Welcome to the CLU-IN Internet Seminar

Practical Models to Support Remediation Strategy Decision-Making - Part 1

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

Delivered: October 11, 2012, 2:00 PM - 4:00 PM, EDT (18:00-20:00 GMT)

Instructors:

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Moderator:

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1

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2

Although I'm sure that some of you have these rules memorized from previous CLU-IN events, let's run through them quickly for our new participants.

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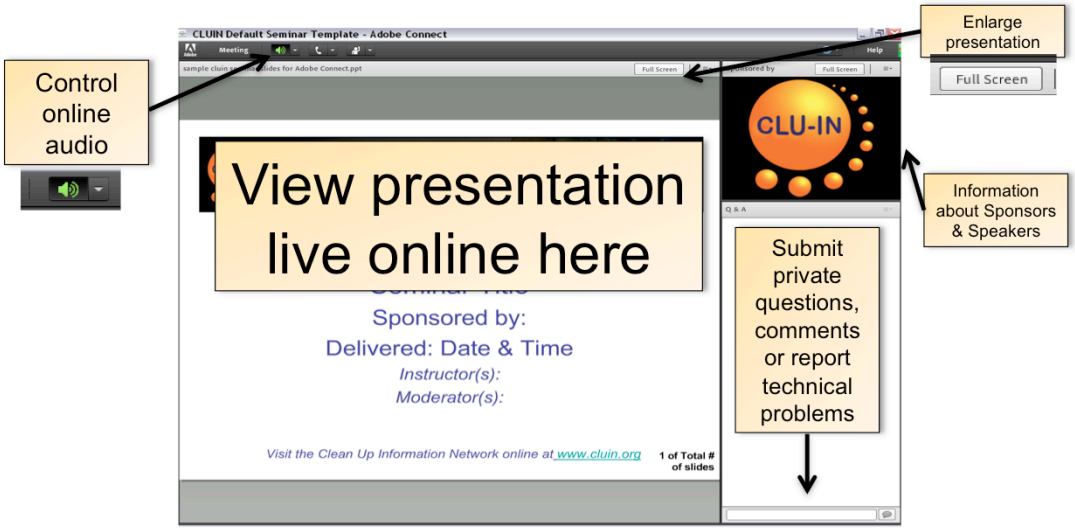
You should note that throughout the seminar, we will ask for your feedback. You do not need to wait for Q&A breaks to ask questions or provide comments. To submit comments/questions and report technical problems, please use the ? Icon at the top of your screen. You can move forward/backward in the slides by using the single arrow buttons (left moves back 1 slide, right moves advances 1 slide). The double arrowed buttons will take you to 1st and last slides respectively. You may also advance to any slide using the numbered links that appear on the left side of your screen. The button with a house icon will take you back to main seminar page which displays our agenda, speaker information, links to the slides and additional resources. Lastly, the button with a computer disc can be used to download and save today's presentation materials.

With that, please move to slide 3.

New online broadcast screenshot



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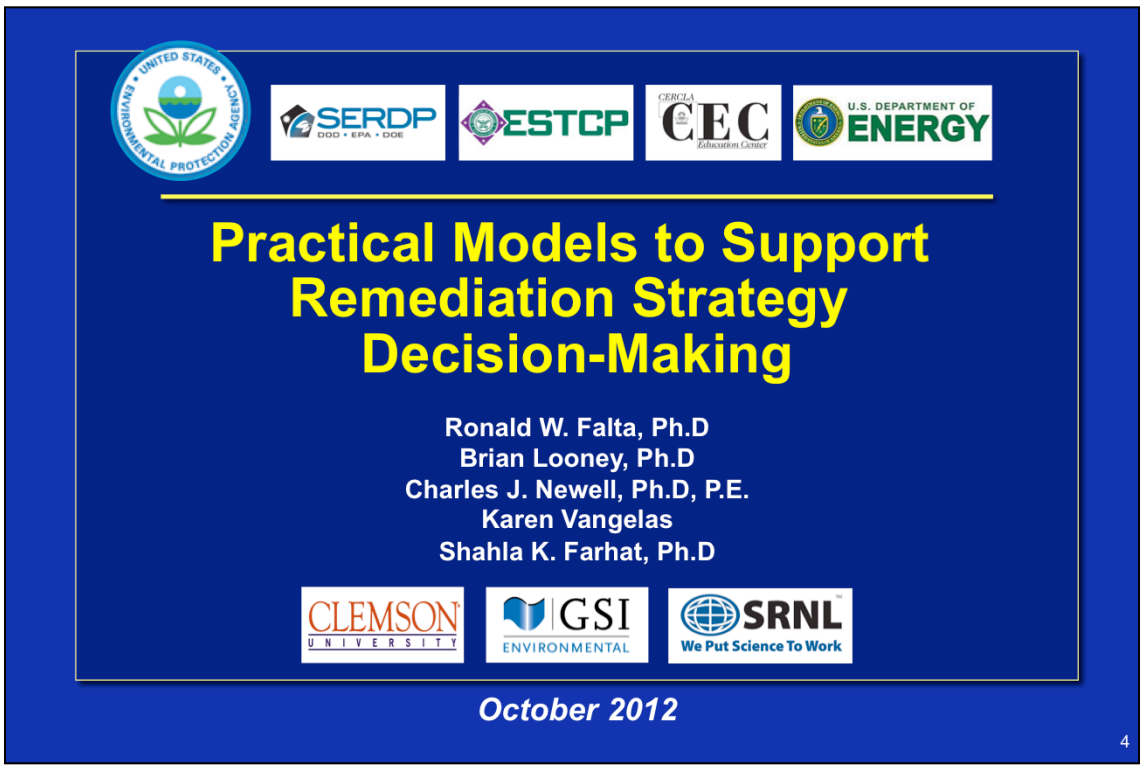
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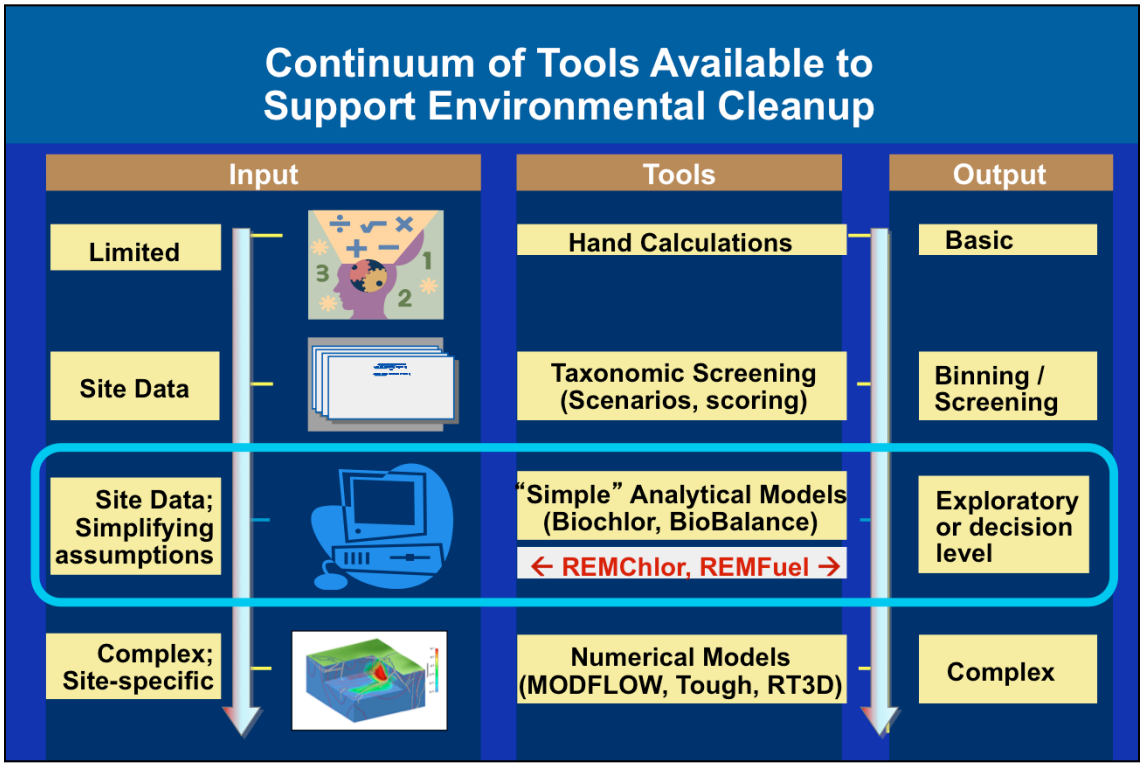
U.S. DEPARTMENT OF
ENERGY
Practical Models to Support Remediation Strategy Decision-Making
Ronald W. Falta, Ph.D
Brian Looney, Ph.D
Charles J. Newell, Ph.D, P.E.
Karen Vangelas
Shahla K. Farhat, Ph.D
CLEMSON
UNIVERSITY
GSI
ENVIRONMENTAL
SRNL
We Put Science To Work
October 2012
4

