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Practical Models to Support Remediation Strategy Decision-Making – Part 2

Sponsored by: U.S. EPA Office of Superfund Remediation and Technology Innovation

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With that, please move to slide 3.

New online broadcast screenshot

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Practical Models to Support Remediation Strategy Decision-Making

Ronald W. Falta, Ph.D
Brian Looney, Ph.D
Charles J. Newell, Ph.D, P.E.
Karen Vangelas
Shahla K. Farhat, Ph.D

Module 2 - October 2012

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Seminar Disclaimer

- **The purpose of this presentation is to stimulate thought and discussion.**
- **Nothing in this presentation is intended to supersede or contravene the National Contingency Plan**

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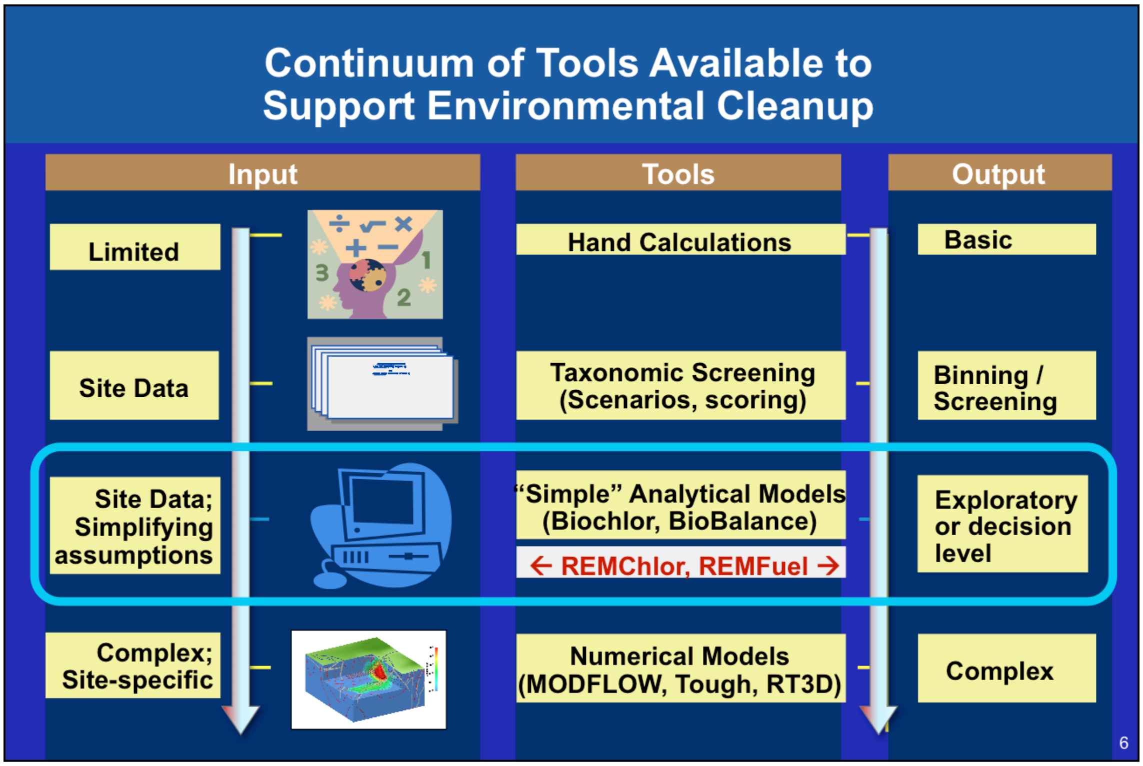
Continuum of Tools Available to
Support Environmental Cleanup
Input
Tools
Output
Limited
Hand Calculations
Basic
Site Data
Taxonomic Screening
(Scenarios, scoring)
Binning /
Screening
Site Data;
Simplifying
assumptions
"Simple" Analytical Models
(Biochlor, BioBalance)
← REMChlor, REMFuel →
Exploratory
or decision
level
Complex;
Site-specific
Numerical Models
(MODFLOW, Tough, RT3D)
Complex
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INSTRUCTORS: *Ron Falta, Ph.D.*

CLEMSON UNIVERSITY

- **Professor, Dept. of Environmental Engineering & Earth Sciences, Clemson University**
  - Ph.D. Material Science & Mineral Engineering, U. of California, Berkley
  - M.S., B.S. Civil Engineering Auburn University
- **Instructor for subsurface remediation, groundwater modeling, and hydrogeology classes**
- **Developer of REMChlor and REMFuel Models**
- **Author of Numerous technical articles**
- **Key expertise:** Hydrogeology, contaminant transport/ remediation, and multiphase flow in porous media

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INSTRUCTORS: *Charles J Newell,* Ph.D., P.E.

- **Vice President, GSI Environmental Inc.**
  - Diplomate in American Academy of Environmental Engineers
  - NGWA Certified Ground Water Professional
  - Adjunct Professor, Rice University
- **Ph.D. Environmental Engineering, Rice Univ.**
- **Co-Author 2 environmental engineering books; 5 environmental decision support software systems; numerous technical articles**
- **Expertise:** Site characterization, groundwater modeling, non-aqueous phase liquids, risk assessment, natural attenuation, bioremediation, software development, long term monitoring, non-point source studies

INSTRUCTORS: *Vangelas, Looney, Farhat*

- **Karen Vangelas, Savannah River National Lab**
  - M.S. Environmental Engineering, Penn State
  - Groundwater, remediation
- **Brian Looney, Savannah River National Lab**
  - Ph.D. Environmental Engineering, U. of Minnesota
  - Vadose zone, remediation, groundwater modeling
- **Shahla Farhat, GSI Environmental**
  - Ph.D. Environmental Engineering, U. of North Carolina
  - Decision support tools, remediation, modeling

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BREAK FOR DISCUSSION OF HOMEWORK EXERCISE 1 AND RESPONSES TO MODULE 1 QUESTIONS FROM PARTICIPANTS

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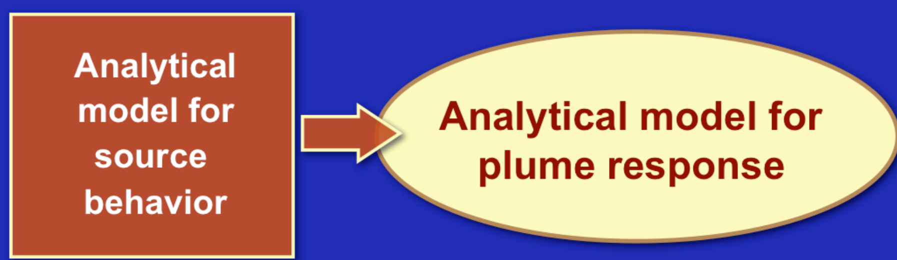
Explanation of How the *Plume* Works in REMChlor



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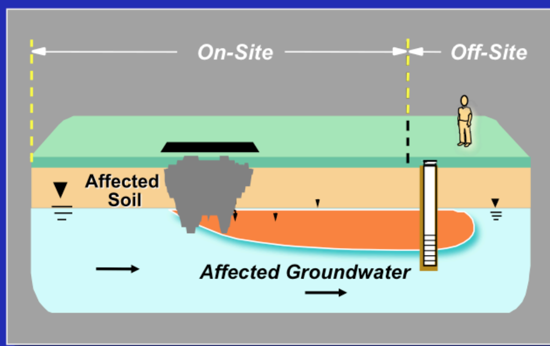
Key Concept 2: Plumes



Key Driver

- Discharge from source

Key Processes

- Advection
- Dispersion
- Adsorption
- Degradation

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Key Material Balance Equations - Plume

Plume equation solved for each species. Equations are linked through the chemical reaction terms.

First-Order Decay reactions

$$R\frac{\partial C_i}{\partial t} = -v\frac{\partial C_i}{\partial x} + \alpha_x v\frac{\partial^2 C_i}{\partial x^2} + \alpha_y v\frac{\partial^2 C_i}{\partial y^2} + \alpha_z v\frac{\partial^2 C_i}{\partial z^2} + rxn_i$$

Retardation Coefficient

Longitudinal Dispersivity

Transverse Dispersivity

Vertical Dispersivity

Groundwater Seepage Velocity

$$V = \frac{K\,i}{n_e}$$

Hydraulic Conductivity

Hydraulic Gradient

Effective Soil Porosity

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Groundwater Transport Processes - *Biodegradation*

- Indigenous micro-organisms are capable of degrading many contaminants.
- Need electron donor and electron acceptor.
- ***Fuels*** like benzene serve as **electron donor.** Oxygen, nitrate, sulfate, iron are **electron acceptor.**
- ***Chlorinated solvents*** act as **electron acceptor.** Hydrogen/acetate serve as **electron donor.**

