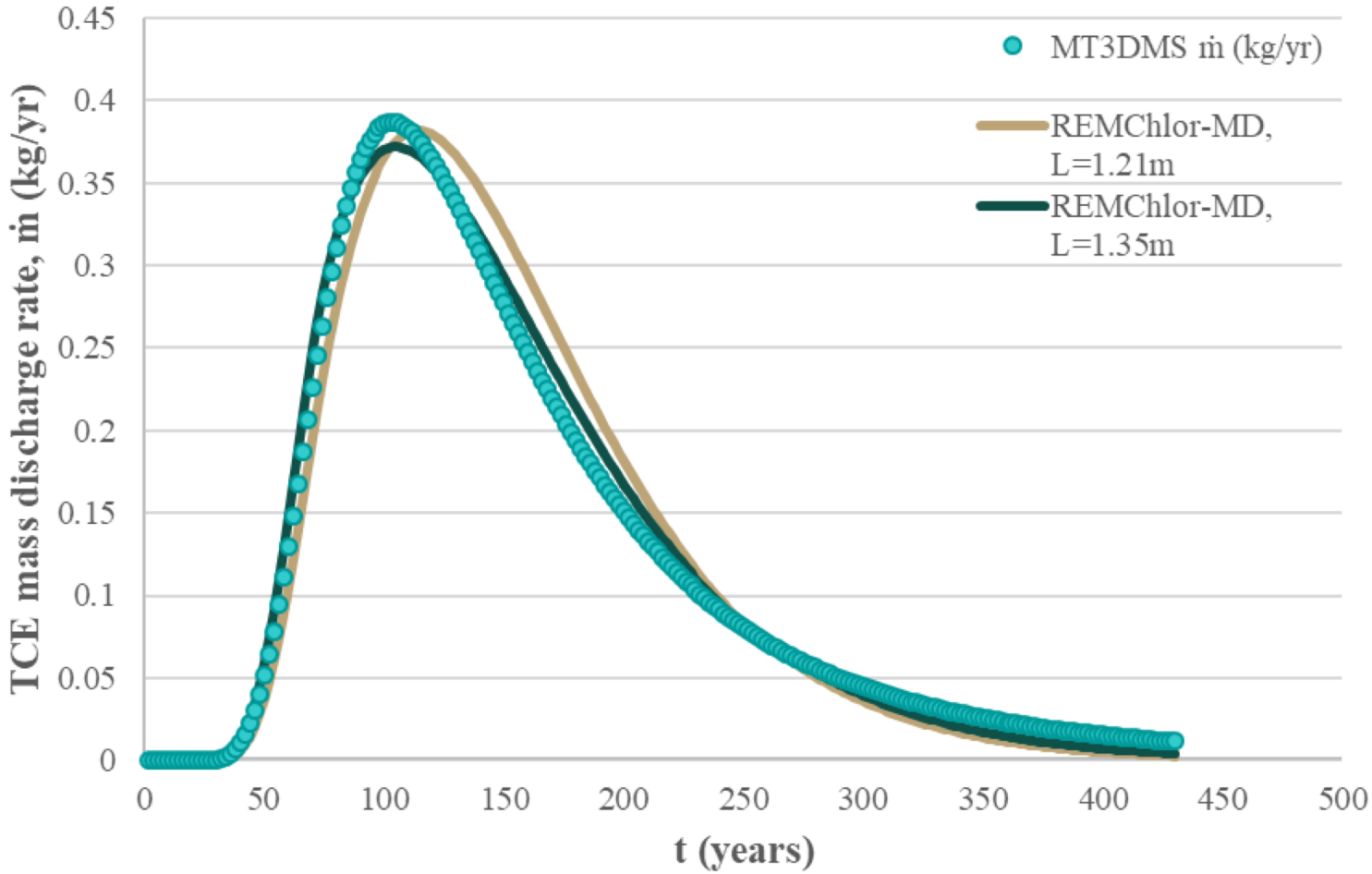
30 years



130 years

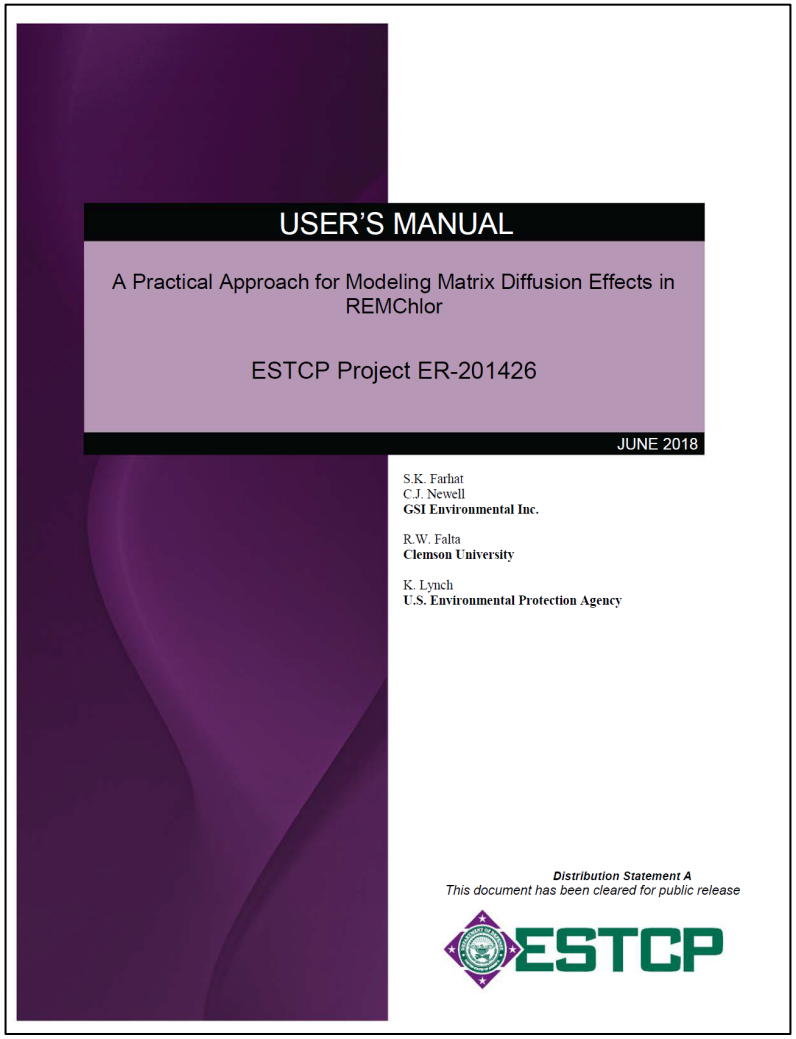


Comparison of Mass Discharge at Downstream Face (x=3000 ft)