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**

5


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

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

7

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

8

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

9

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?
- **Wrap-Up**

10

Enabling Objectives

- Introduce publicly available analytical models and tools and how these tools can be used in combination to address questions/issues relevant to remediating chlorinated solvents and hydrocarbon fuel sites
- Present options for developing and diversifying metrics for success in supplementing traditional concentration-based goals

11

Enabling Objectives Cont'd

- **Encourage decision processes that match environmental technologies to site specific and time specific conditions, supporting the overarching need to transition activities until the various plume segments (e.g. source to aqueous plume, aqueous plume, and distal plume) achieve remediation goals – Combined Remedies.**
- **Explore how mass balance and mass flux approaches support plume evaluation, remedial decisions, and understanding remediation performance.**
- **Provide a glimpse on how REMChlor and REMFuel are applied to solve problems**

12

CLASS OBJECTIVES: *What Do I get from Source and Plume Remediation?*

- This is not a simple question; the answer depends on both the site conditions, as well as on the remediation goals.
- Easy to use, mathematically rigorous tools are now available to help answer this question.
- These tools are mainly based on the mass-balance approach, where the source and plume mass and mass fluxes are key variables.

13

Related Question:

Is My Groundwater Monitoring System OK?

- **Do I have the information I need to make the correct decisions?**
- Is the plume growing, shrinking, or stable?
- Is most of the contaminant mass in the source area or in the plume?
- What is the mass discharge (flux) into the plume?

14

Administrative Issues

- How and when to ask questions
- Three types of learning:
  - *Slides*
  - *Homework exercises*
  - *Demo of running the Models*

15

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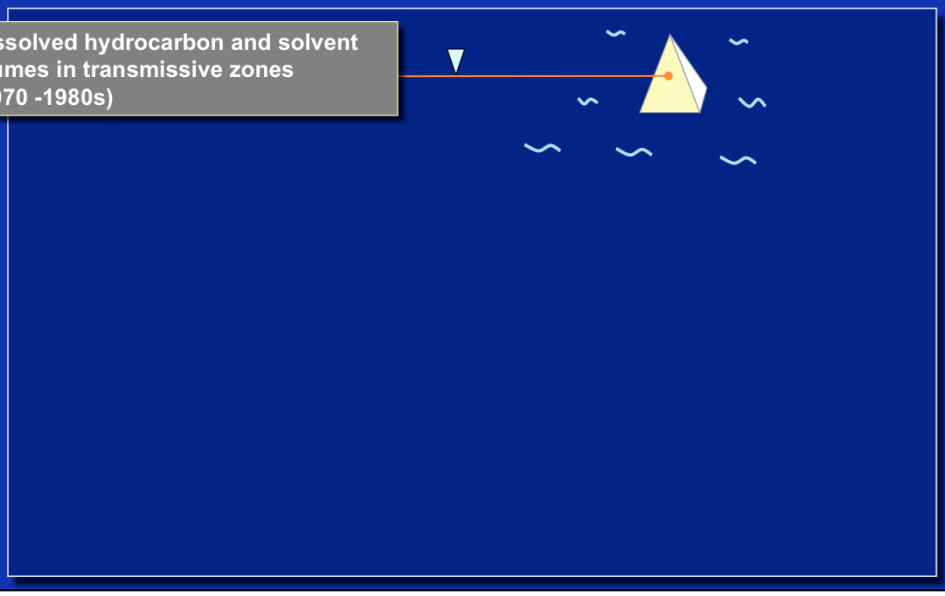
16

Emerging Picture of Groundwater Remediation Challenges

Dissolved hydrocarbon and solvent plumes in transmissive zones (1970 -1980s)



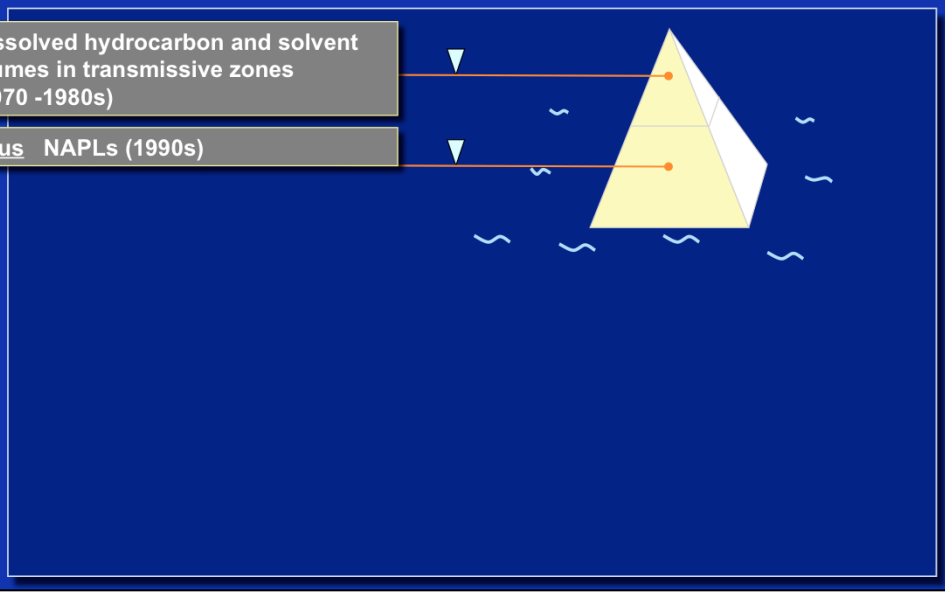
Adapted from: Chlorinated Solvent FAQs

17

Emerging Picture of Groundwater Remediation Challenges

Dissolved hydrocarbon and solvent plumes in transmissive zones (1970 -1980s)

Plus NAPLs (1990s)



Adapted from: Chlorinated Solvent FAQs

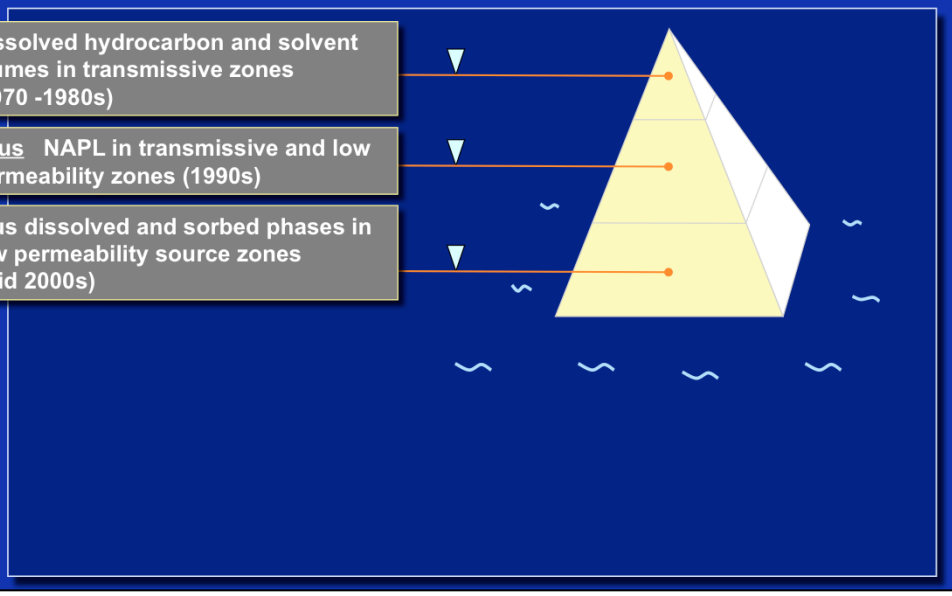
18

Emerging Picture of Groundwater Remediation Challenges

Dissolved hydrocarbon and solvent plumes in transmissive zones (1970 -1980s)