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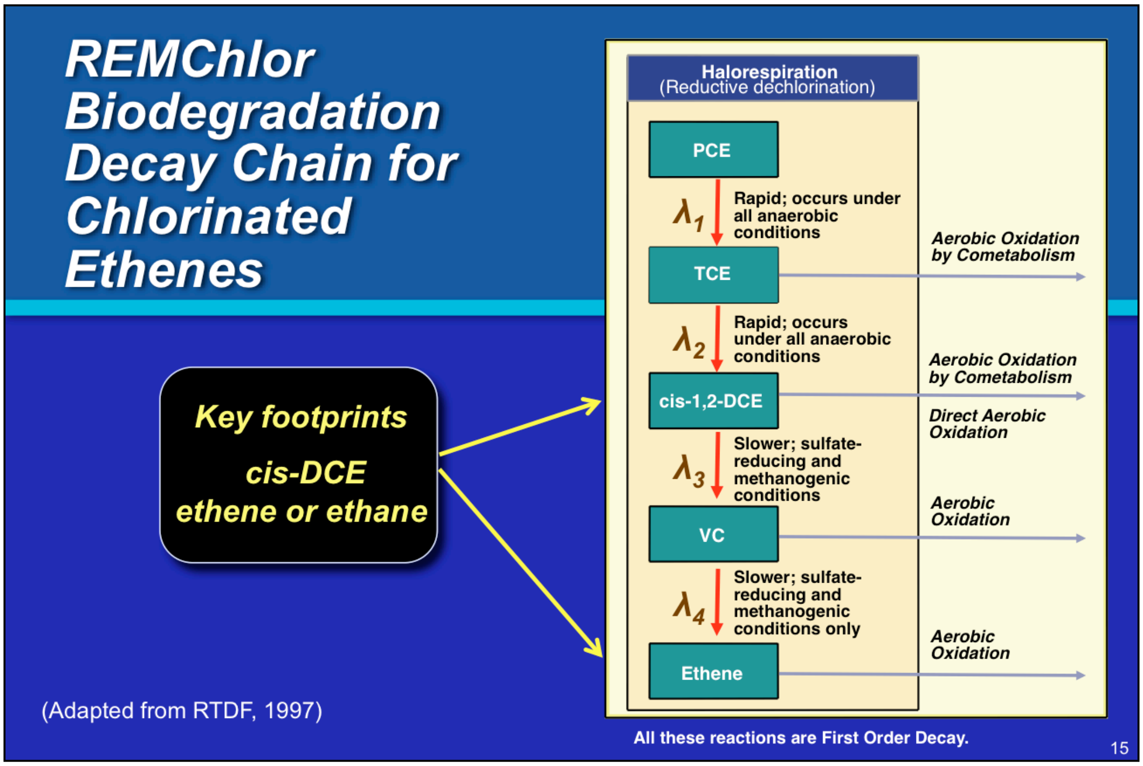
REMChlor Biodegradation Decay Chain for Chlorinated Ethenes
Key footprints
cis-DCE
ethene or ethane
Halorespiration
(Reductive dechlorination)
PCE
λ1
Rapid; occurs under all anaerobic conditions
TCE
Aerobic Oxidation by Cometabolism
λ2
Rapid; occurs under all anaerobic conditions
cis-1,2-DCE
Aerobic Oxidation by Cometabolism
Direct Aerobic Oxidation
λ3
Slower; sulfate-reducing and methanogenic conditions
VC
Aerobic Oxidation
λ4
Slower; sulfate-reducing and methanogenic conditions only
Ethene
Aerobic Oxidation
(Adapted from RTDF, 1997)
All these reactions are First Order Decay.
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Example REMChlor Sequential Reactions

λ_1 λ_2 λ_3 λ_4

PCE → TCE → DCE → VC → ETH

$$Rate_{PCE} = -\lambda_1 C_{PCE}$$

$$Rate_{TCE} = \lambda_1 y_1 C_{PCE} - \lambda_2 C_{TCE}$$

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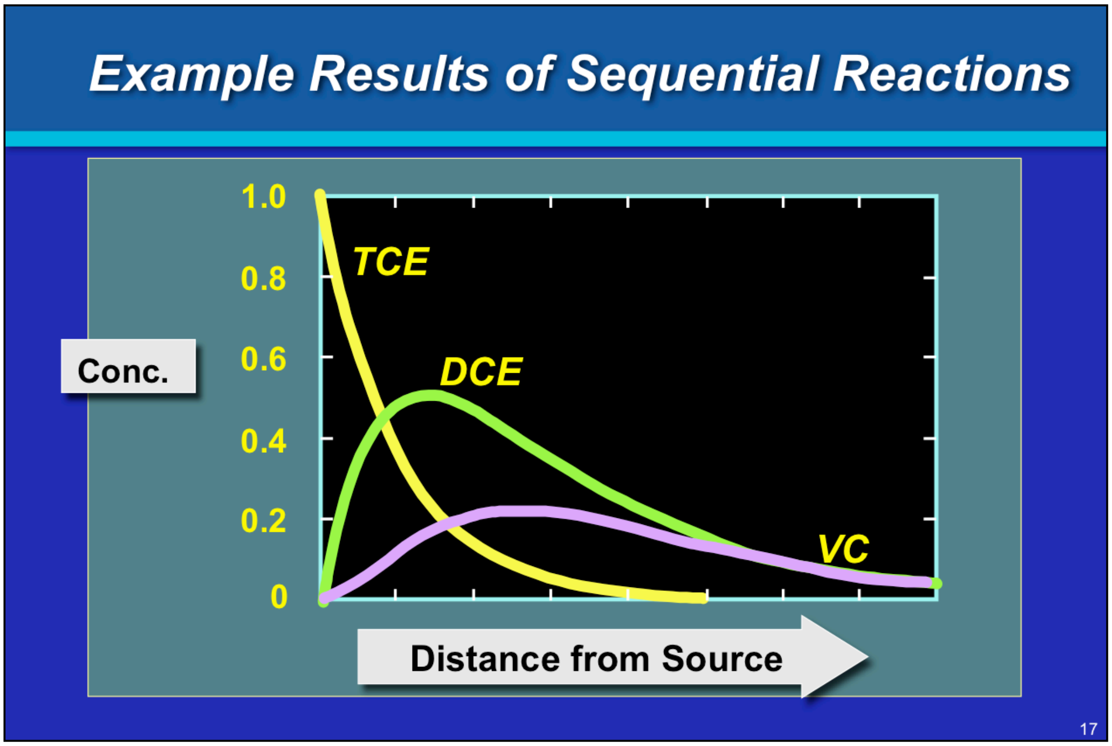
Example Results of Sequential Reactions
Conc.
1.0
0.8
0.6
0.4
0.2
0
TCE
DCE
VC
Distance from Source
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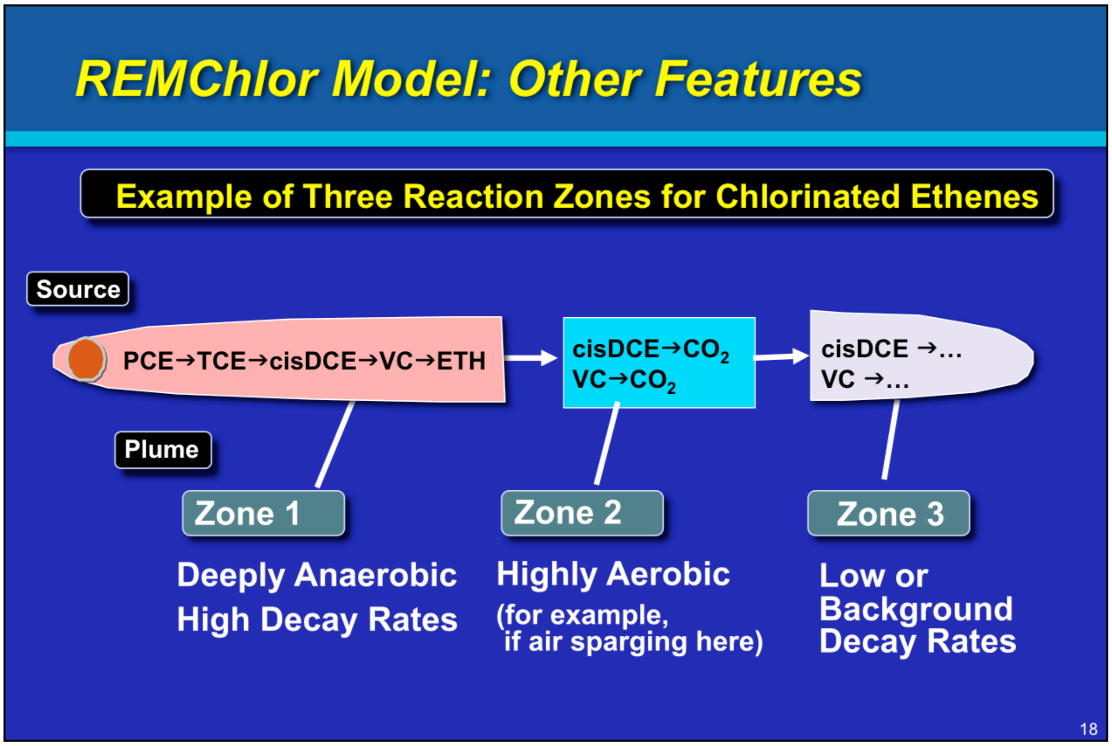
REMChlor Model: Other Features
Example of Three Reaction Zones for Chlorinated Ethenes
Source
PCE→TCE→cisDCE→VC→ETH
cisDCE→CO2
VC→CO2
cisDCE →…
VC →…
Plume
Zone 1
Zone 2
Zone 3
Deeply Anaerobic
High Decay Rates
Highly Aerobic
(for example,
if air sparging here)
Low or
Background
Decay Rates
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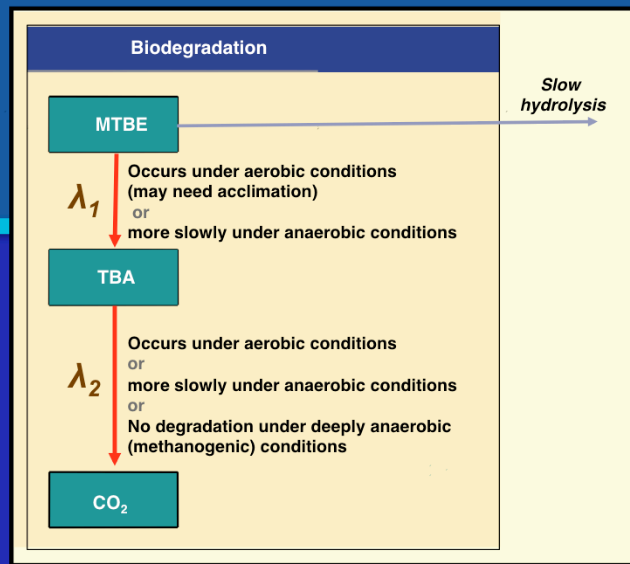
REMFuel Simplified Biodegradation Decay Chain for MTBE

Key footprint: TBA



All these reactions are First Order Decay.