Download REMChlor-MD Model and User's Guide for Free from ESTCP

- 108-page manual describes theory and all input and output variables
- Chemical and geologic parameter databases are included
- Three case studies and six appendices


USER'S MANUAL

A Practical Approach for Modeling Matrix Diffusion Effects in REMChlor

ESTCP Project ER-201426

JUNE 2018

S.K. Farhat
C.J. Newell
GSI Environmental Inc.

R.W. Falta
Clemson University

K. Lynch
U.S. Environmental Protection Agency

Distribution Statement A
This document has been cleared for public release

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Q&A Session 1

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ESTCP

Using REMChlor-MD

Dr. Chuck Newell
Dr. Shahla Farhat
GSI Environmental, Inc.

SERDP
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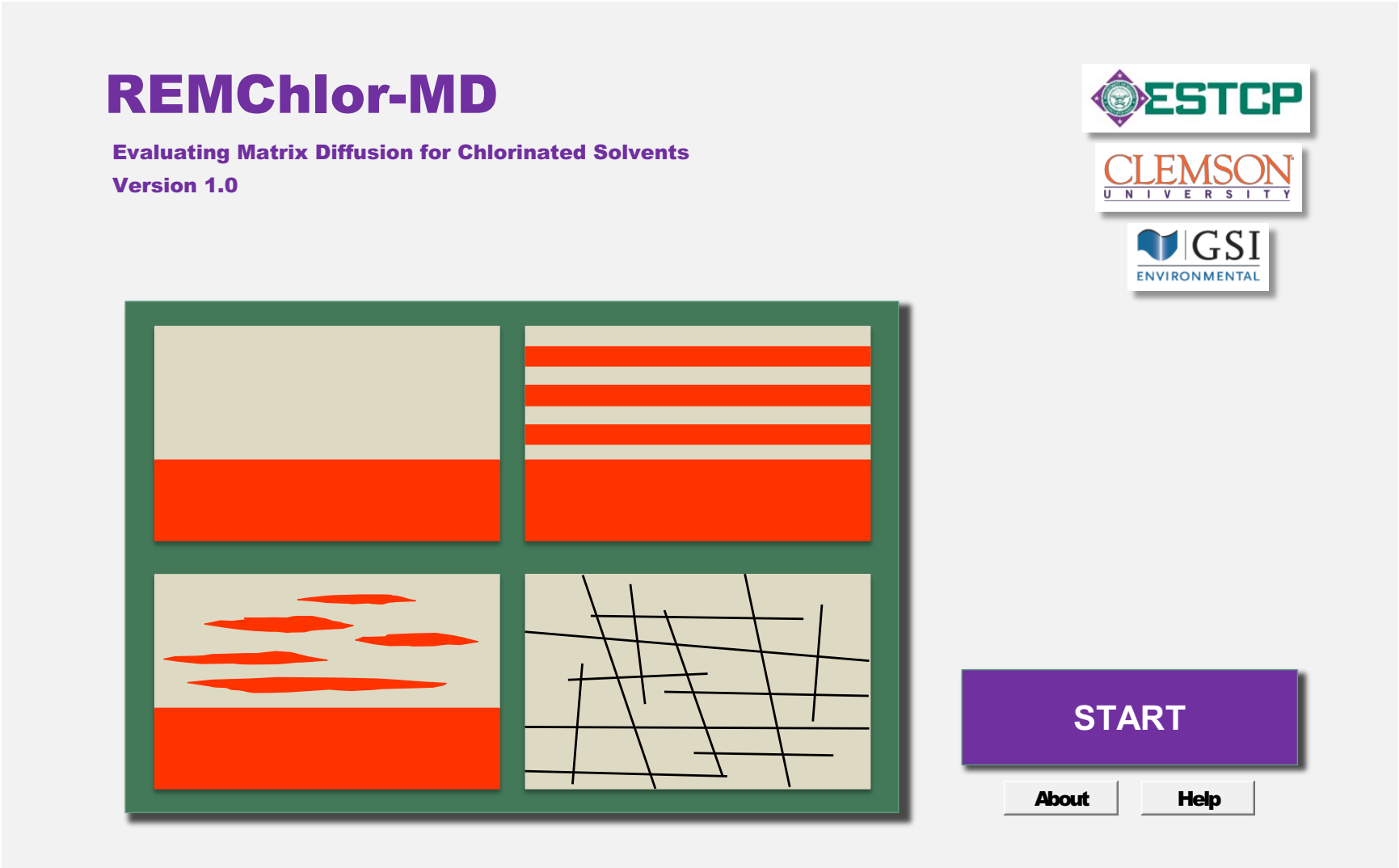
REMChlor-MD Main Screen



Main Data Input Screen

REMChlor-MD Data Input Screen

Version 1.0

Site Location and ID: REMChlor Tutorial 7

1. STARTING INFORMATION — SI Units | English Units | Unconsolidated | Fractured Rock/Media

2. MODEL CONFIGURATION

	Cell Size	Model Size	
X-Direction (in direction of groundwater flow)	20	2000	(m)
Y-Direction (transverse to groundwater flow)	10	200	(m)
Z-Direction (vertical) (all layers have same hydrogeology)	3	15	(m)

Observation Well Location: X-Value 205.0 (m) Y-Value 23.0 (m)

Obs. Well Z-Value Top of Screen (model bottom is at Z=0) 6.2 (m) Bottom of Screen 0.8 (m)

Starting Year of Simulation (year the source started) 1970 (YYYY year)

Ending Year of Simulation 2070 (YYYY year)