Plus NAPL in transmissive and low permeability zones (1990s)

Plus dissolved and sorbed phases in low permeability source zones (mid 2000s)



Adapted from: Chlorinated Solvent FAQs

19

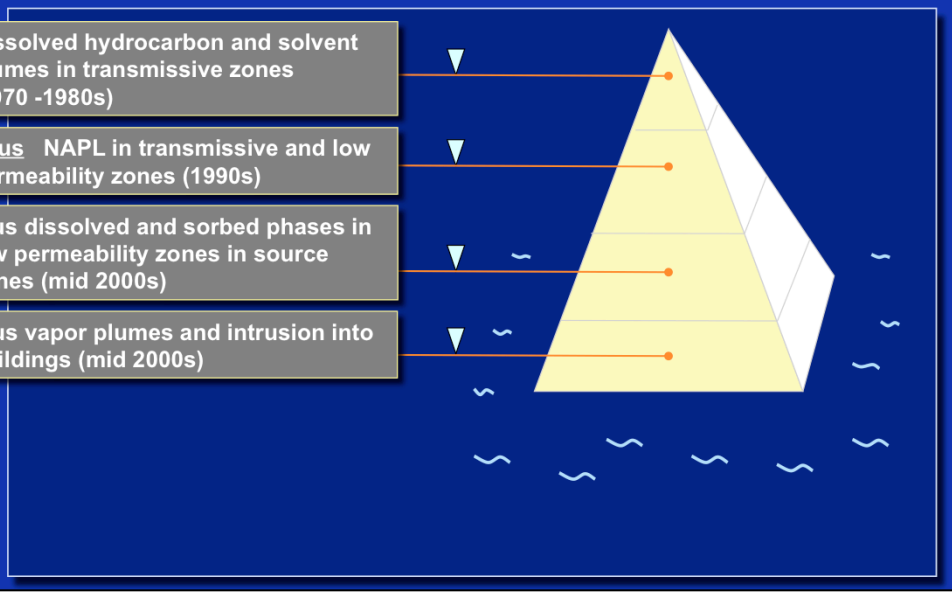
Emerging Picture of Groundwater Remediation Challenges

Dissolved hydrocarbon and solvent plumes in transmissive zones (1970 -1980s)

Plus NAPL in transmissive and low permeability zones (1990s)

Plus dissolved and sorbed phases in low permeability zones in source zones (mid 2000s)

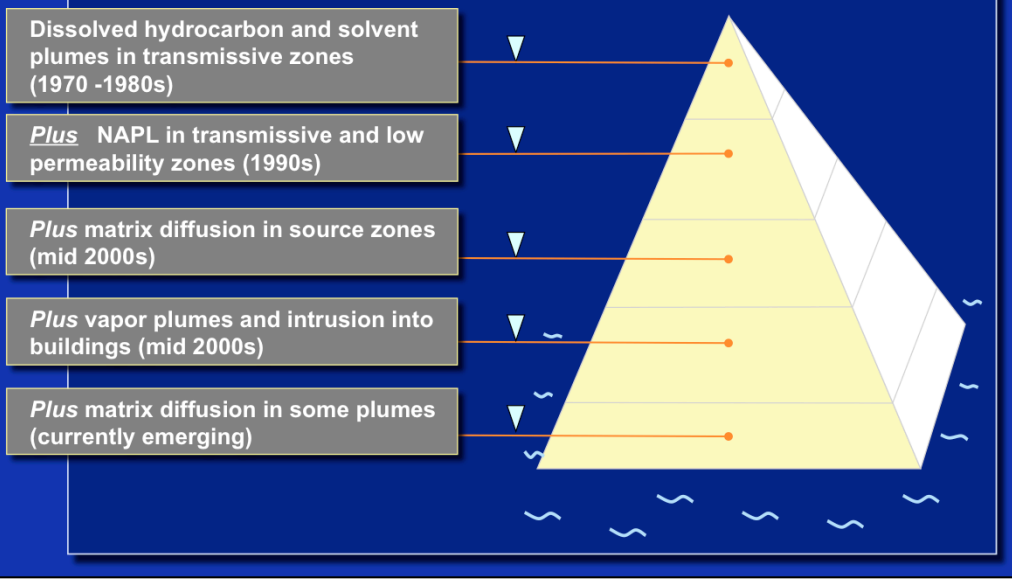
Plus vapor plumes and intrusion into buildings (mid 2000s)



Adapted from: Chlorinated Solvent FAQs

20

Emerging Picture of Groundwater Remediation Challenges



Adapted from: Chlorinated Solvent FAQs

21

Why has Remediation Been Difficult?

Some possible reasons:

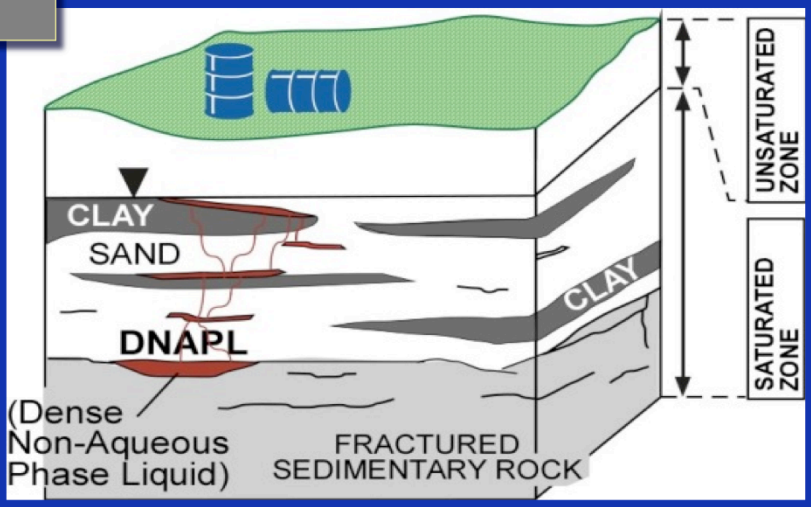
- Poor design.
- Poor understanding of what technologies do.
- Misunderstanding the extent / distribution.
- Poor recognition of the uncertainties inherent in remediation design.
- Remedial objectives that can only be achieved over long periods of time at some sites