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REMFuel Sequential Reactions

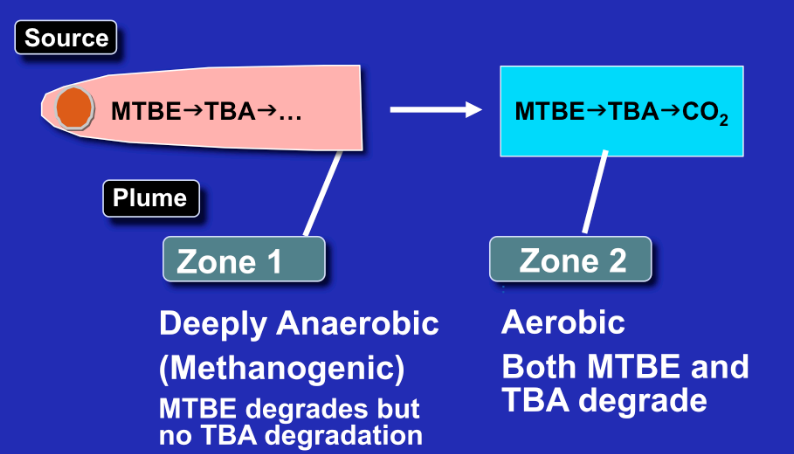
$$MTBE \xrightarrow{\lambda_1} TBA \xrightarrow{\lambda_2} CO_2$$

$$Rate_{MTBE} = -\lambda_1 C_{MTBE}$$

$$Rate_{TBA} = \lambda_1 y_1 C_{MTBE} - \lambda_2 C_{TBA}$$

REMFuel Model: Other Features

Example Using Two Reaction Zones for MTBE / TBA



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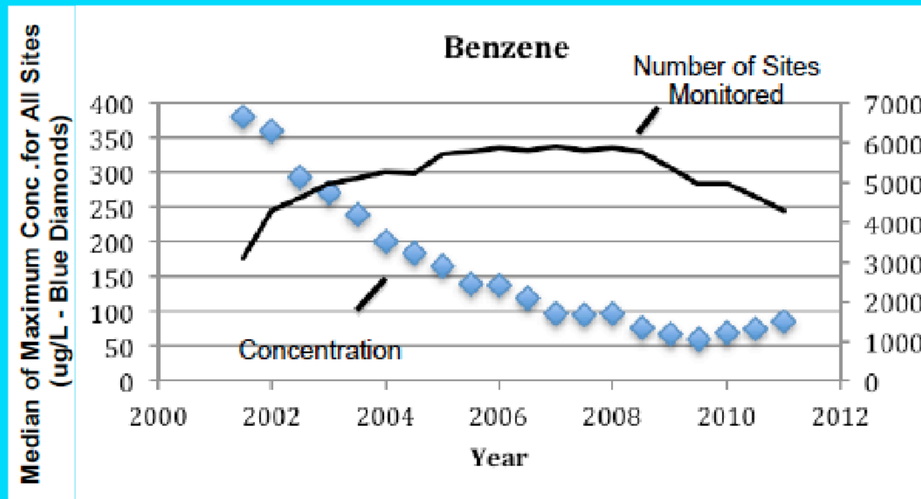
Maximum Site Concentrations Over Time California Geotracker Database (most with some type of remediation)



McHugh et al., 2012

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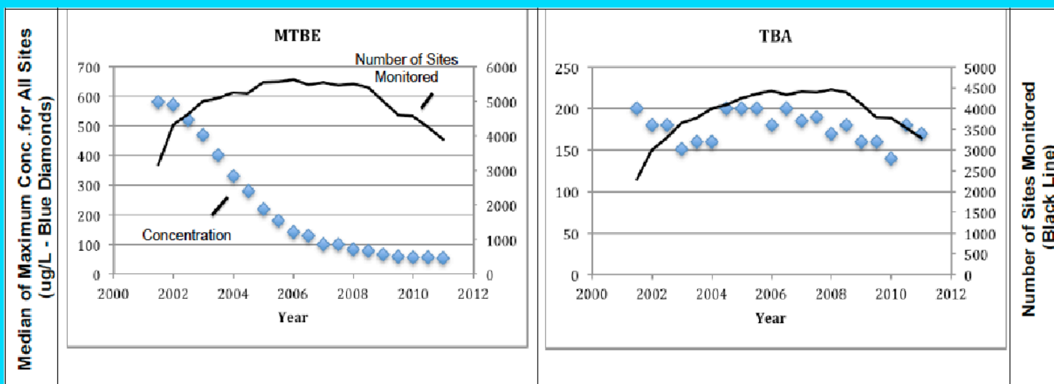
Maximum Site Concentrations Over Time California Geotracker Database (most with some type of remediation)

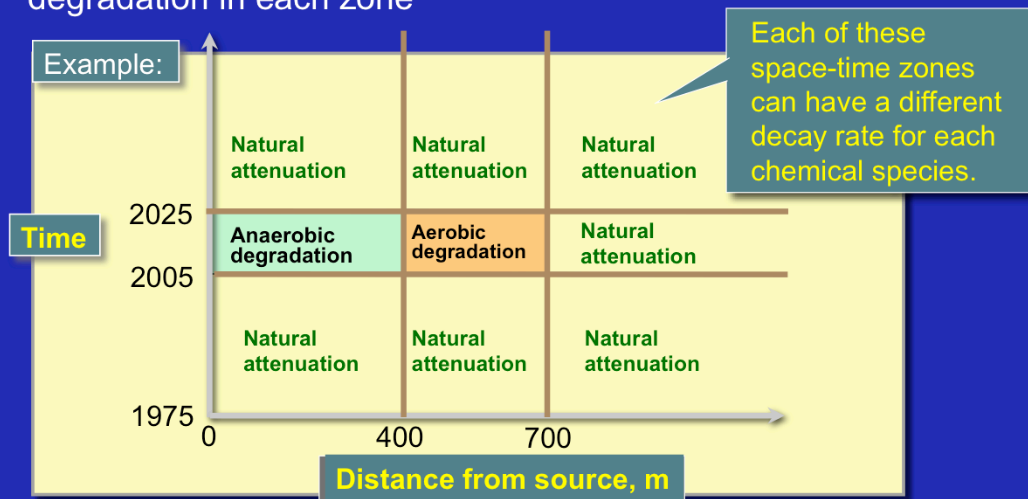


Note: Charts show median of maximum concentration for all sites vs. time for UST sites in California with any monitoring data available between 2001 and 2011.

McHugh et al., 2012

REM's Plume Remediation Model

Divide space and time into "reaction zones", solve the coupled parent-daughter reactions for chlorinated solvent degradation in each zone



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Wrap-Up: *Describing Your Plume's "Space-Time Story" With REMC and F*

1. Both models allows plume to develop for any number of years before remediation (Neat!) (Very Important).
2. You can simulate three natural reaction zones.
3. You can remediate all or part of the plume by increasing degradation rates for three specific time periods (1 year? 5 years? You pick).
4. The plume will respond to all of these factors:

natural attenuation processes

+ plume remediation

+ source decay

+ source remediation (eventually!)

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Agenda

- Class Objectives
- What Tools are Out There?
- ***What Are the Key Questions?***
  - *Will Source Remediation Meet Site Goals?*
  - *What Will Happen if No Action is Taken?*
  - *Should I Combine Source and Plume Remediation?*
  - *What is the Remediation Time-Frame?*
  - *What is a Reasonable Remediation Objective?*

Note: Many of these questions are interrelated!

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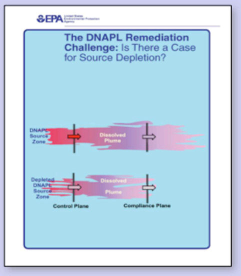
Will Source Remediation Meet Site Goals?
What are the Goals? Two Examples

U.S. EPA DNAPL Challenge (2003)

- Reduce potential for DNAPL migration
- Reduce long-term management requirements
- Enhance natural attenuation
- Reduce loading to receptor
- Attain MCLs
- “Stewardship”



ITRC LNAPL Guidance (2009)

- Reduce LNAPL to residual saturation range
- Terminate/reduce potential LNAPL body migration
- Abate/reduce unacceptable soil vapor and/or dissolved phase concentrations from LNAPL
- Aesthetic LNAPL concern Abated (saturation or (composition)

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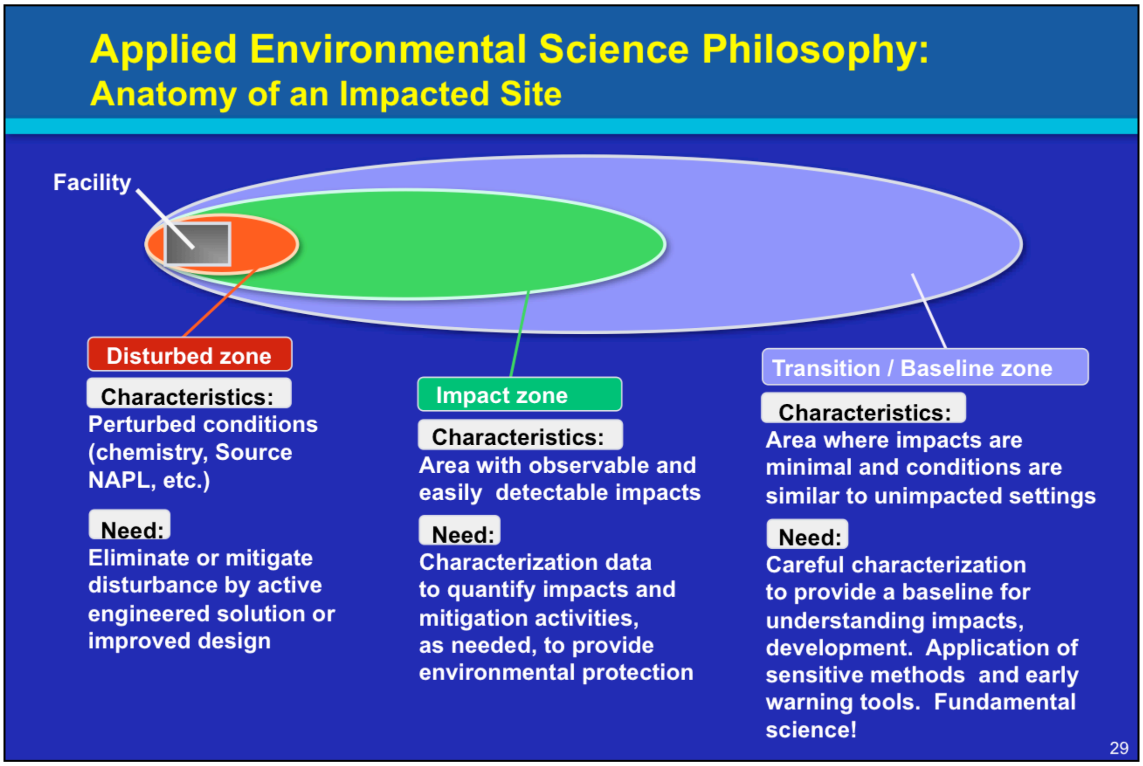
Will Source Remediation Meet Site Goals?