Start Year (release yr) — T1 (Sect. 6) — T2 (Sect. 6) — Ending Year

3. MEDIA CHARACTERISTICS (uniform for all cells)

	Soil Type	Hydr. Cond. (m/yr)	Porosity (-)	Tortuosity (-)
Transmissive Zone (T-Zone)	Sand	1.25E+04	0.33	0.70
Low Permeability Zone (Low-k)	Clay	1.00E+00	0.4	0.70

T-Zone Hydraulic Gradient 0.0020 (-)

T-Zone Groundwater Darcy Velocity 2.50E+01 (m/yr)

Default Tortuosity

4. MATRIX DIFFUSION

Calculate Heterogeneity

Average Darcy Velocity (including low-k units)	1.00E+01	(m/yr)
Transmissive Zone Volume Fraction	4.00E+01	(%)
Average Diffusion Length	5.00E-01	(m)
Surface Area of Low-k Interfaces	7.20E+02	(m2)

5. CONTAMINANTS AND SOURCE TERM

	Parent	Deg. Prod. 1	Deg. Prod. 2	Deg. Prod. 3	
Constituent (use dropdown menu)	PCE	TCE	cis-DCE	Vinyl Chloride	
Initial Source Concentration	1.00E+02	0.00E+00	0.00E+00	0.00E+00	(mg/L)
Source Mass at Time of Release	1.62E+03	0.00E+00	0.00E+00	0.00E+00	(kg)
Retardation Factor in T-Zone	2	2	2	2	(-) Calc R
Retardation Factor in Low-k	2	2	2	2	(-) Calc R'

Source Width (REMChlor-MD will round to nearest whole cell) 10 (m)

Z-Value for Top of Source (model bottom is at Z=0) 3 (m)

Z-Value for Bottom of Source 0 (m)

General Molecular Diffusion Coefficient for all Constituents 1.00E-09 (m2/sec)

Next Step: Show Graph | Show Previous Results | New Site/Clear Data | Paste Example | HELP | Return to Main Screen | Save/Export Data | Load Data

DATA INPUT INSTRUCTIONS

Enter value directly. Toolkit default value. OK to overwrite.
Value calculated by Toolkit. Cell cannot be edited.

6. PLUME DEGRADATION

(Both T-Zone and Low-k Zone)

Degradation First Order Decay Rates — Enter Custom Microbial Yield Terms

Time (yrs)		PCE	TCE	cis-DCE	Vinyl Chloride
Model ends here		Zone 1	Zone 2	Zone 3	
	Period 3	Decay Rate (1,3)	Decay Rate (2,3)	Decay Rate (3,3)	
		4.00E-01	4.00E-01	4.00E-01	T-Zone (1/yr)
		4.00E-01	4.00E-01	4.00E-01	Low-k (1/yr)
50.00 (yrs) Time Period 2 (T2)	Period 2	Decay Rate (1,2)	Decay Rate (2,2)	Decay Rate (3,2)	
		4.00E-01	4.00E-01	4.00E-01	T-Zone (1/yr)
		4.00E-01	4.00E-01	4.00E-01	Low-k (1/yr)
40.00 (yrs) Time Period 1 (T1)	Period 1	Decay Rate (1,1)	Decay Rate (2,1)	Decay Rate (3,1)	
		4.00E-01	4.00E-01	4.00E-01	T-Zone (1/yr)
Model starts here		4.00E-01	4.00E-01	4.00E-01	Low-k (1/yr)

X1 300 X2 700

Distance From Source (m)

7. PLUME TRANSPORT

	Longitudinal	Transverse	Vertical
Dispersivity (m)	0	0.5	0.1

Dispersivity Calculator

8. SOURCE ZONE REMEDIATION

Percent Source Mass Removed by Remediation	90	(%)
Remediation Started in Year	30.00	(yrs)
Remediation Ended in Year	31.00	(yrs)
Mass-Flux/Remaining-Mass Term (Gamma, Γ)	1	(-)
Natural Source Decay Rate	0	(1/yr)