Source: Chlorinated Solvent FAQs

22

Another Reason, Particularly for Chlorinated Solvent Sites

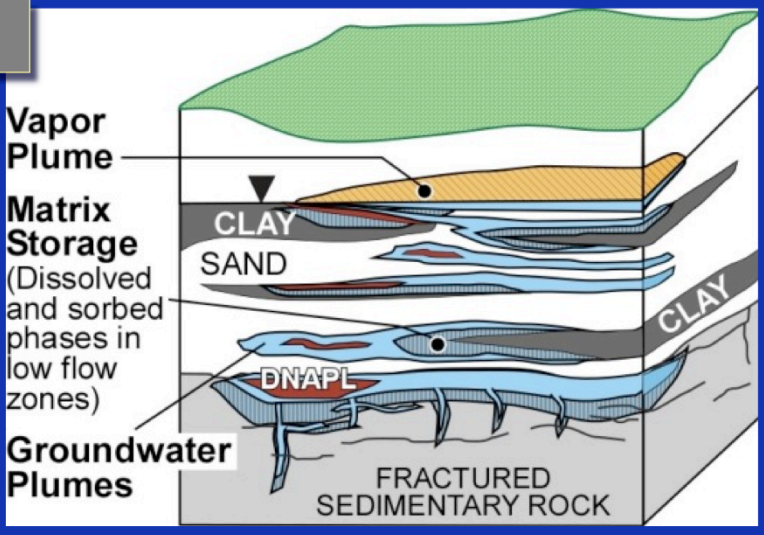
EARLY STAGE



23

Another Reason, Particularly for Chlorinated Solvent Sites

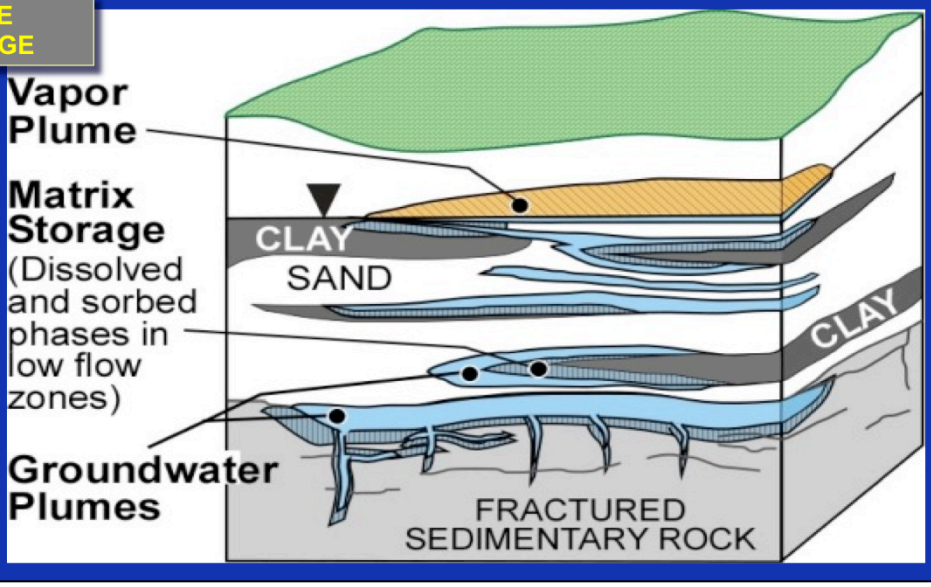
MIDDLE STAGE



Source: Chlorinated Solvent FAQs

Another Reason, Particularly for Chlorinated Solvent Sites

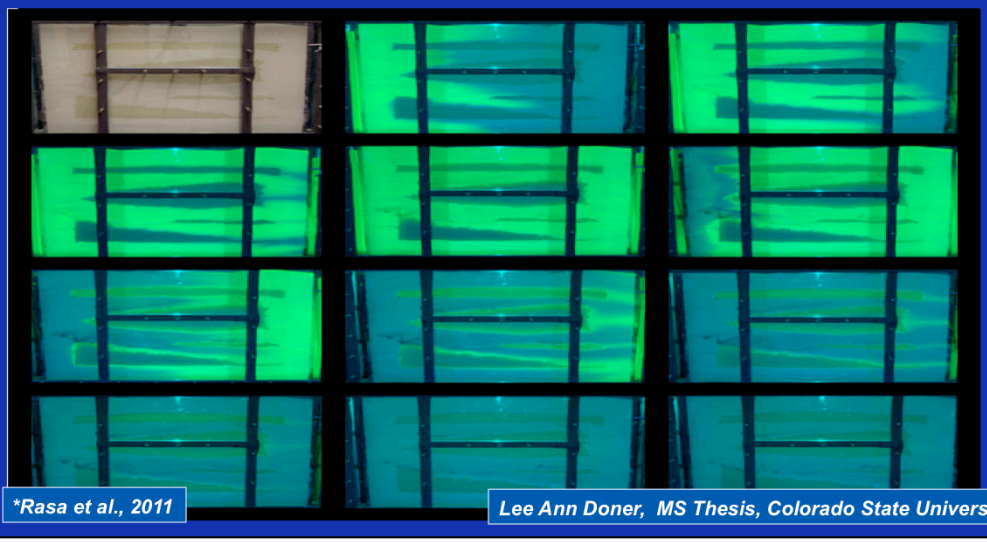
LATE STAGE



25

Quick Time Out: Matrix Diffusion

Important at certain chlorinated solvent sites.
Maybe less important for BTEX sites?
One recent paper* on matrix diffusion and MTBE



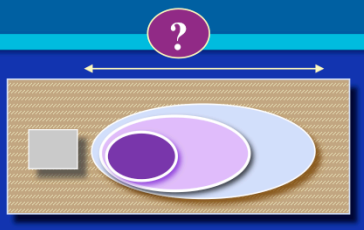
*Rasa et al., 2011

Lee Ann Doner, MS Thesis, Colorado State University

26

Colorado State Tank Study – Let's Go to the Movies!

Key Concept 1: Sources

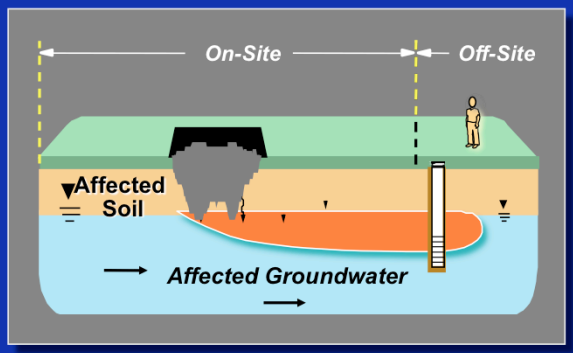


- Most dissolved plumes can be traced back to a concentrated "source area," where the original release occurred.
- The source area is usually small compared to the plume footprint.
- The source may contain NAPL, and/or it may consist of high concentrations of dissolved contaminants in low permeability zones.
- ***The mass of contaminant in the source zone, and the mass discharge of contaminant out of the source zone play a central role in the evolution of dissolved plumes.***

28

Key Concept 2: Plumes

Applies to Both Solvent and Hydrocarbon Sites



Key Driver

- Discharge from source

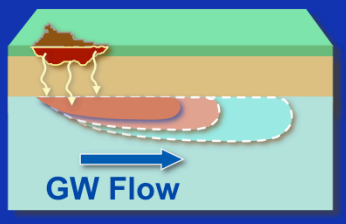
Key Processes

- Advection
- Dispersion
- Adsorption
- Degradation

29

Key Concept 2: Plumes

- Plumes are fed by the source, and move with the groundwater flow with some dispersion.
- The dissolved contaminants may also adsorb or diffuse into aquifer materials.

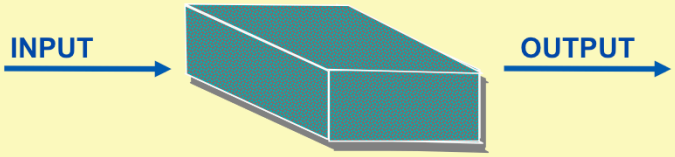


- The groundwater pore velocity (Darcy velocity divided by porosity) and the rate at which the chemical degrades play a central role the nature of the plume.
- High velocities with low decay rates = large plumes.
- Low velocities with high decay rates = small plumes.

30

Key Concept 3: Mass Balance

(Change in Accumulation)



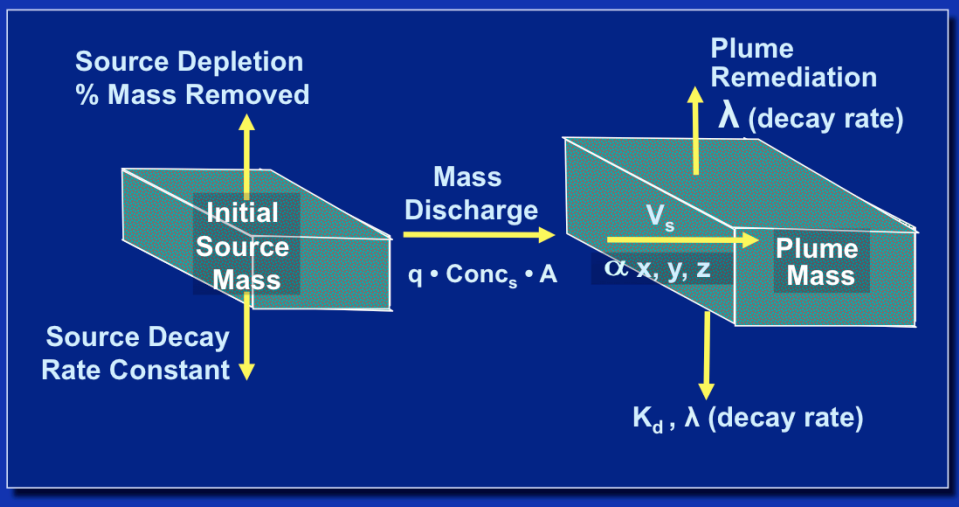
Source: D. Reible

- First expressed by Lavoisier
- Also called "material balance"
- Basic tool for modeling system behavior
- Used to determine mass flows based on inputs and outputs

31

Developing the Mass Balance

Label known flows, concentrations, and fate processes



32

Questions to be Addressed by Mass Balance Type Modeling

- What will happen if no action is taken?
- *Will source remediation meet site goals? How effective must the source remediation be?*
- Will enhanced biodegradation of the plume meet site goals? How effective (and long-lived) must the plume treatment be?
- *Should I combine source and plume remediation? How much of each do I need before I get to transition to MNA?*
- What is the remediation time-frame?
- *What is a reasonable remediation objective?*

33

Key Concept 4: Groundwater Modeling

Source

$$\frac{dM}{dt} = -Q(t)C_s(t) - \lambda_s M \qquad C_s(t) = C_0\left(\frac{M(t)}{M_0}\right)^{\Gamma}$$

Plume

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

34

BREAK FOR QUESTIONS FROM PARTICIPANTS

35

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?*

36

How Do We Get Some Answers

- We need some source and plume characterization data – the more the better.
- We need estimates of the source mass, the source discharge, the groundwater velocity, and plume decay rates.
- We need some understanding of source and plume remediation efficiency (% removal, cost, etc.).
- We can then run simple models such as REMChlor and REMFuel to test what would happen with source remediation, plume remediation, or some combination of the two.