General Characteristics of Sites

Where is the bulk of the contaminant mass?	What is the nature of the plume over time? (assume that plume is relatively large)	How much concentration reduction is needed (maximum /desired)
SOURCE-DOMINATED Mostly in the NAPL source zone	Growing	Factor of ten
MIXED SOURCE/PLUME Partly in the source zone and partly in the dissolved plume	Stable	Factor of five hundred
PLUME-DOMINATED Mostly in the dissolved plume	Shrinking	Factor of ten thousand


Applied Environmental Science Philosophy:
Anatomy of an Impacted Site
Facility
Disturbed zone
Characteristics:
Perturbed conditions (chemistry, Source NAPL, etc.)
Need:
Eliminate or mitigate disturbance by active engineered solution or improved design
Impact zone
Characteristics:
Area with observable and easily detectable impacts
Need:
Characterization data to quantify impacts and mitigation activities, as needed, to provide environmental protection
Transition / Baseline zone
Characteristics:
Area where impacts are minimal and conditions are similar to unimpacted settings
Need:
Careful characterization to provide a baseline for understanding impacts, development. Application of sensitive methods and early warning tools. Fundamental science!
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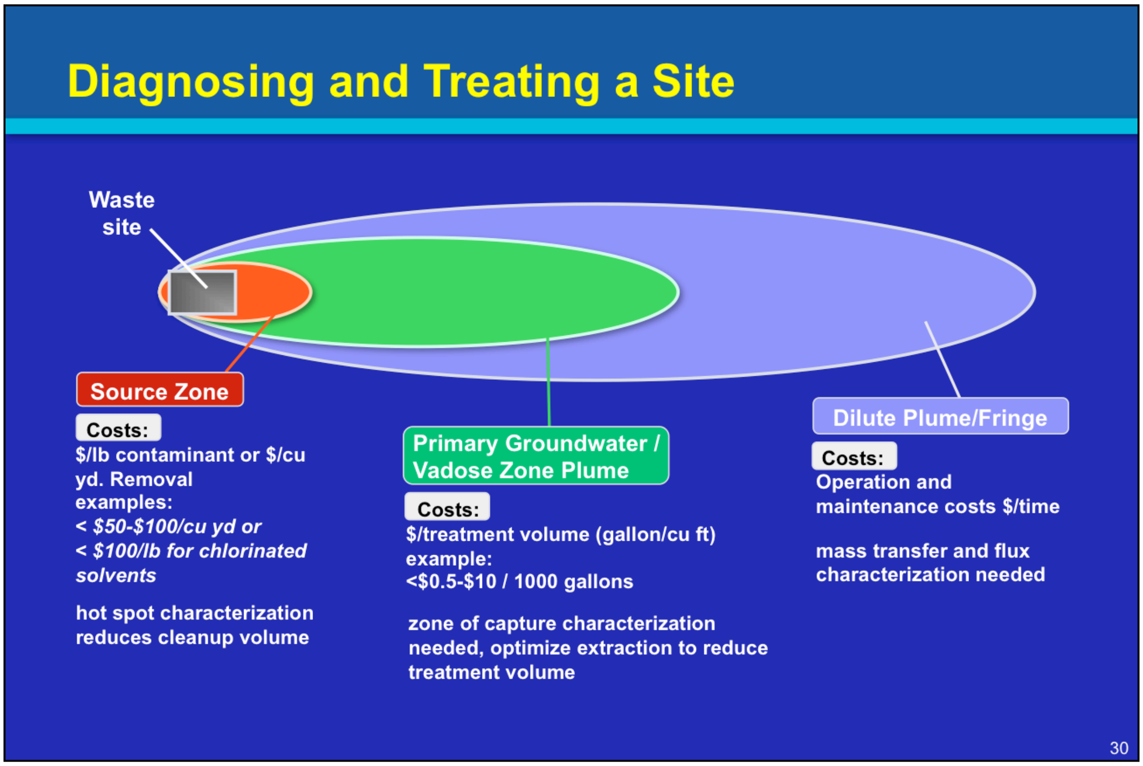
Diagnosing and Treating a Site
Waste site
Source Zone
Costs:
$/lb contaminant or $/cu yd. Removal examples:
< $50-$100/cu yd or
< $100/lb for chlorinated solvents
hot spot characterization reduces cleanup volume
Primary Groundwater / Vadose Zone Plume
Costs:
$/treatment volume (gallon/cu ft) example:
<$0.5-$10 / 1000 gallons
zone of capture characterization needed, optimize extraction to reduce treatment volume
Dilute Plume/Fringe
Costs:
Operation and maintenance costs $/time
mass transfer and flux characterization needed
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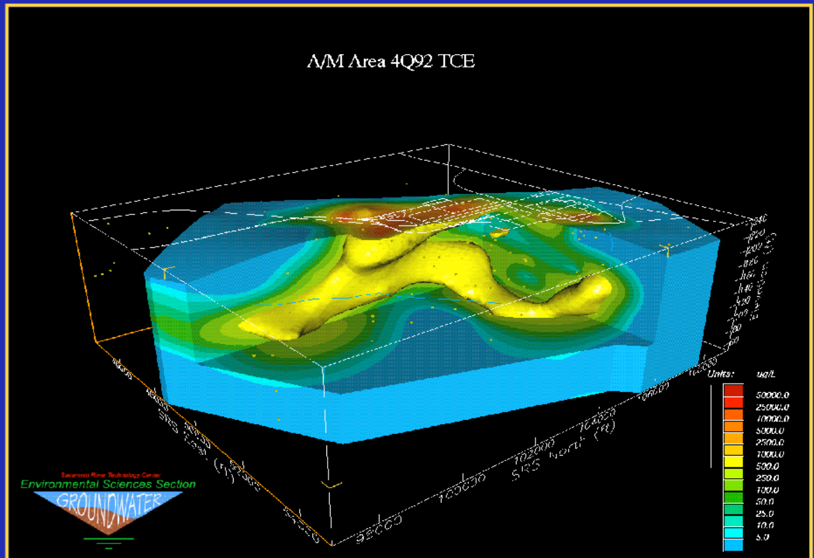
Real World Plume



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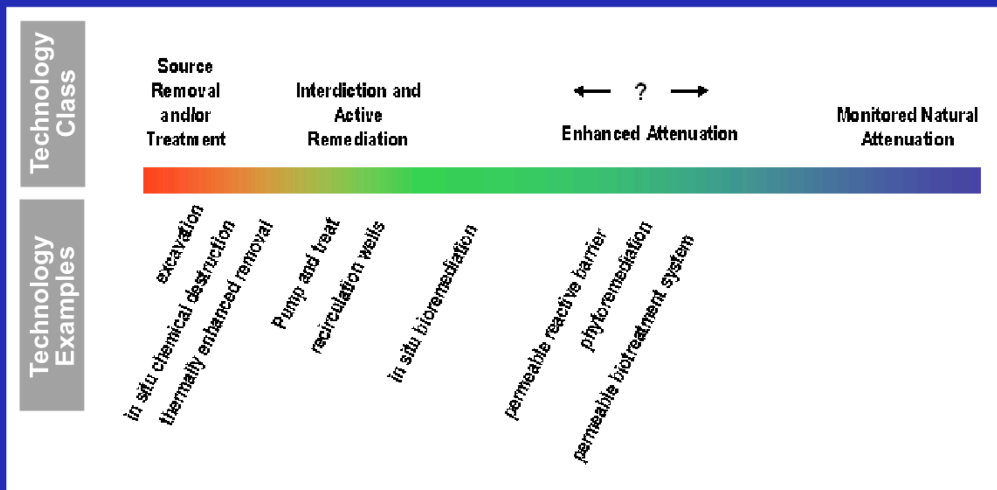
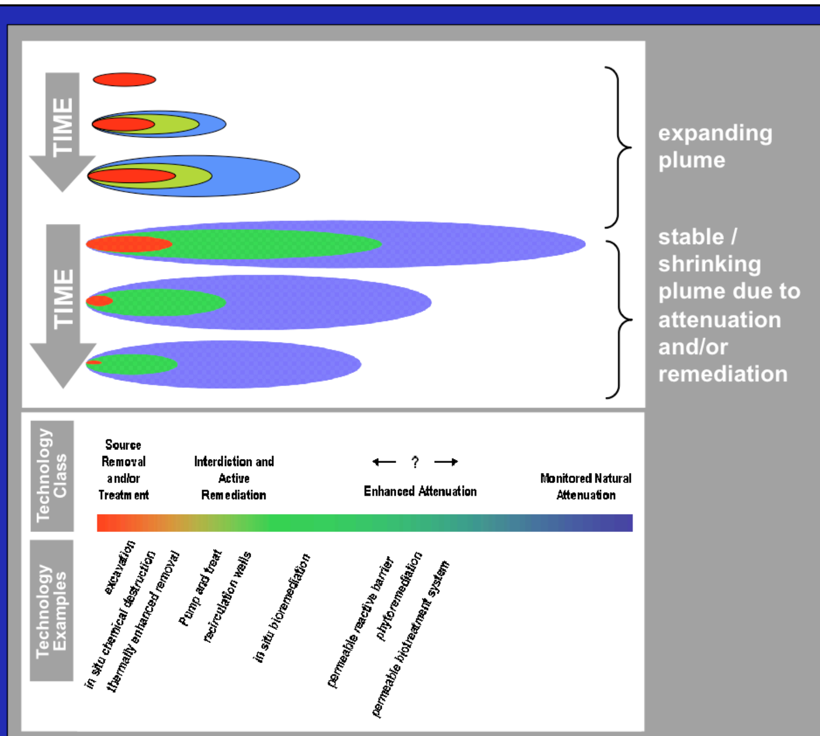
Continuum of Remediation Technologies/ Strategies/Options



a) **Simplified representations of a groundwater plume in space and time**



b) **Potential remedial technologies**

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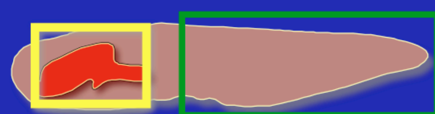
Technology Coupling

- Three types: temporal, spatial, simultaneous
- IDSS team experience most common approaches:
  - Intensive technology followed by passive
  - Different technology for Source versus Plume
  - Any technology followed by MNA
- In past, “opposing” combinations (ISCO then bio) were thought to be incompatible. This has proven to not be *always* the case.