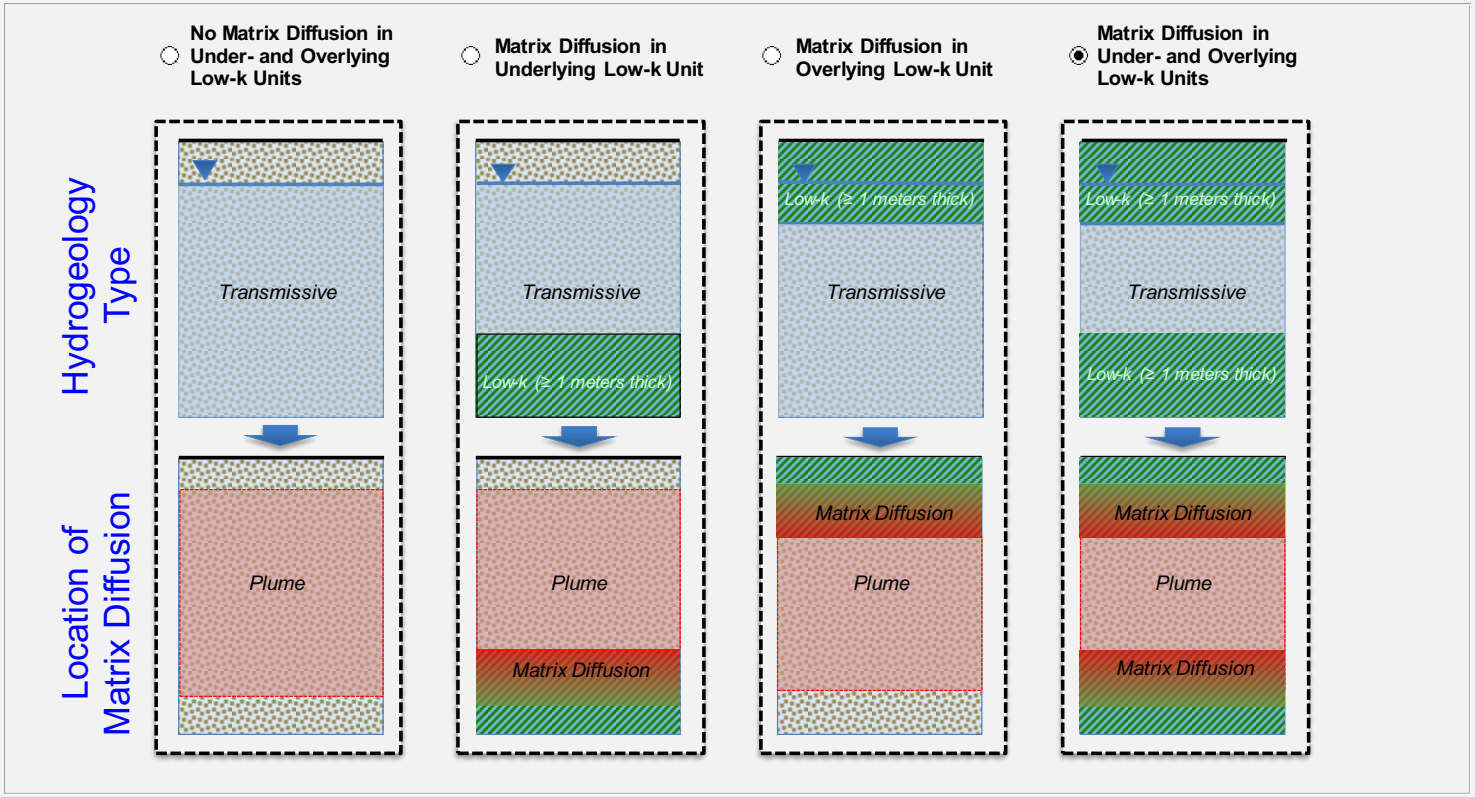
9. MODELING PARAMETERS

Timestep Size	1	(yr)
Maximum Number of Iterations	500	(-)
Convergence Tolerance	1.00E-05	(mg/L)
See Results Every	10	(yr)

Matrix Diffusion: Heterogeneity Calculator – Unconsolidated, Step 1

REMChlor-MD Heterogeneity Calculator - Unconsolidated Media *Version 1.0*

STEP 1. Pick One of These Three Basic Top/Bottom Conditions for Your Plume



Next: Go to Step 2

Return to Main Input Screen

HELP

Matrix Diffusion: Heterogeneity Calculator – Unconsolidated, Step 2

REMChlor-MD Heterogeneity Calculator - Unconsolidated Media

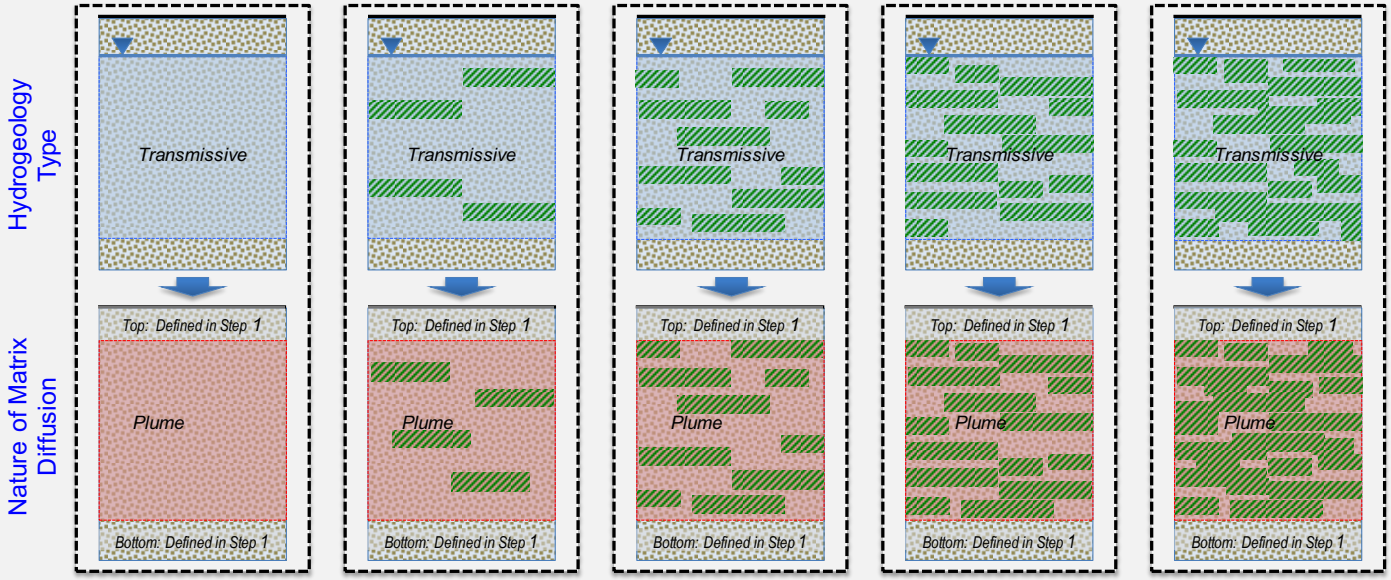
Version 1.0

STEP 2. **Pick an option for the embedded layering between the top and bottom of your plume that best represents your Site.**

(Note: Don't count the top and bottom Low-k layers; just the in-between embedded layers.)

Simple Method: Pick one of these five options:

- ○ **~0% of Plume Thickness is in Low-k Material** (not counting top, bottom
- ○ **~20% of Plume Thickness is in Low-k Material** (not counting top, bottom
- ○ **~40% of Plume Thickness is in Low-k Material** (not counting top, bottom
- ◉ **~60% of Plume Thickness is in Low-k Material** (not counting top, bottom
- ○ **~80% of Plume Thickness is in Low-k Material** (not counting top, bottom



OR pick one of these two options:

- ○ Use Site-Specific Boring Log Data (More complicated, but more accurate)
- ○ Enter Heterogeneity Parameters Manually