37

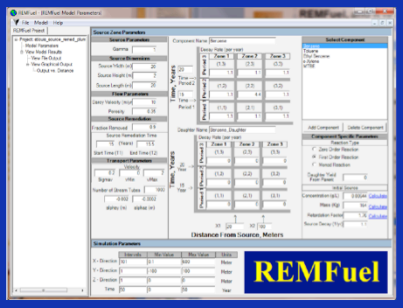
How Do We Move Forward?

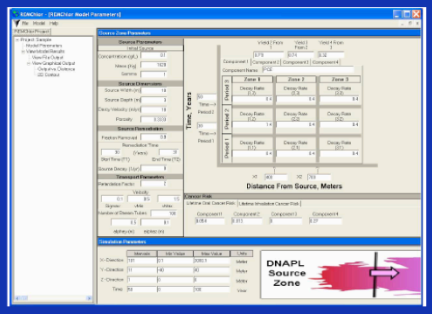
- Look at what has happened at other sites - particularly *multiple - site studies*
- Practice a flexible, feedback-based decision process *(Observational Approach)*
- Use *practical tools* to help understand the site

38

REMFuel and REMChlor

- Combine Source and Plume Models Together
- Easier to use than numerical models





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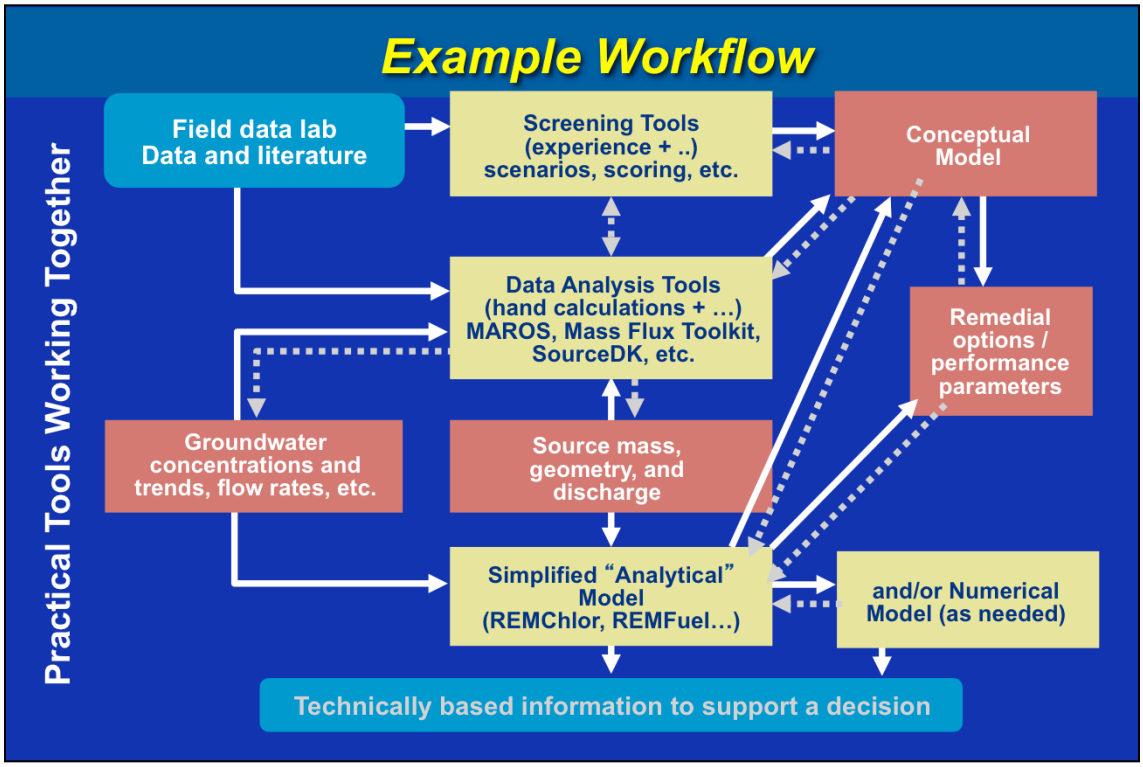
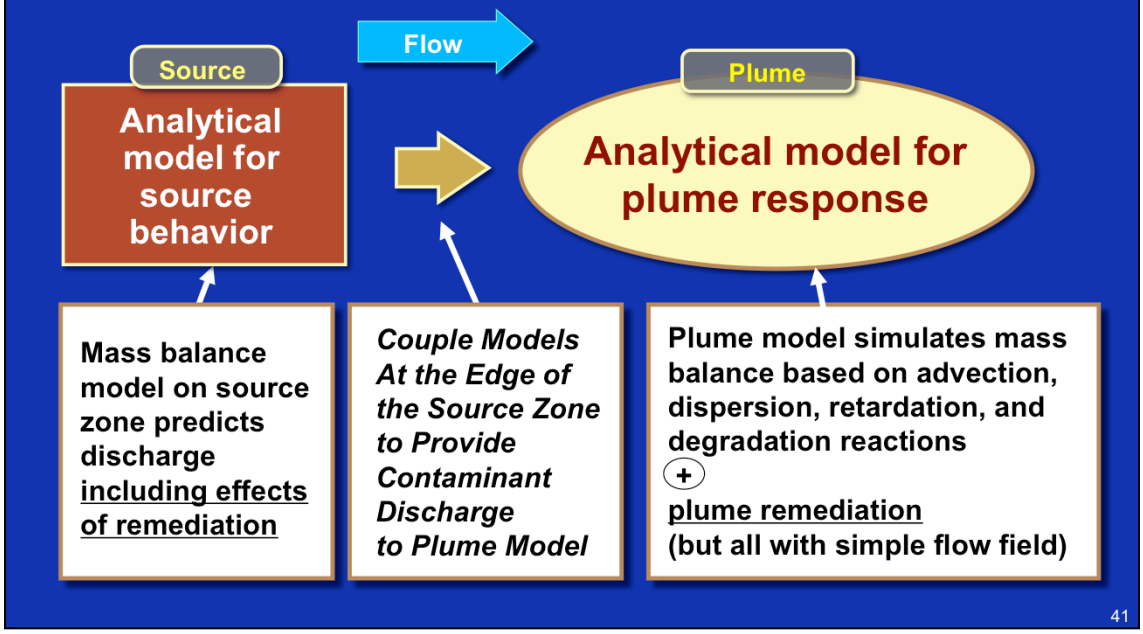

Example Workflow
Practical Tools Working Together
Field data lab
Data and literature
Screening Tools
(experience + ..)
scenarios, scoring, etc.
Conceptual
Model
Data Analysis Tools
(hand calculations + …)
MAROS, Mass Flux Toolkit,
SourceDK, etc.
Remedial
options /
performance
parameters
Groundwater
concentrations and
trends, flow rates, etc.
Source mass,
geometry, and
discharge
Simplified "Analytical"
Model
(REMChlor, REMFuel…)
and/or Numerical
Model (as needed)
Technically based information to support a decision

What Makes REM-C and REM-F So Special?



REMFuel and REMChlor

WHAT:

Analytical groundwater transport models that combines source behavior with solute transport in the plume

HOW:

1. **Enter site data.**
2. **Try to match existing site data (calibration).**
3. **Ask questions (up to you!).**
4. **Change variable and see what happens** (based on hydrogeology, biodegradation, sorption, source decay, and other key processes at the site).