From ITRC Integrated DNAPL Site Strategy training materials

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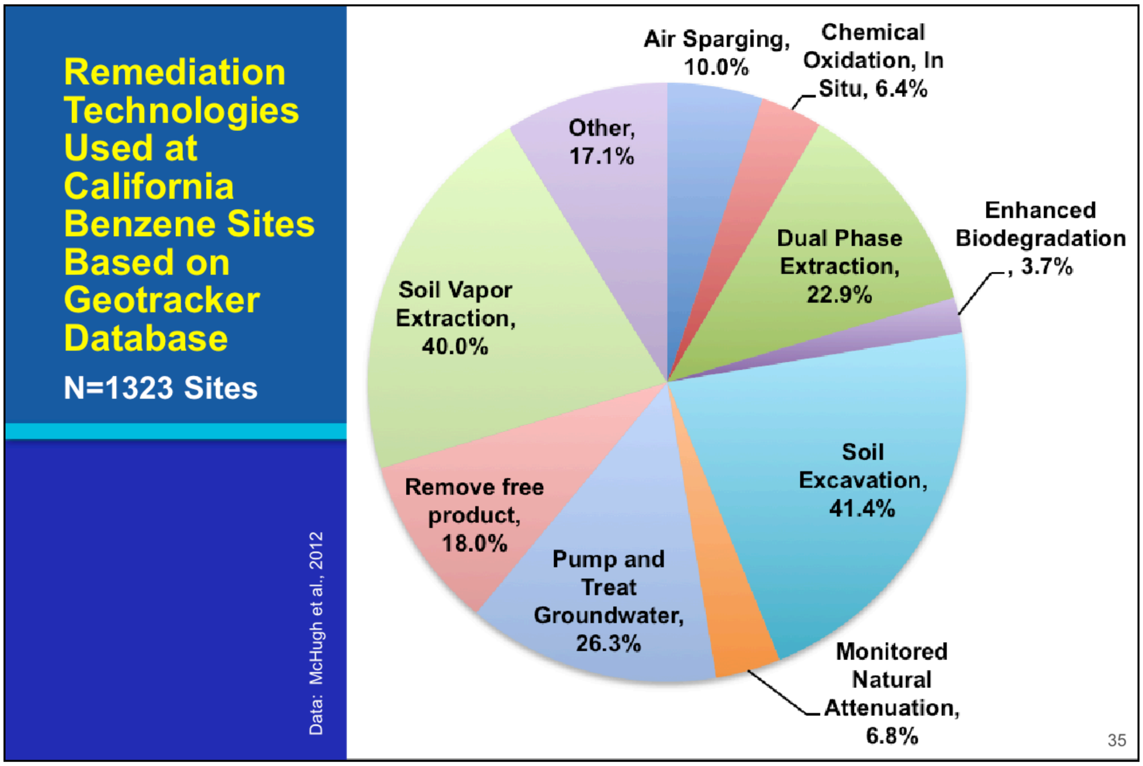
Remediation Technologies Used at California Benzene Sites Based on Geotracker Database
N=1323 Sites
Data: McHugh et al., 2012
Air Sparging, 10.0%
Chemical Oxidation, In Situ, 6.4%
Other, 17.1%
Dual Phase Extraction, 22.9%
Enhanced Biodegradation, 3.7%
Soil Vapor Extraction, 40.0%
Soil Excavation, 41.4%
Remove free product, 18.0%
Pump and Treat Groundwater, 26.3%
Monitored Natural Attenuation, 6.8%
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Multiple Site Performance Studies
(This and next 3 slides apply to chlorinated solvent sites)

Strong point about these studies …

- **Strong point about these studies…**
- **Independent researchers, careful before/after evaluation**
- **Repeatable, consistent comparison methodology**
- **Describes spectrum of sites**
- **Real data, not anecdotal**
- **Several studies described in peer reviewed papers:**

Ground Water Monitoring&Remediation

Performance of DNAPL Source Depletion Technologies at 59 Chlorinated Solvent-Impacted Sites

by Travis M. McGuire, James M. McDade, and Charles J. Newell

Multiyear Temporal Changes in Chlorinated Solvent Concentrations at 23 Monitored Natural Attenuation Sites

Charles J. Newell, P.E., M.ASCE[1]; Iain Cowie[2]; Travis M. McGuire[3]; and Walt W. McNab Jr.[4]

Abstract: Long-term (e.g., 5–15 years) groundwater concentration versus time records were compiled from 47 near-source zone monitoring wells at 23 chlorinated solvent sites (52 total records). Chlorinated volatile organic compound (CVOC) concentrations decreased significantly in most of the 52 temporal records, with a median reduction in concentration of 74%. A statistical method based on a Mann–Kendall analysis also showed that most sites had statistically significant decreasing concentration trends over time. Median point

Ground Water Monitoring&Remediation

ISCO for Groundwater Remediation: Analysis of Field Applications and Performance

by Friedrich J. Krembs, Robert L. Siegrist, Michelle L. Crimi, Reinhard F. Furrer, and Benjamin G. Petri

Ground Water Monitoring&Remediation

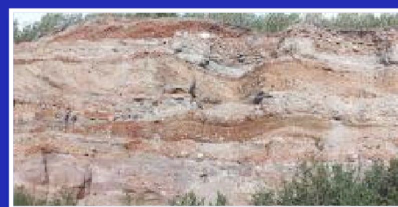
State-of-the-Practice Review of In Situ Thermal Technologies

by Jennifer L. Triplett Kingston, Paul R. Dahlen, and Paul C. Johnson

From ITRC Integrated DNAPL Site Strategy training materials

Order of Magnitude are Powers of 10
Why Use OoMs for Remediation?

- Hydraulic conductivity is based on OoMs
- VOC concentration is based on OoMs
- Remediation performance (concentration, mass, Md) can be also evaluated using OoMs ….
  - 90% Reduction: 1 OoM reduction
  - 99.9% Reduction: 3 OoM reduction
  - 70% Reduction: 0.5 OoM reduction
- Example:
  - Before concentration 50,000 ug/L
  - After concentration 5 ug/L
  - Need 4 OoMs (99.99% reduction)



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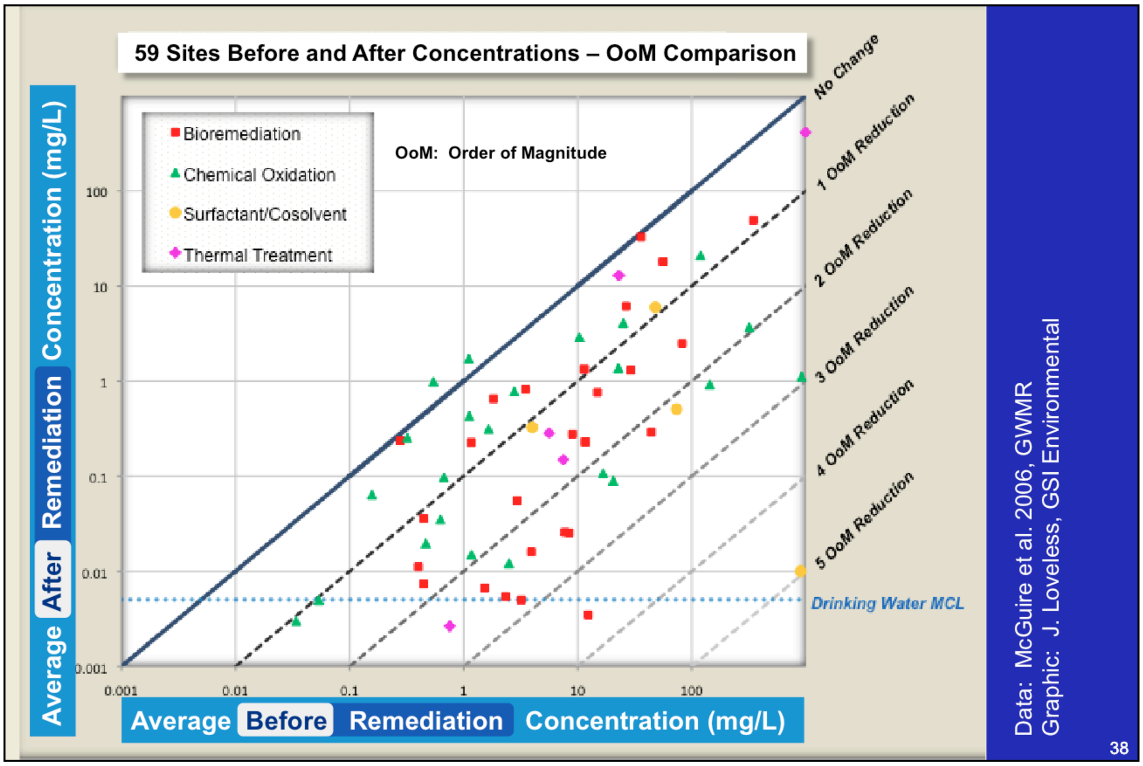
59 Sites Before and After Concentrations – OoM Comparison
Bioremediation
Chemical Oxidation
Surfactant/Cosolvent
Thermal Treatment
OoM: Order of Magnitude
No Change
1 OoM Reduction
2 OoM Reduction
3 OoM Reduction
4 OoM Reduction
5 OoM Reduction
Drinking Water MCL
Average After Remediation Concentration (mg/L)
Average Before Remediation Concentration (mg/L)
0.001
0.01
0.1
1
10
100
Data: McGuire et al. 2006, GWMR
Graphic: J. Loveless, GSI Environmental
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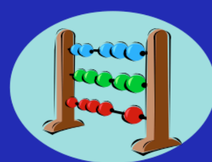
Others Say Use Caution….

- Not site specific
- Some lump pilot scale, full scale
- May not account for intentional shutdowns (i.e. they stopped when they got 90% removal)
- Don't account for different levels of design/experience
- We are a lot better now….



From ITRC Integrated DNAPL Site Strategy training materials

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BREAK FOR QUESTIONS FROM PARTICIPANTS

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How to Use REMChlor and REMFuel

1. Collect input data.
2. Determine things you don't know and make best estimate.
3. Run model and compare results to available data (such as most recent sampling event).
4. Adjust model parameters to fit data (plume length is most common calibration parameter). Typical things to adjust are parameters in Step 2 above, particularly:
   - Initial source concentration
   - Source mass
   - Biodegradation rate in plume
   - Seepage velocity
5. Run sensitivity analysis (vary several parameters and see which ones are important).

