



Welcome to the CLU-IN Internet Seminar

Practical Models to Support Remediation Strategy Decision-Making - Part 3

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

Delivered: October 24, 2012, 1:00 PM - 3:00 PM, EDT (17:00-19:00 GMT)

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

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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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With that, please move to slide 3.

New online broadcast screenshot

The screenshot displays the 'CLUIN Default Seminar Template - Adobe Connect' interface. A large central text box reads 'View presentation live online here'. To the left, a 'Control online audio' callout points to a speaker icon. To the right, an 'Enlarge presentation' callout points to a 'Full Screen' button. Below this, a 'Submit private questions, comments or report technical problems' callout points to a text input field. Further right, an 'Information about Sponsors & Speakers' callout points to a section of the presentation. The presentation content includes fields for 'Sponsored by:', 'Delivered: Date & Time', 'Instructor(s):', and 'Moderator(s):', along with a URL 'Visit the Clean Up Information Network online at www.cluin.org' and a slide indicator '1 of Total # of slides'.

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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.

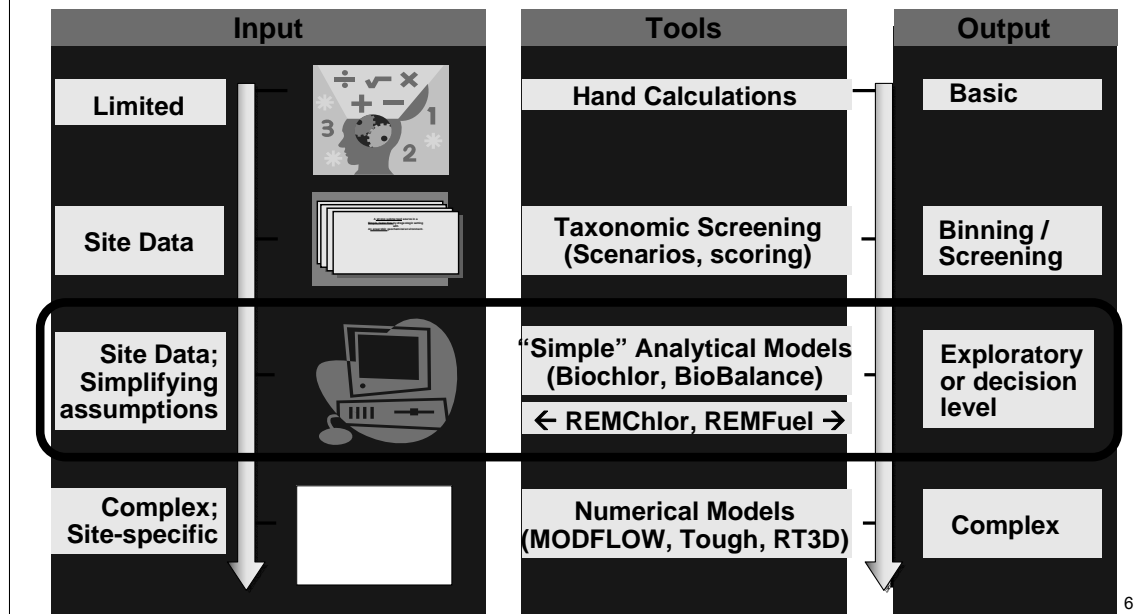


Module 3 - October 2012

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**

Continuum of Tools Available to Support Environmental Cleanup



Ron Falta, Ph.D.



- **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

Charles J Newell, Ph.D., P.E.