42

REMFuel and REMChlor

WHERE: Free download from EPA Webpage

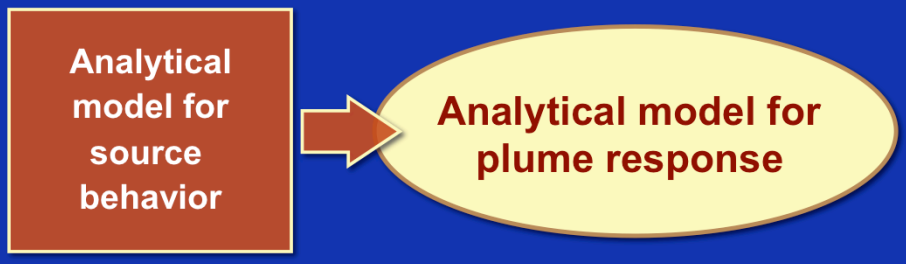
- http://www.epa.gov/nrmrl/gwerd/csmos/models/remchlor.html
- http://www.epa.gov/nrmrl/gwerd/csmos/models/remfuel.html

WHEN: Both available now

WHO: Dr. Ron Falta, Clemson University
plus
Stacy, Ahsanuzzaman, Wang, Earle, and Wilson
(EPA co-authors - R.S. Kerr Lab, Ada, OK)

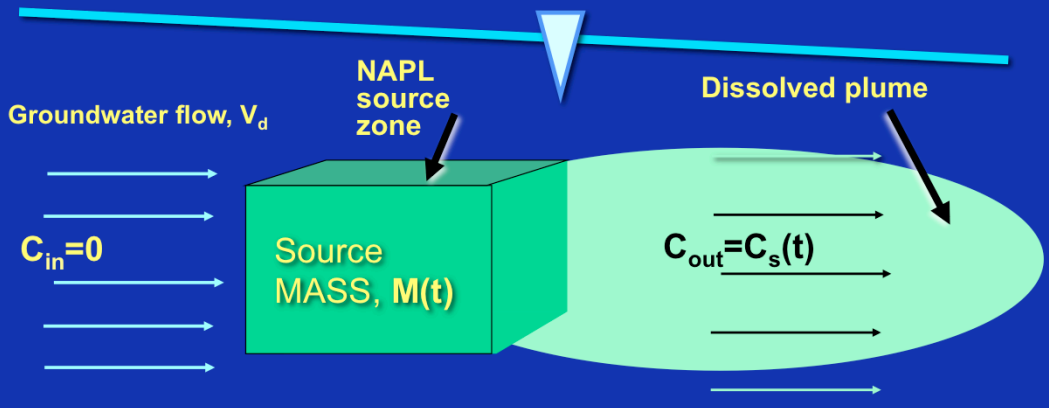
43

Explanation of How the *Source Term* Works in REMCHLOR and REMFuel



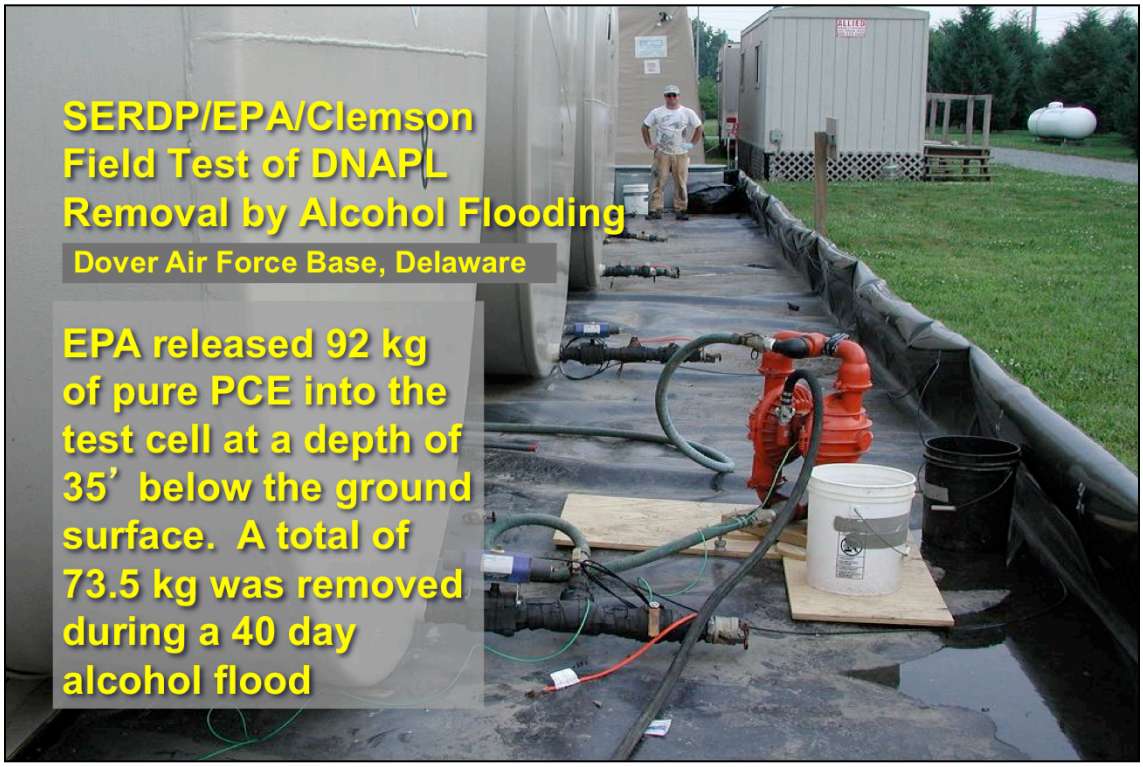
44

The Discharging Concentration (C_s) Depends on the Mass Remaining in the Source Zone, (M)

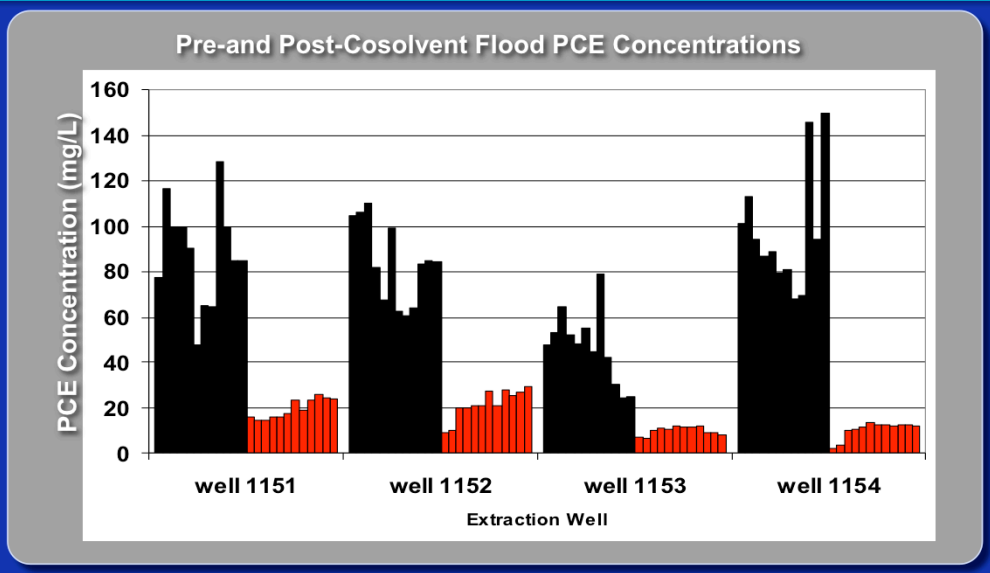


$$\frac{dM}{dt} = -Q(t)C_s(t) - \lambda_s M \qquad \frac{C_s(t)}{C_0} = \left(\frac{M(t)}{M_0}\right)^{\Gamma}$$

45


SERDP/EPA/Clemson
Field Test of DNAPL
Removal by Alcohol Flooding
Dover Air Force Base, Delaware
EPA released 92 kg
of pure PCE into the
test cell at a depth of
35’ below the ground
surface. A total of
73.5 kg was removed
during a 40 day
alcohol flood