Show Me How It Works

NUMBER 1

REMChlor and the TCE Plume

♦

REMChlor Case Study: TCE Plume at a Manufacturing Plant in North Carolina

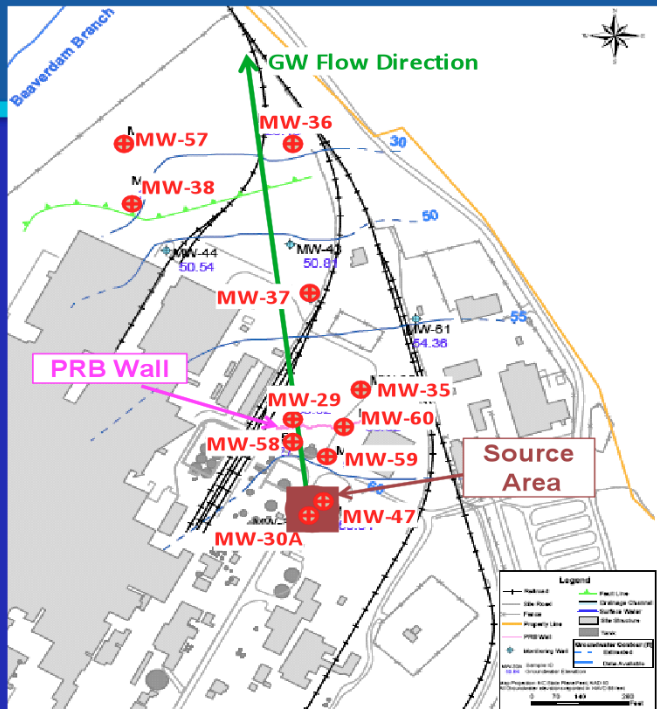
- **Plant in eastern NC, currently produces Dacron polyester resin and fibers.**
- **TCE contamination of groundwater discovered in the late 1980's; ~ stable plume about 1250 ft long (380 m).**
- **Release date unknown, but before 1980.**
- **Plume is dominated by TCE; small amounts of cis-1,2-DCE are present and VC is essentially absent.**
- **Groundwater velocity is slow, less than 100 ft/yr seepage velocity.**

from Liang et al., Ground Water Monitoring and Remediation, Winter, 2012

REMChlor Case Study: TCE Plume at a Manufacturing Plant in North Carolina

- Source zone TCE mass estimated at 300 lbs (136 kg), source zone concentrations up to ~6,000 ug/L.
- Source remediation took place in 1999, consisting of ZVI injection throughout the suspected source zone. Although source mass removal was reported as 95%, wells in the source zone have not seen large reductions in concentration.
- A 5 inch thick permeable reactive barrier (PRB) using ZVI was installed 290 ft downgradient of the source in 1999.

Will Source Remediation Meet Site Goals? Should We Combine Source and Plume Remediation?



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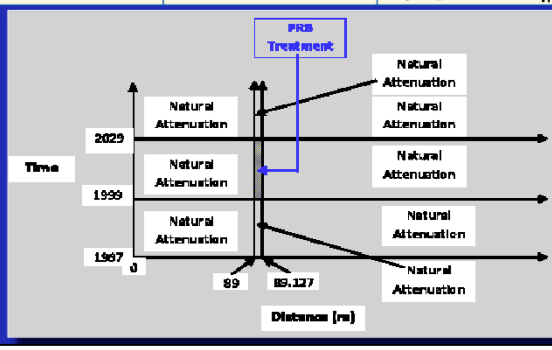
REMChlor Model Parameters for Transport/Natural Attenuation

Parameter	Value	Comment
Initial Source Conc., C_o	6,000 ug/L	Estimated from source wells
Initial Source Mass, M_o	136 kg	From site reports; assume 1967 release date
Source function exponent, Γ	1	Estimated
Source Width, W	8 m	From site reports
Source Depth, D	3.5 m	From site reports
Darcy velocity, V	8 m/yr	Calibrated; reports had estimated 1.5 to 4.6 m/yr
Porosity, φ	0.33	From site reports
Retardation Factor, R	2	Estimated
Longitudinal dispersivity, α_l	x/20	Calibrated
Transverse dispersivity, α_t	x/50	Calibrated
Vertical dispersivity, α_v	x/1000	Estimated
TCE decay rate in plume, λ	0.125 yr^{-1}	Calibrated (equal to $t_{1/2}$ of 5.5 yrs)

REMChlor Model Parameters for Source and Plume Remediation

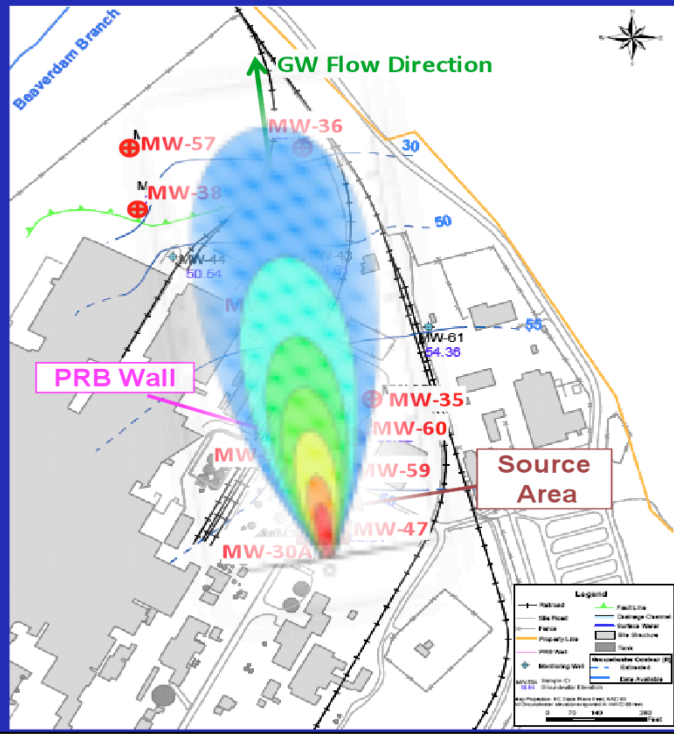
Parameter	Value	Comment
Fraction of source removed in 1999, X	95%	From site reports (but large uncertainty)
PRB wall thickness (after 1999)	0.127m (5")	From site reports
TCE decay rate in PRB	435 yr^{-1}	Estimated from well data (equal to $t_{1/2}$ of 14 hours)



Will Source Remediation Meet Site Goals? Should We Combine Source and Plume Remediation?

Simulated TCE concentrations In 1999 prior to source remediation or PRB wall installation

Contours at 5, 20, 50,100, 200, 500, and 1000 ug/L

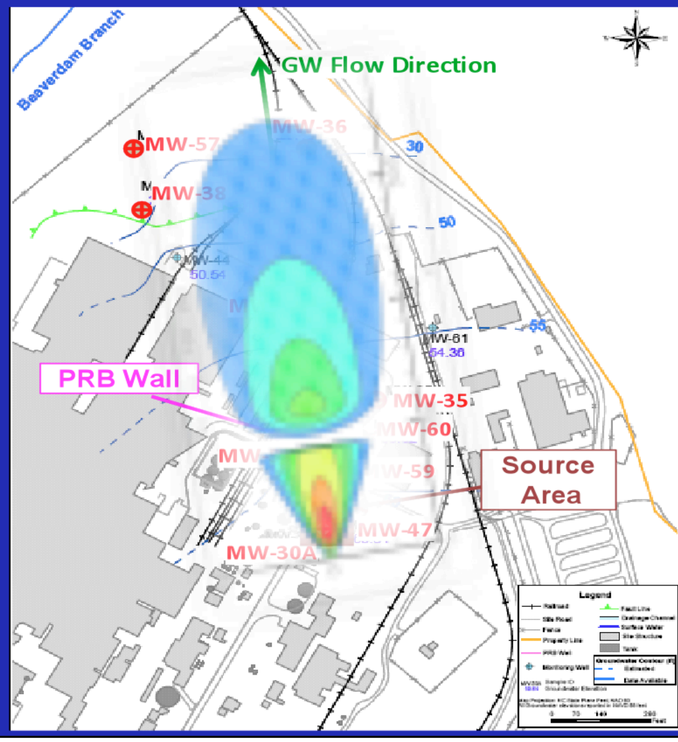


48

Will Source Remediation Meet Site Goals? Should We Combine Source and Plume Remediation?

Simulated TCE concentrations In 2001, 2 years after source remediation and PRB wall installation