■ **Vice President, GSI Environmental Inc.**

- Diplomat 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

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




**BREAK FOR RESPONSES TO
MODULE 2 QUESTIONS
FROM
PARTICIPANTS**

Question 1: Will Source Remediation Meet Site Goals? General Conclusions

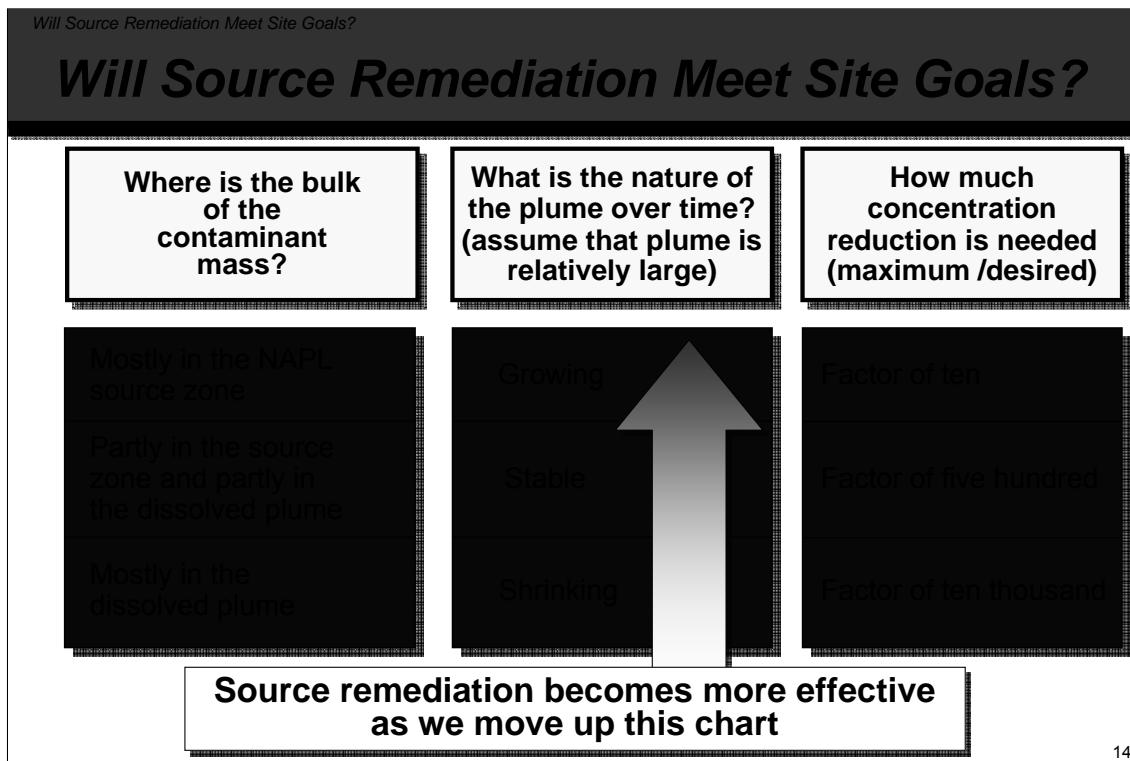
- **Source remediation can often remove 90% to 99.9% of a contaminant from the target volume.**
- **Source remediation can be expensive.**
- **Source remediation reduces the contaminant discharge that feeds the plume.**
- **It takes time for the plume to respond.**

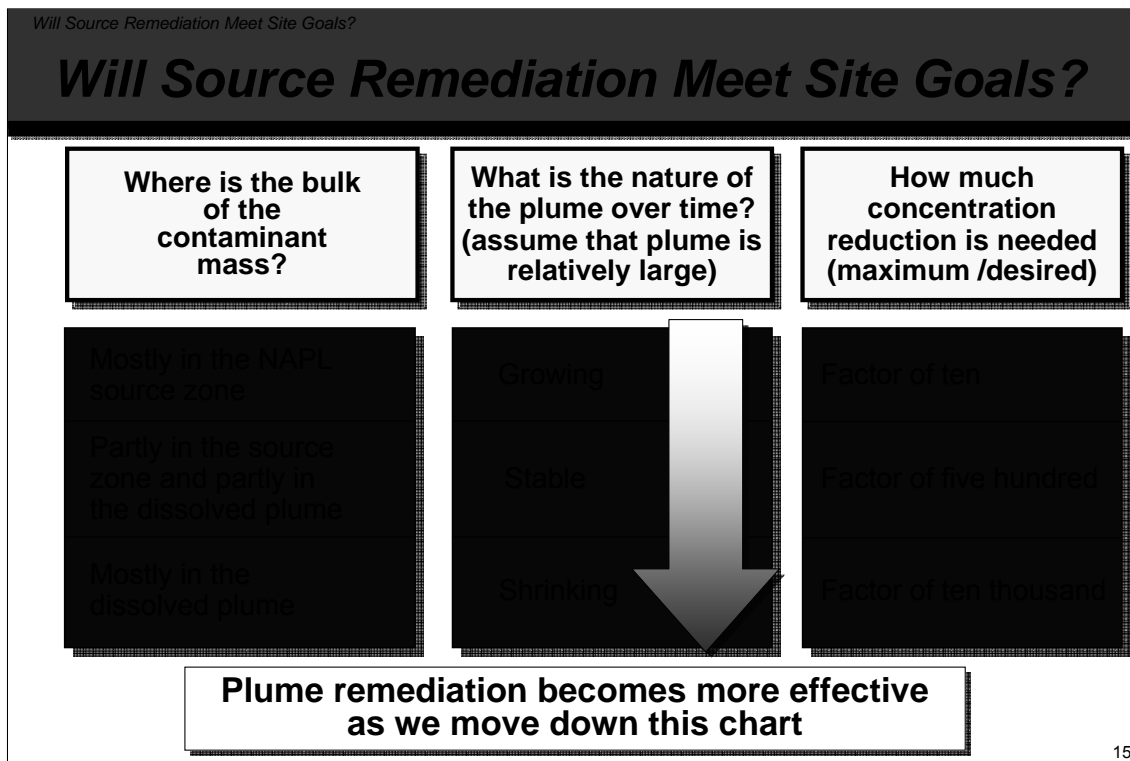
Question 1: Will Source Remediation Meet Site Goals? (cont'd)