Next: Go to Step 3

Return to Step 1

Return to Main Input Screen

HELP

Matrix Diffusion: Heterogeneity Calculator – Unconsolidated, Step 3

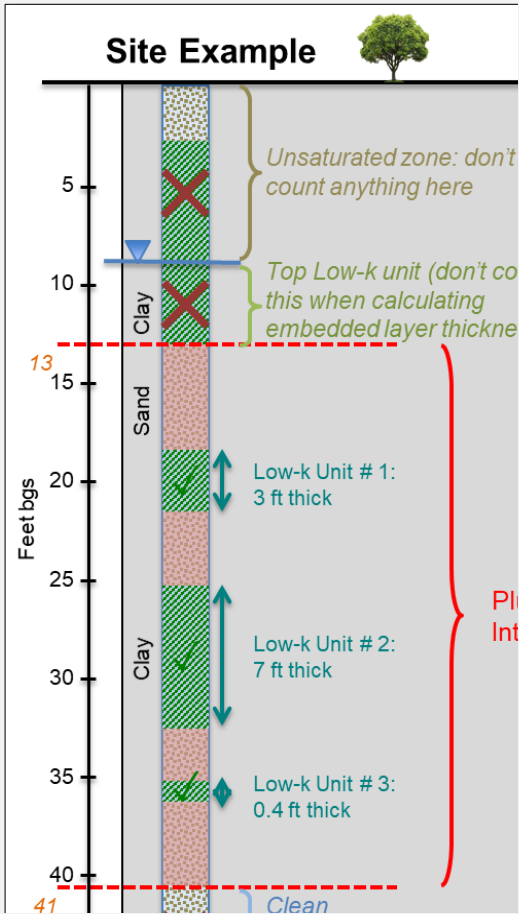
REMChlor-MD Heterogeneity Calculator - Unconsolidated Media *Version 1.0*

STEP 3. Estimate Site-Specific Heterogeneity Parameters

1. Number of wells to be used 3 *(≤ 100 wells)*
2. Enter the top and bottom of the plume and the thickness for each separate low-k unit. *Leave blank if you have entered data for all the low-k units in the boring log.*

	Plume Top (m bgs)	Plume Bottom (m bgs)	Low-k Unit Thickness (m) 1	2	3	4	5	6	7	8	9	10
Well 1	10.00	38.00	0.50	1.00	2.00							
Well 2	10.00	38.00	2.00	0.50	1.00							
Well 3	10.00	38.00	0.50	1.00	2.00							

Next Step: Calc Heterogeneity | **Return to Step 1** | **Return to Step 2** | *Clear All Data* | ***HELP***



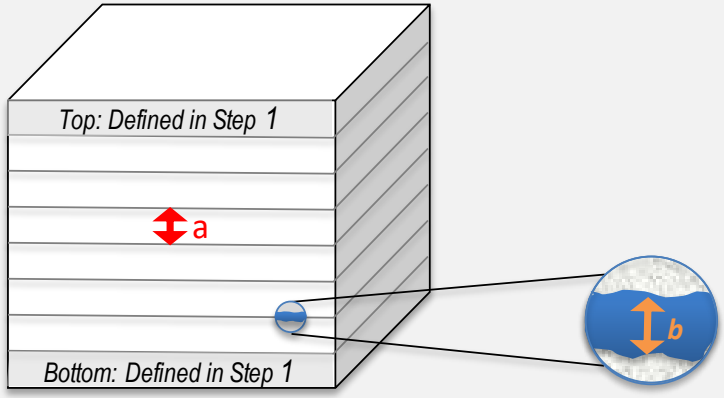
V_f Volume fraction of high permeability material in a gridblock

A_{md} Interfacial area between the high and low permeability zones in a gridblock of volume V_T