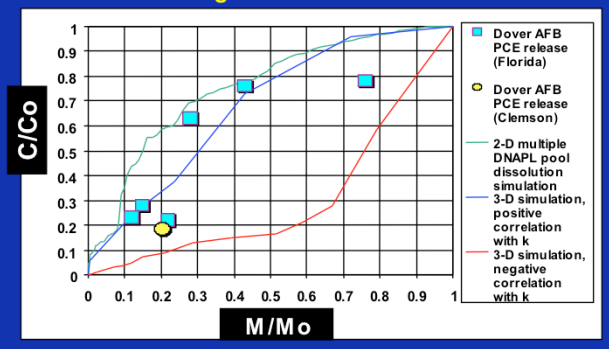
80% Source Removal Resulted in 81% Reduction in Groundwater Concentration



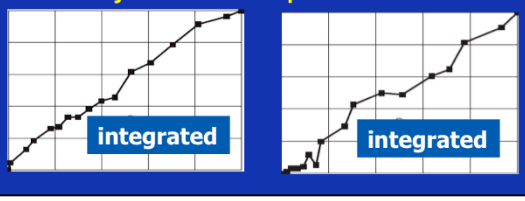
47

Source Mass Reduction Leads to Discharge Reduction

Field and Modeling Data



Laboratory dissolution experiments

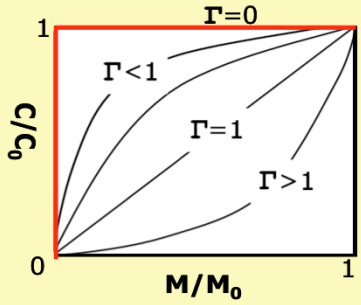


(Jawitz et al.)

Power function model

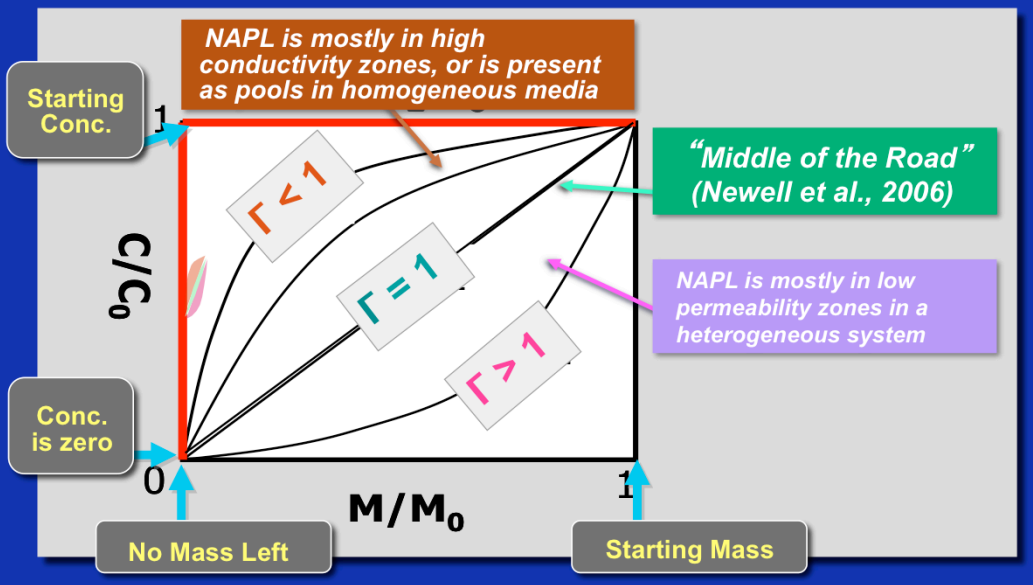
[Rao et al., 2001; Parker and Park, 2004; Zhu and Sykes, 2004]

$$\frac{C}{C_0} = \left(\frac{M}{M_0}\right)^{\Gamma}$$



48

Source Power Function – *What's That?*



49

LNAPLs are Usually Multi-component NAPLs

The dissolution of components (such as benzene or MTBE) from gasoline can be calculated using partitioning coefficients:

$$C_w = K_{pnw} C_n$$

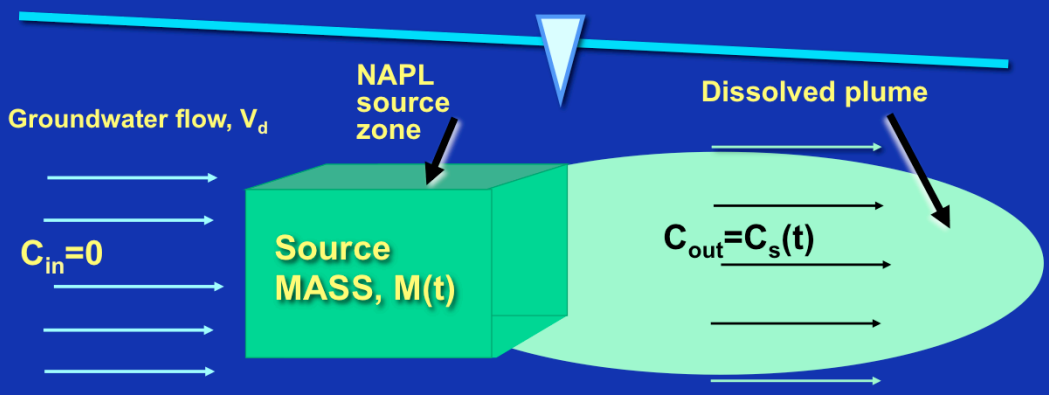
The dissolved concentration in groundwater is equal to the NAPL-water partition coefficient for the component, multiplied by the concentration in the NAPL (this is equivalent to Raoult's Law)

Over time, as the Component Washes Out of the LNAPL, Concentrations Drop

Because the dissolved groundwater concentration is directly proportional to the concentration remaining in the LNAPL, it responds like our power function model, with an exponent of Γ=1

$$\frac{C}{C_0} = \left(\frac{M}{M_0}\right)^{\Gamma}$$

The Discharging Concentration (C_s) Depends on the Mass Remaining in the Source Zone, (M)

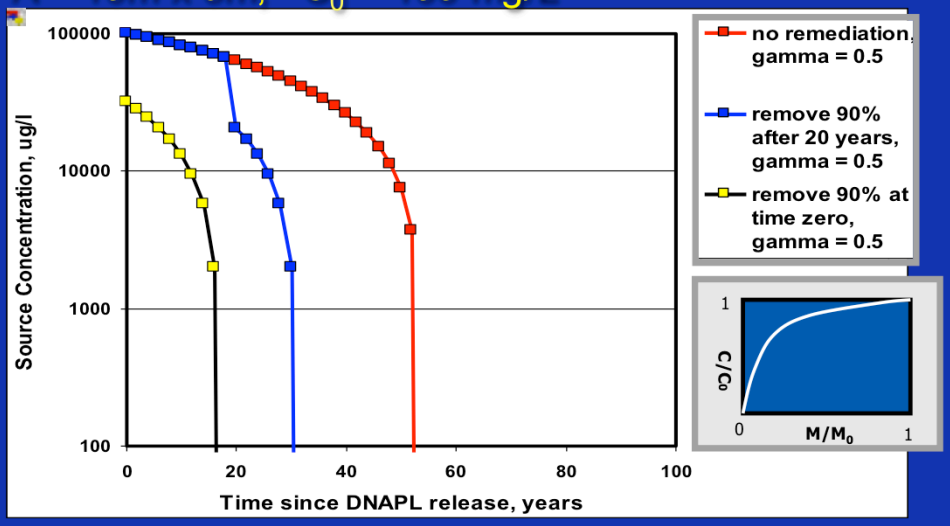


$$\frac{dM}{dt} = -Q(t)C_s(t) - \lambda_s M \qquad \frac{C_s(t)}{C_0} = \left(\frac{M(t)}{M_0}\right)^{\Gamma}$$