- **Source remediation shortens the life of the source.**
- **Source remediation rarely achieves drinking water standards in the source zone immediately after deployment.**
- **The likely response of a plume to source remediation can be modeled using REMChlor or REMFuel.**

Will Source Remediation Meet Site Goals? <i>General Characteristics of Sites</i>		
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 NAPL 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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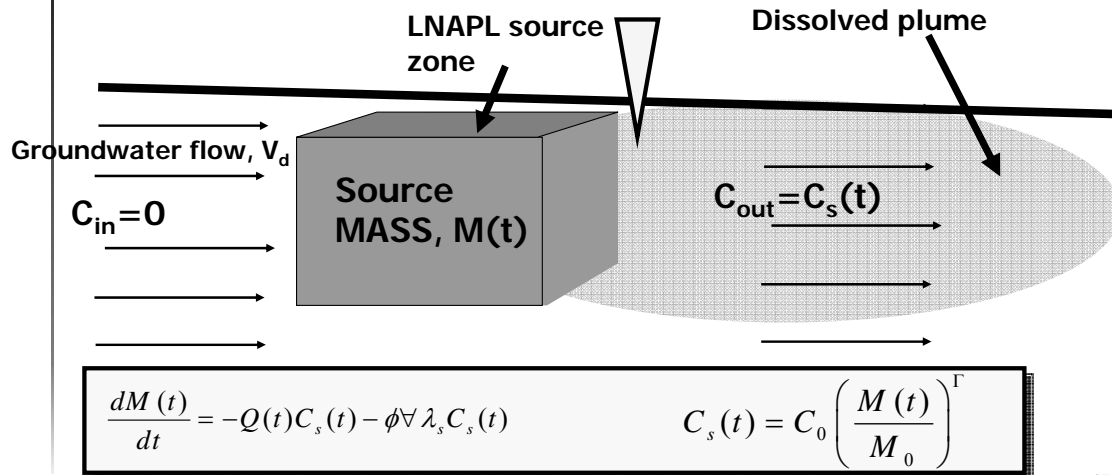




REMFuel

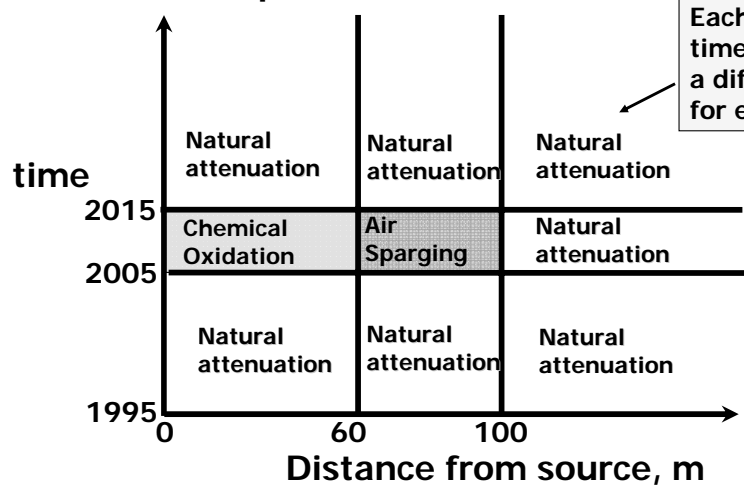
- ▶ New EPA model for UST sites (2012)
- ▶ **It's FREE** - download from EPA website
- ▶ Based on the REMChlor model for chlorinated sites (released in 2007)
- ▶ REMFuel extends REMChlor capability to model multiple hydrocarbons (BTEX) and additives (MTBE, EDB, DCA)
- ▶ Considers remediation of both the LNAPL source and the dissolved plumes