L Characteristic maximum diffusion length

Matrix Diffusion: Heterogeneity Calculator – Fractured Media, Step 2

REMChlor-MD Heterogeneity Calculator - Fractured Rock/Media *Version 1.0*



Next: Continue

Return to Step 1

Return to Main Input Screen

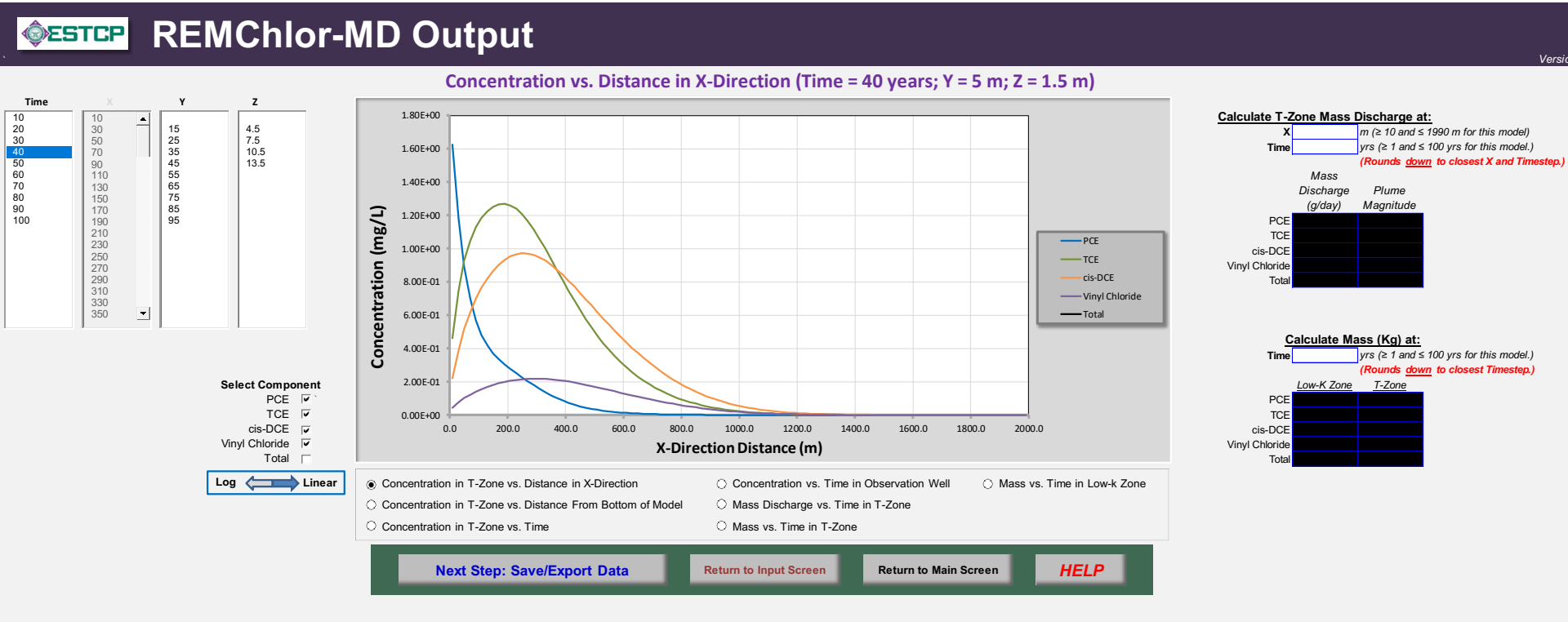
Clear Data

HELP

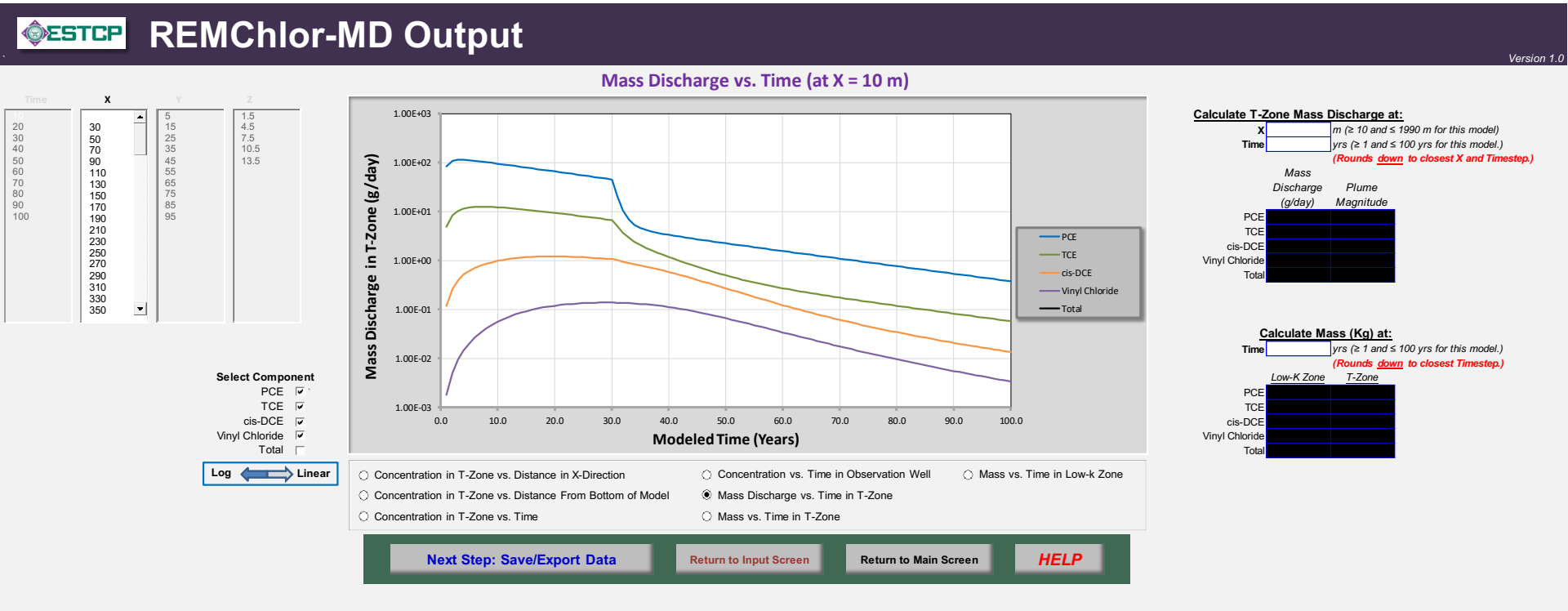
STEP2. Enter Fracture Data

1. Typical distance between parallel fractures ("a")	1.00E+00	*(m)*
2. Typical thickness of aperture/fracture ("b")	1.00E-04	*(m)*