Contours at 5, 20, 50,100, 200, 500, and 1000 ug/L



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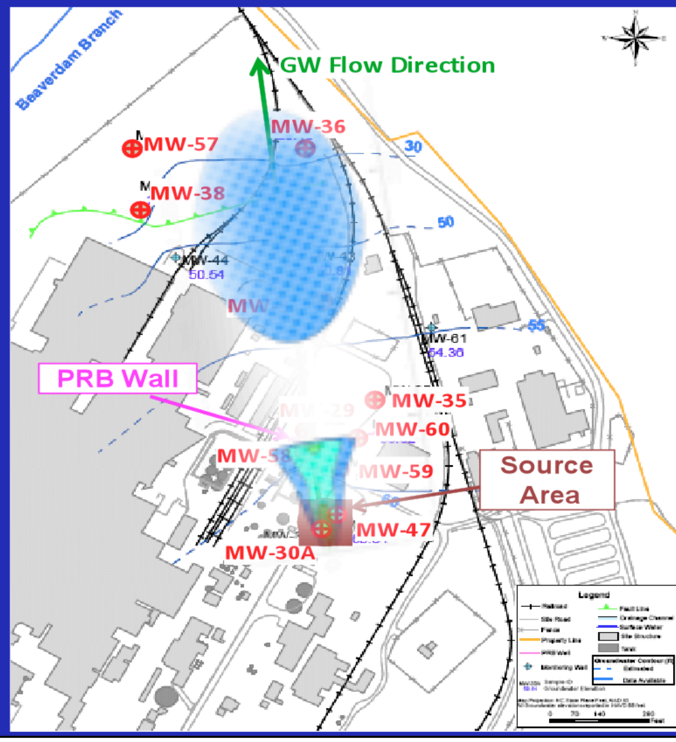
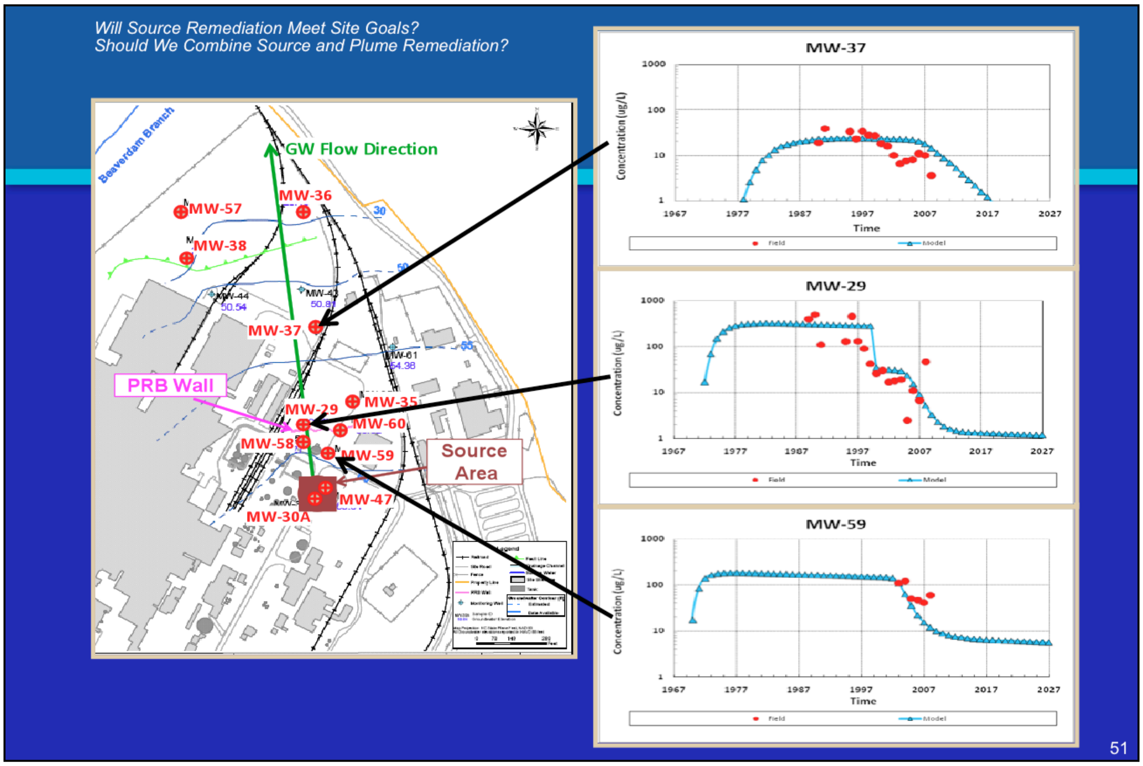
Will Source Remediation Meet Site Goals?
Should We Combine Source and
Plume Remediation?

Simulated TCE concentrations In 2009, 10 years after source remediation and PRB wall installation

Contours at 5, 20, 50,100, 200, 500, and 1000 ug/L



50


Will Source Remediation Meet Site Goals?
Should We Combine Source and Plume Remediation?
Beaverdam Branch
GW Flow Direction
MW-57
MW-36
MW-38
MW-37
PRB Wall
MW-29
MW-35
MW-60
MW-58
MW-59
Source
Area
MW-47
MW-30A
MW-37
MW-29
MW-59
Concentration (ug/L)
Time
Field
Model
51

REMChlor Key Points

1. REMChlor allows plume to develop for any number of years before remediation (Neat!) (Very Important).
2. You can simulate three natural reaction zones.
3. You can remediate all or part of the plume by increasing degradation rates for three specific time periods (1 year? 5 years? You pick).
4. The plume will respond to all of these factors:

natural attenuation processes

+ plume remediation

+ source decay

+ source remediation (eventually!)

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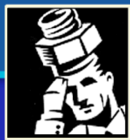
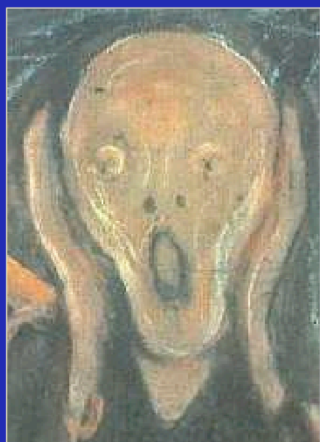


Hands-On Computer Exercise



NUMBER 1

Now You Try Using REMChlor For a Site

♦

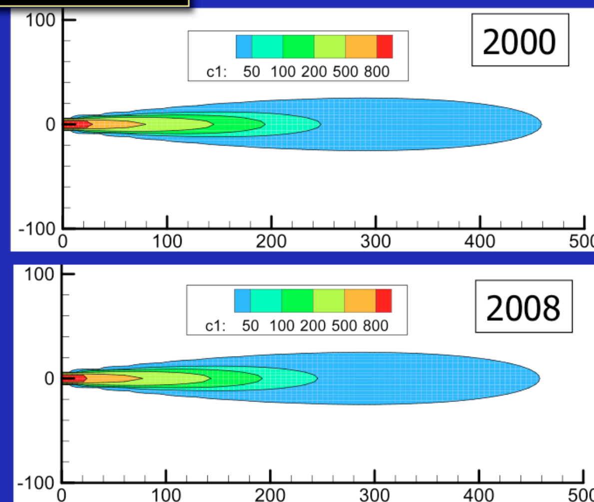
Questions answered:
What will happen if no action taken?
Will source remediation meet site goals?

Will Source Remediation Meet Site Goals?

Case #1

200 kg release of 1,2-DCA in 1980

- ***Initial source concentration is 1 mg/L***
- ***Groundwater pore velocity is 60 m/yr***
- ***1,2-DCA plume biodegradation half life is 2 years***
- ***Plume is stable, but not shrinking***



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Will Source Remediation Meet Site Goals?

Case #1

Where is the bulk of the contaminant mass?	What is the nature of the plume over time? (assume that plume is relatively large)	How much concentration reduction is needed (maximum /desired)
Mostly in the DNAPL source zone	Growing	Factor of ten
Partly in the source zone and partly in the dissolved plume	Stable	Factor of five hundred
Mostly in the dissolved plume	Shrinking	Factor of ten thousand

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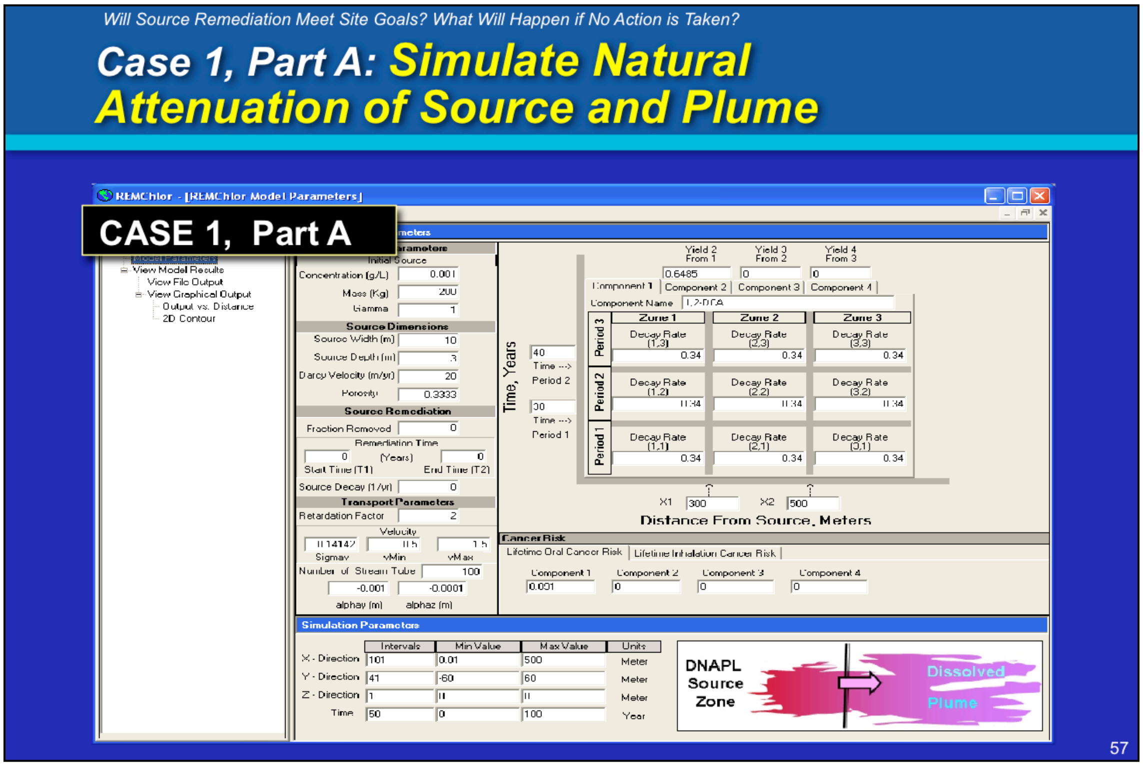
First Step in Analysis

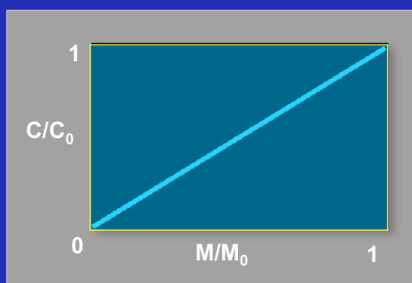
Assess what will happen if no action is taken.

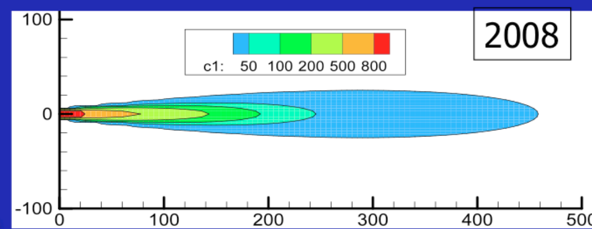
- Run REMChlor without any source or plume remediation.
- The source still depletes due to water flushing, but the depletion may be very slow.
- If the natural source depletion rate is fast, then source remediation may not be needed.