52

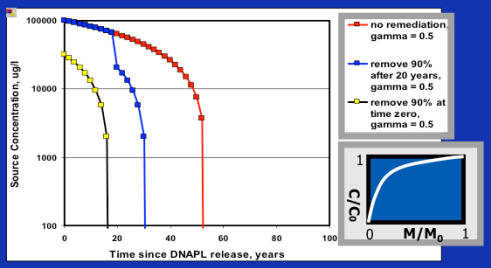
Source Behavior

Γ= 0.5, M_0 = 1,620 kg, V = 20 m/yr,
A = 10m x 3m, C_0 = 100 mg/L

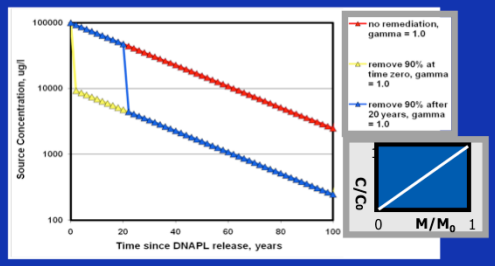


53

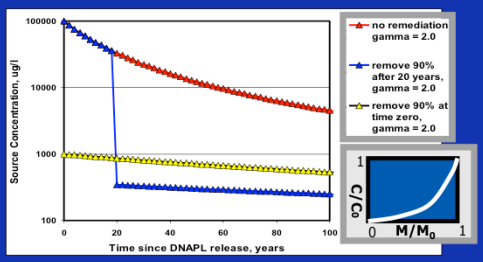
Source Behavior



Γ = 0.5



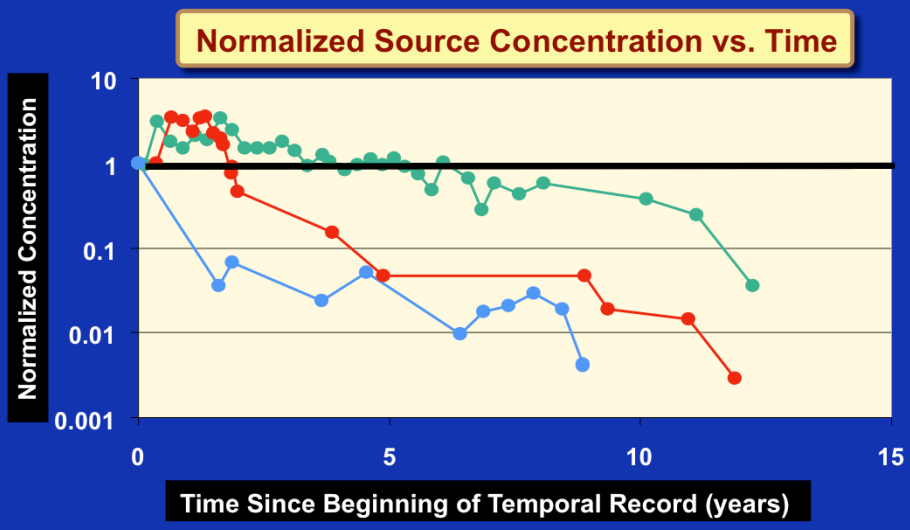
Γ = 1.0



Γ = 2.0

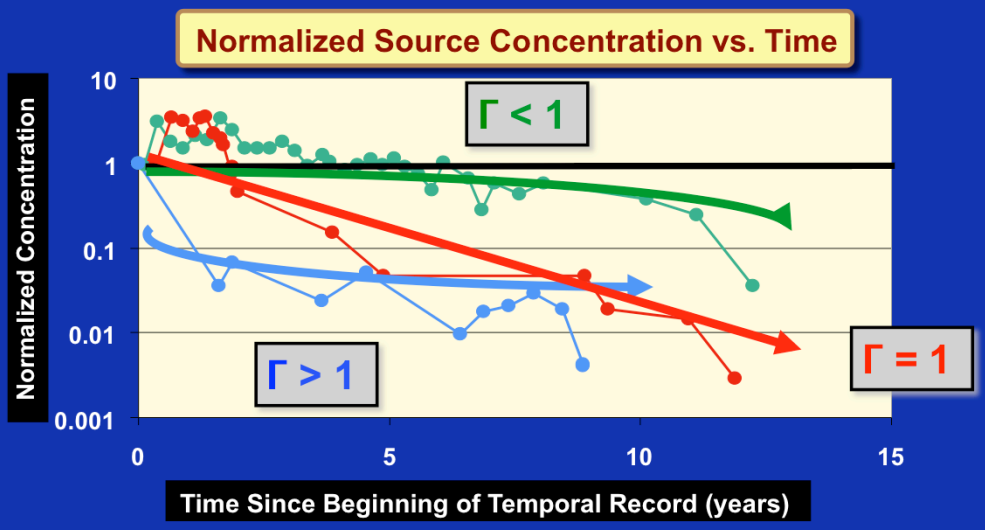
54

Take a Look at Data: 3 TCE Sites



55

Take a Look at Data: 3 TCE Sites



56

Summary: *Describing Your Source Zone ("Source Zone Architecture")*

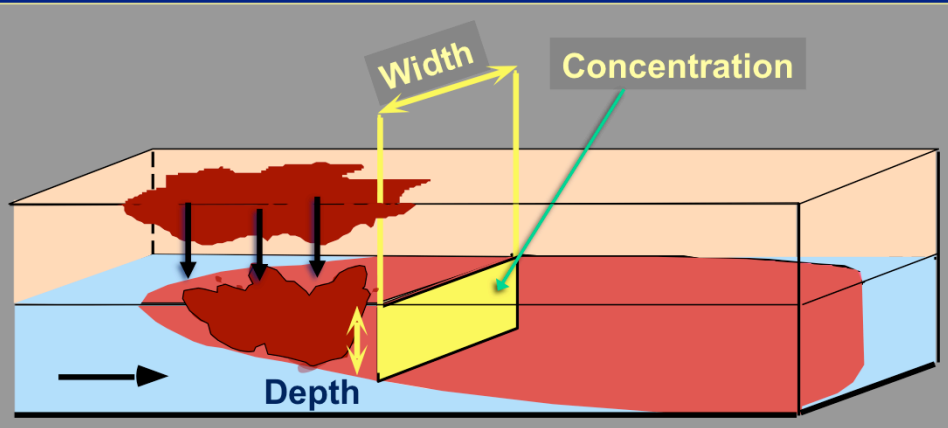
1. Need to pick a gamma (Γ)
2. Thought to range from Γ = 0.5 to Γ = 2.0
3. If you think you know something about source architecture, use these rules:

Might use Γ < 1.0	Might use Γ = 1.0	Might use Γ > 1.0
- Lots of pools of NAPL - NAPL mostly in high conductivity zones - Concentration vs. time shows long plateau (over many years)	- multicomponent LNAPL - Don't know much about source architecture - Want to use "Middle of Road" value Most Commonly Used Approach	- NAPL is in low permeability zone - There are (or will be) strong matrix diffusion effects (lots of low-permeability material in source zone) - Concentration vs. time shows obvious decline, (over many years)

57

Source Term Configuration

Assumed to be Vertical Plane. ***Need these data:***



58

Wrap-Up: Answering Questions About the Source Zone Using REMChlor and REMFuel

1. Pick a gamma (Γ) to reflect how source zone will decay (mass vs. mass flux). Note that gamma applies to both natural attenuation and remediation).
2. If you don't know, use middle of the road Γ = 1.0. This value is suggested for multicomponent LNAPLs
3. Put in the starting date and mass released. If mass is unknown, use best guess!
4. Run REMChlor/REMFuel and compare to site data (concentration and/or mass discharge).
5. Take out 90% of the mass (or any amount you want to simulate) to model the effects of source zone remediation. The post-remediation concentration will be determined by gamma.
6. See what happens to the plume!

59

Homework Assignment: Download and install REMChlor and REMFuel

- Download from EPA website:
- http://www.epa.gov/nrmrl/gwerd/csmos/models/remchlor.html
- http://www.epa.gov/nrmrl/gwerd/csmos/models/remfuel.html
- To run these, you will probably need to right-click on the icon, and then *"run as administrator"*
- A complete user's manual is available as a pdf in the help section
- It is always a good idea to print out the manual, and keep it handy

60

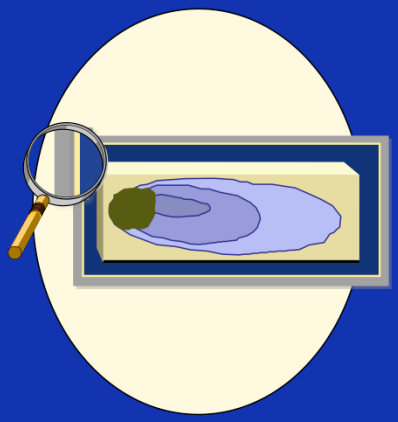
Homework Exercise

NUMBER 1

Plume gets shorter by how much?

♦

Text and Calculations



BREAK FOR QUESTIONS FROM PARTICIPANTS

62

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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

63

Resources & Feedback

- To view a complete list of resources for this seminar, please visit the **Additional Resources**
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