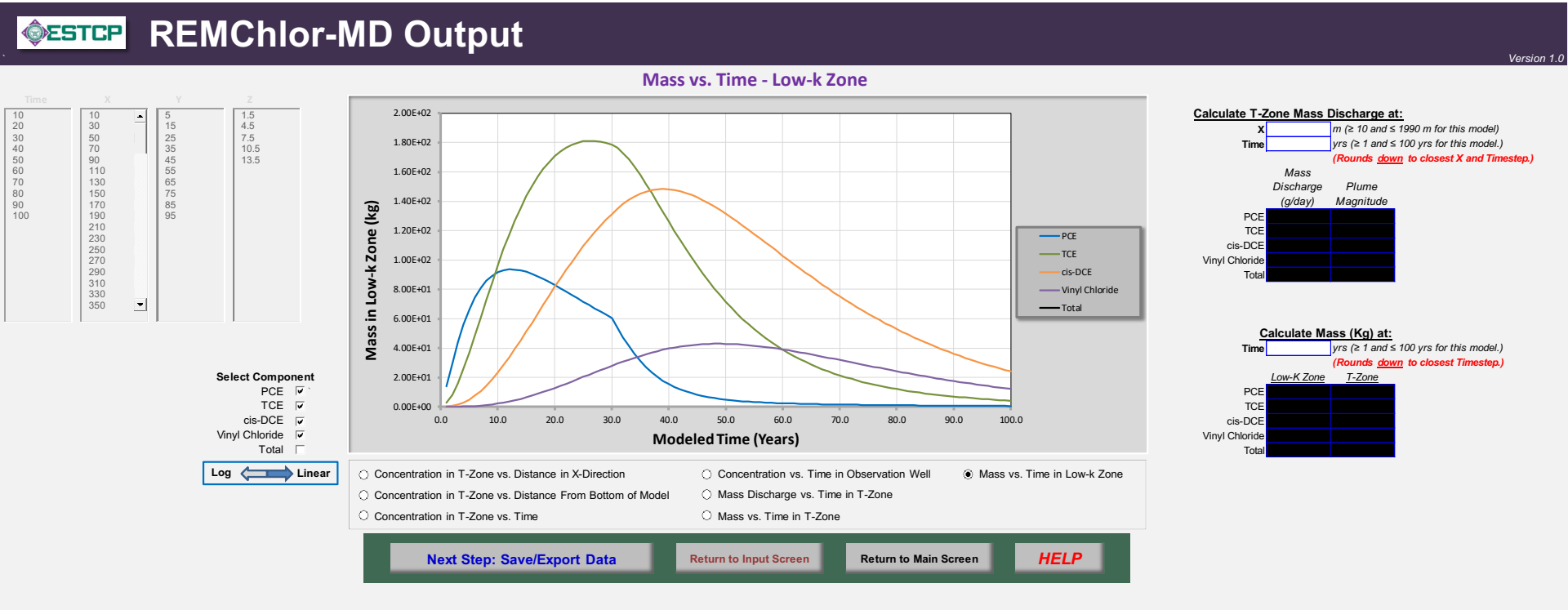
Model Output



Model Output

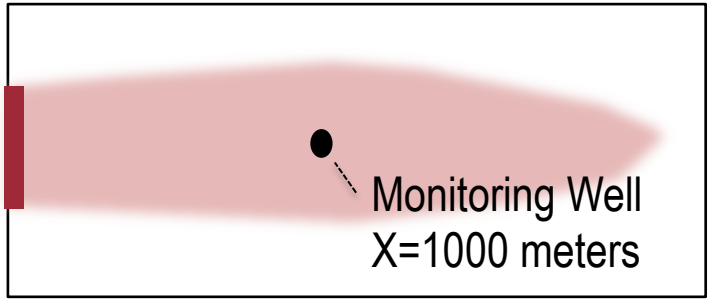


Model Output

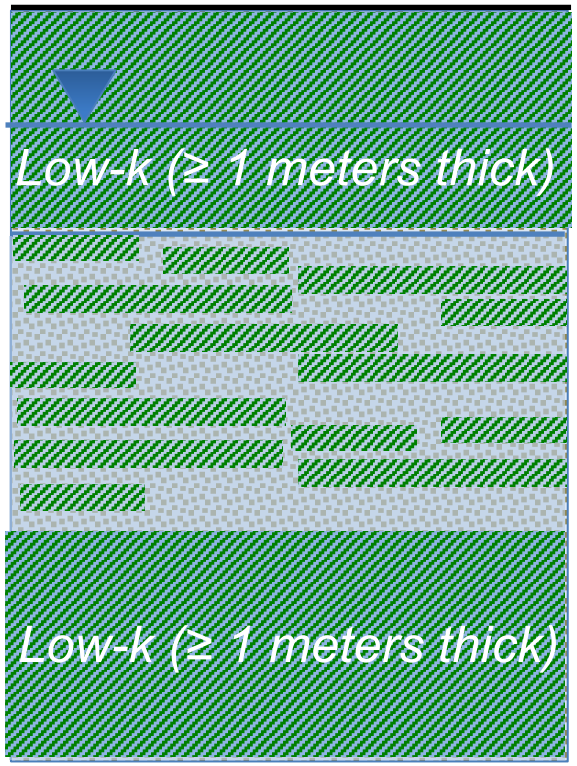


How Important is All This?

Old REMChlor vs. REMChlor-MD



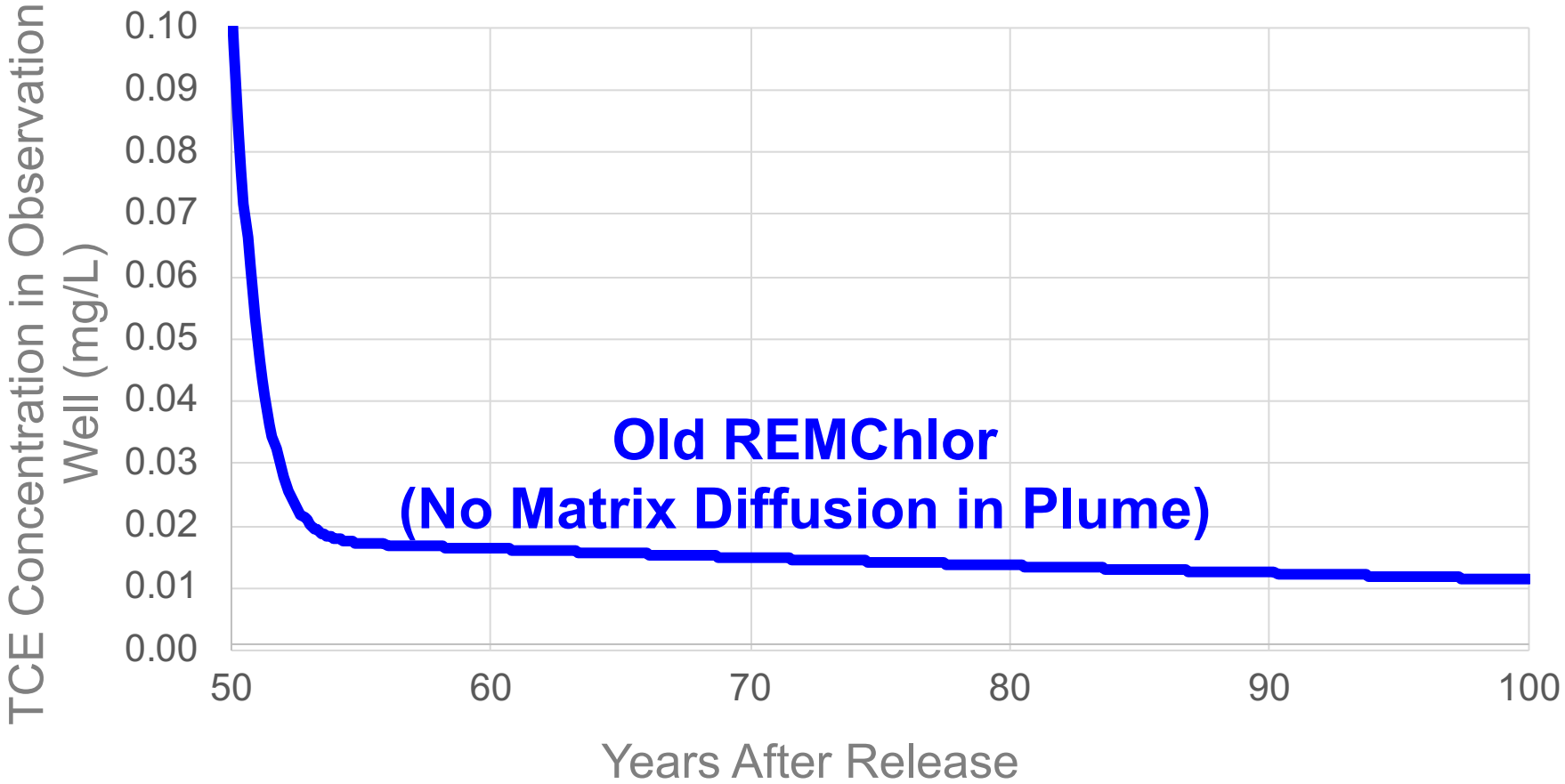
- TCE source: 100 mg/L
- Decaying source (gamma = 1)
- Source remediation: 99% Removal 30 years
- No plume biodegradation
- Retardation factor = 2