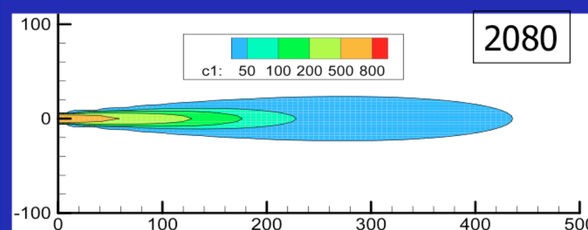

Will Source Remediation Meet Site Goals? What Will Happen if No Action is Taken?
Case 1, Part A: Simulate Natural Attenuation of Source and Plume
CASE 1, Part A
Time, Years
Distance From Source, Meters
DNAPL Source Zone
Dissolved Plume
57

Case 1, Part A: Natural Attenuation of Both Source and Plume

In 2080, plume is nearly the same size, and ~74% of the original DNAPL source mass remains.





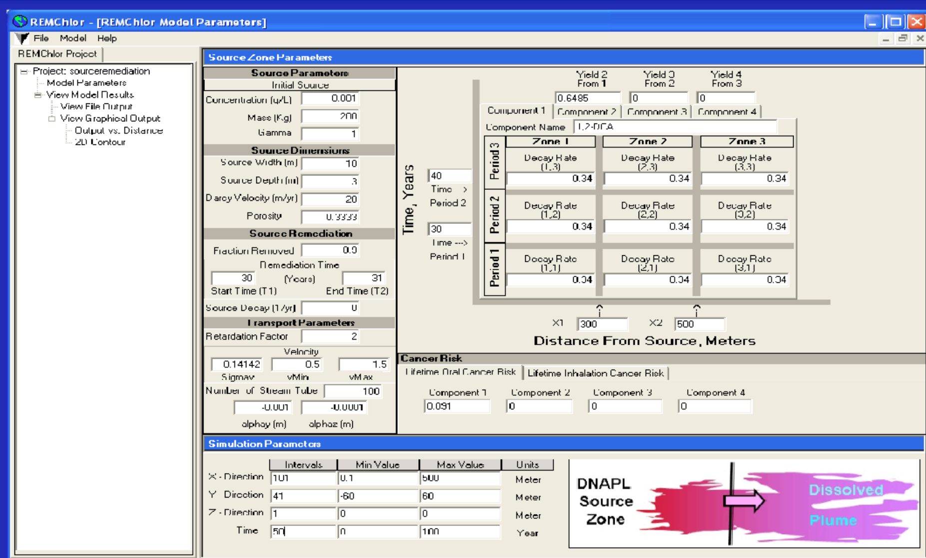


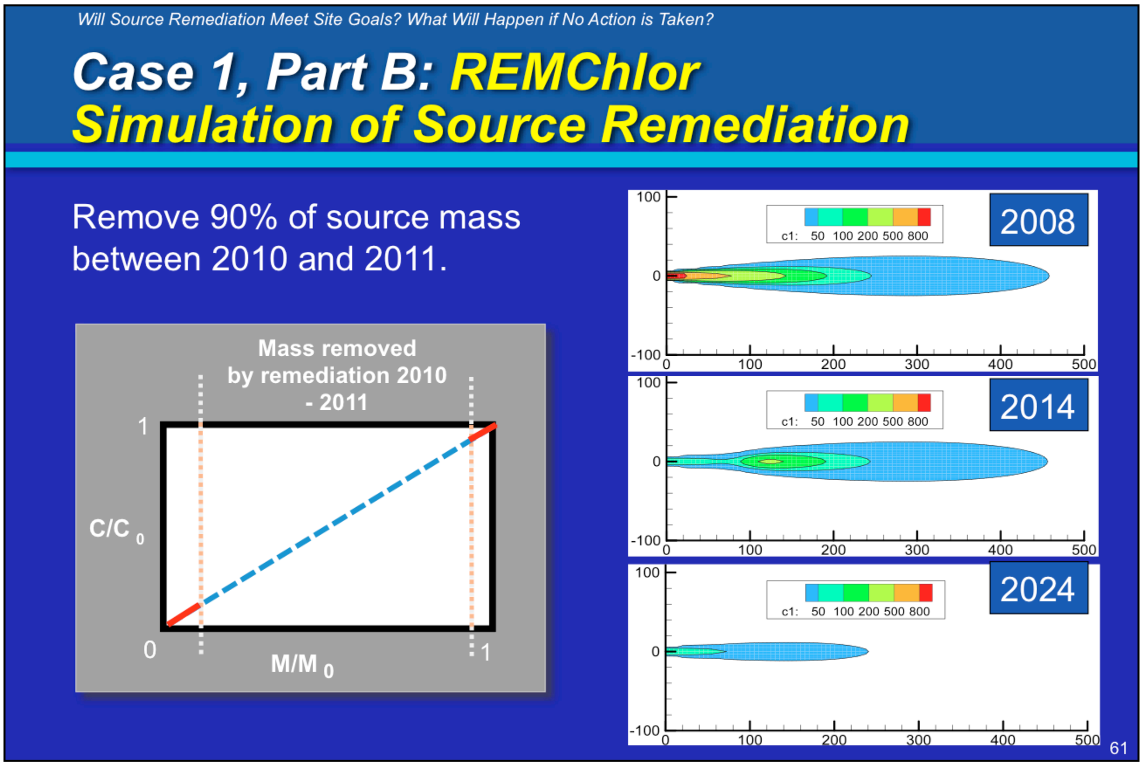
Next Step in Analysis:
Run Source Remediation

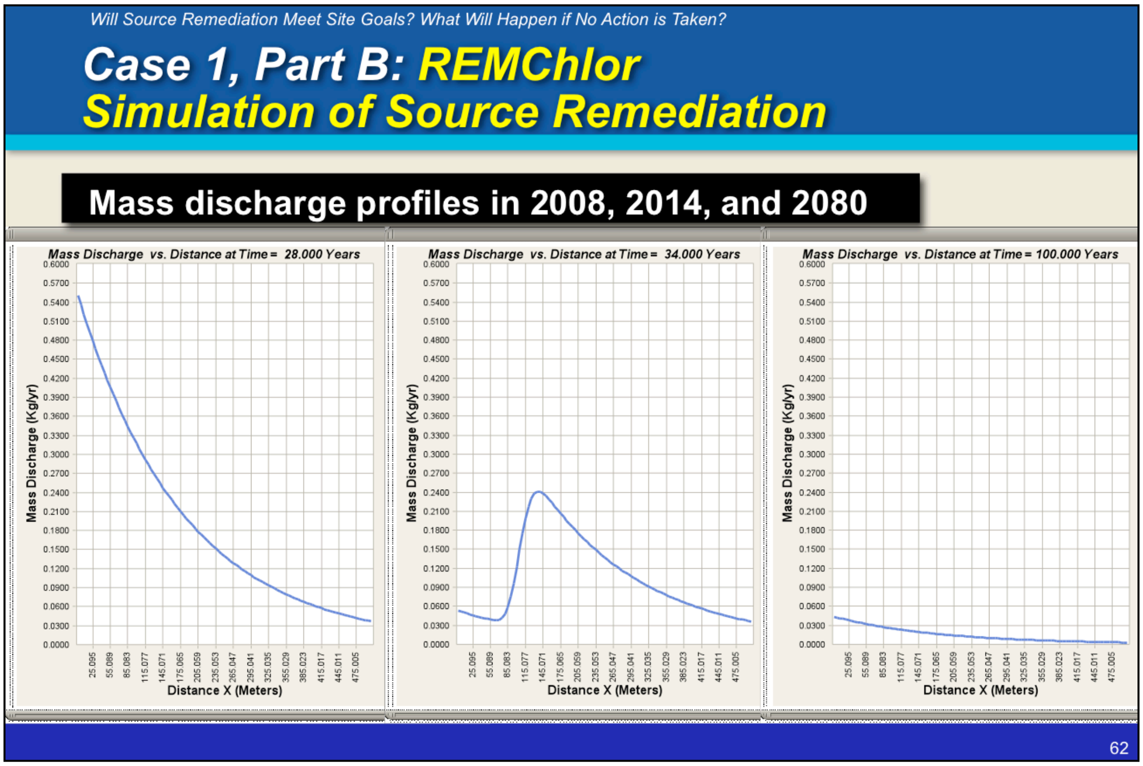
- Try source remediation.
- We have assumed that we can remove 90% of the source.
- Model source remediation between 2010 and 2011.
- Note that we could combine source and plume remediation, but in this simulation, we look at source remediation alone.

Will Source Remediation Meet Site Goals? What Will Happen if No Action is Taken?

Case 1, Part B: Source Remediation Simulation




Will Source Remediation Meet Site Goals? What Will Happen if No Action is Taken?
Case 1, Part B: REMChlor Simulation of Source Remediation
Remove 90% of source mass between 2010 and 2011.
Mass removed by remediation 2010 - 2011
C/C 0
M/M 0
2008
2014
2024
c1: 50 100 200 500 800
61


Will Source Remediation Meet Site Goals? What Will Happen if No Action is Taken?
Case 1, Part B: REMChlor
Simulation of Source Remediation
Mass discharge profiles in 2008, 2014, and 2080
Mass Discharge vs. Distance at Time = 28.000 Years
Mass Discharge vs. Distance at Time = 34.000 Years
Mass Discharge vs. Distance at Time = 100.000 Years
Mass Discharge (Kg/yr)
Distance X (Meters)
62

It Appears that Source Remediation Would Permanently Shrink this Plume

- The plume does not respond instantly to source remediation.
- The beneficial effect of source remediation "washes" downstream until the plume has readjusted to the reduced contaminant discharge.
- Source remediation often results in a detached plume.
- Unless the source treatment is perfect (100%), there will still be a plume, but it will be smaller.
- The degree of plume shrinkage depends not only on the fraction removed, but also on the amount of concentration reduction that is needed.

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BREAK FOR QUESTIONS FROM PARTICIPANTS

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- Follow CLU-IN on Facebook, LinkedIn, or Twitter

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https://twitter.com/#!/EPACleanUpTech

http://www.linkedin.com/groups/Clean-Up-Information-Network-CLUIN-4405740

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Resources & Feedback

- To view a complete list of resources for this seminar, please visit the **Additional Resources**
- Please complete the **Feedback Form** to help ensure events like this are offered in the future

Need confirmation of your participation today?

Fill out the feedback form and check box for confirmation email.

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