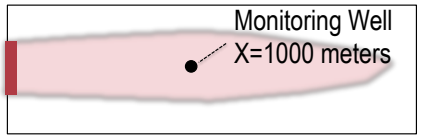


- Matrix diffusion: Top and bottom layers
- 40% aquifer volume is low-K with interbedded layers

Old REMChlor vs. REMChlor-MD

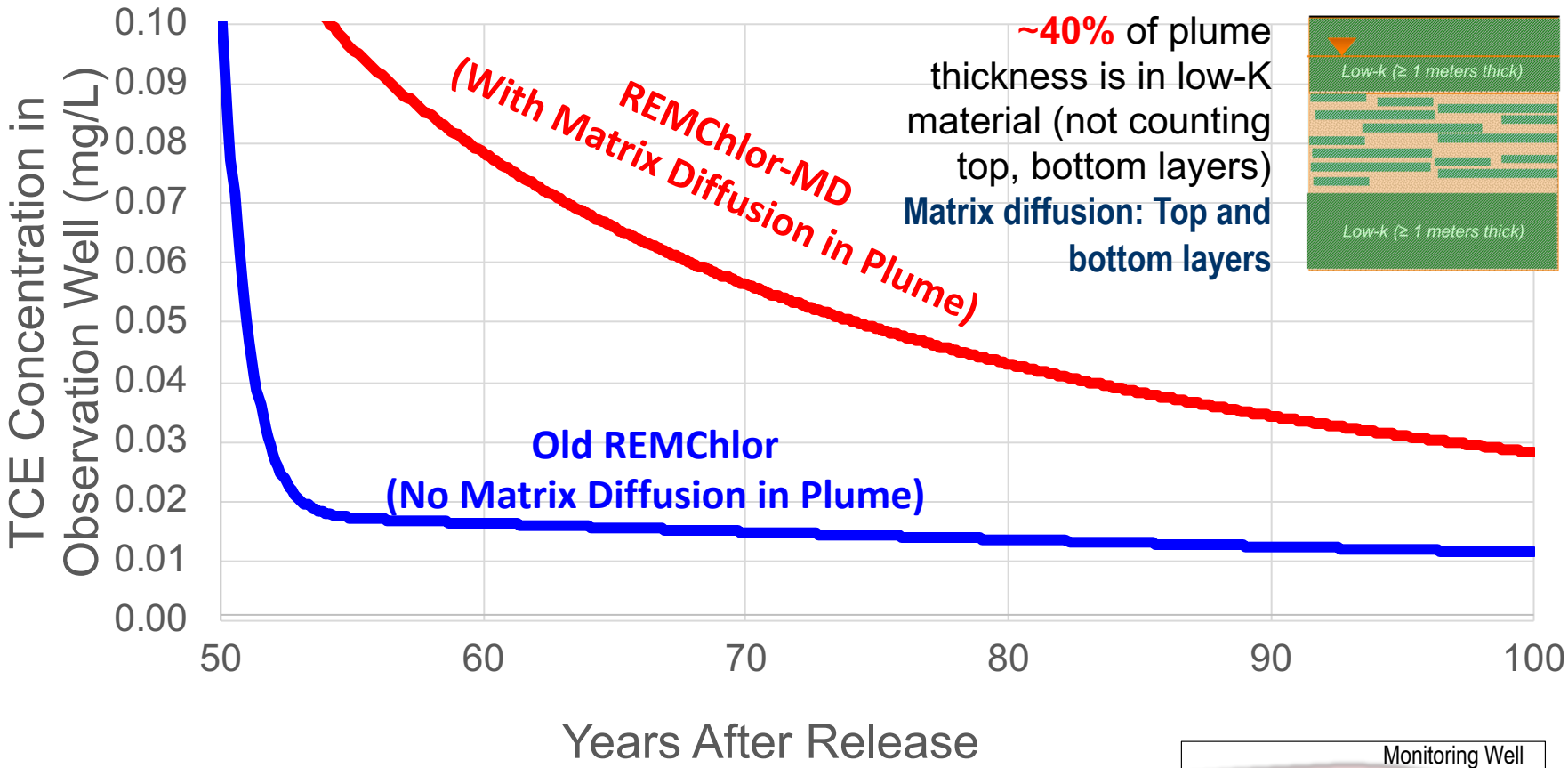
100 mg/L source with 99% removal after 30 years

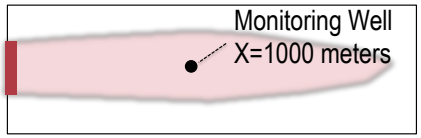




Old REMChlor vs. REMChlor-MD

100 mg/L source with 99% removal at 30 years





Conclusions

- New method for simulating matrix diffusion in aquitards, heterogeneous aquifers, and fractured rocks is developed
- Method is implemented in a new version of the REMChlor source/plume remediation model
- Matrix diffusion can be included in a simulation with minimal effort on the part of the user
- Future work will apply this method to the 3-D MODFLOW 6 flow and transport code

DoD Benefits

- Allows users to quickly asses the effect of matrix diffusion in a screening-level model
- Model can consider both source and plume remediation
- Model only requires 2 parameters related to the low-K zone geometry
- Model can be run with and without matrix diffusion to highlight impact

For additional information, please visit

https://www.serdp-estcp.org/Program-Areas/Environmental-Restoration/Contaminated-Groundwater/Persistent-Contamination/ER-201426

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skfarhat@gsi-net.com; 713-522-6300

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Q&A Session 2

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The next webinar is on February 21, 2019

Utilization of Advanced Conservation Voltage Reduction for Energy Reduction on DoD Installations

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Survey Reminder

Please take a moment to complete the survey that will pop up on your screen when the webinar ends

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