Source conceptual model is the same: Mass is mainly removed by flushing, and biodegradation in aqueous phase. Remediation is simulated by removing a fraction of the source mass at the time of remediation



Plume Remediation Model – divide space and time into “reaction zones”, solve the degradation reactions for each dissolved component in each zone

Example:



Each of these space-time zones can have a different decay rate for each chemical species

Consider coupled parent-daughter reactions in the plume

For example, we could model first order decay of MTBE into TBA:

$$rxn_{MTBE} = -\lambda_{MTBE} C_{MTBE}$$

$$rxn_{TBA} = y_{TBA/MTBE} \lambda_{MTBE} C_{MTBE} - \lambda_{TBA} C_{TBA}$$

We would like for all of these decay rate constants to be functions of distance and time.

REMFuel also can model zero-order and Monod kinetics in the plume zone

CLEMSON
UNIVERSITY

REMFuel

Built-in calculators for LNAPL components – mass, concentration, R. Database is also in User's Guide

The image displays three overlapping software windows for LNAPL calculations. The left window, titled "Benzene Initial Concentration Calculation", shows the formula $\text{Initial Concentration} = X_{\text{napl}} (\text{Mole Fraction}) \cdot C_{\text{max}} (\text{Pure Solubility}) \cdot \text{Dilution Factor}$. Inputs include X_{napl} Mass Fraction (0.006), Molecular Wt. NAPL (105), Molecular Wt. Benzene (88), C_{max} (1.8), and Dilution Factor (0.5). The result is Initial Concentration = 0.00644 (g/L). The right window, also titled "Benzene Initial Concentration Calculation", shows the formula $\text{Initial Mass} = X_{\text{napl}} (\text{Mass Fraction}) \cdot \text{Volume NAPL} \cdot \text{Density of NAPL}$. Inputs include Set Volume of NAPL (1000), Unit (US Gallon), X_{napl} (0.006), and Density of NAPL (0.72). The result is Initial Mass = 164 (kg). The center window, titled "Calculate Retardation Factor", shows inputs for K_{oc} (83), F_{oc} (0.002), Bulk Density (1.6), and Porosity (0.35). The formula $\text{Retardation Factor} = 1 + \frac{(83)(0.002)(1.6)}{0.35}$ is shown, resulting in Retardation Factor = 1.76.

Benzene Initial Concentration Calculation

Select type of NAPL: Gasoline - Unleaded with high MTBE

Initial Concentration = $X_{\text{napl}} (\text{Mole Fraction}) \cdot C_{\text{max}} (\text{Pure Solubility}) \cdot \text{Dilution Factor}$

$X_{\text{napl}} (\text{Mole Fraction}) =$

X_{napl} Mass Fraction: 0.006

Molecular Wt. NAPL: 105

Molecular Wt. Benzene: 88

$C_{\text{max}} (\text{Pure Solubility}) =$ 1.8

Dilution Factor (0.01 - 1.0) = 0.5

Initial Concentration = 0.00644 (g/L)

☒ Significant Digits: 3

Benzene Initial Concentration Calculation

Select type of NAPL: Gasoline - Unleaded with high MTBE

Initial Mass = $X_{\text{napl}} (\text{Mass Fraction}) \cdot \text{Volume NAPL} \cdot \text{Density of NAPL}$

Set Volume of NAPL = 1000 Unit: US Gallon

$X_{\text{napl}} (\text{Mass Fraction}) =$ 0.006

Density of NAPL = 0.72

Initial Mass = 164 (kg)

Calculate Retardation Factor

Retardation Factor

K_{oc} (L/Kg): 83

F_{oc} (-): 0.002

Bulk Density (Kg/L): 1.6

Porosity = 0.35

Retardation Factor = $1 + \frac{(83)(0.002)(1.6)}{0.35}$

Retardation Factor = 1.76

☒ Significant Digits: 3

LNAPL components can be chosen from built-in library or created; REMFuel can handle up to 20 at once (plus a degradation daughter product for each one)

New Component

☒ Use Default variable inputs

Select Compound: Benzene, Toluene, Ethyl Benzene, o-Xylene, m-Xylene, p-Xylene, MTBE, TBA, TAME, DIPE, ETBE, Napthalene, **EDB**

Name: **EDB**

Reaction Type:
☐ Zero Order Reaction
☒ First Order Reaction

Decay Rate: **0.63**

Initial Source:
Concentration (g/L): **0** [Calculate](#)
Mass (Kg): **0** [Calculate](#)

☐ Copy Component variables from existing Component.

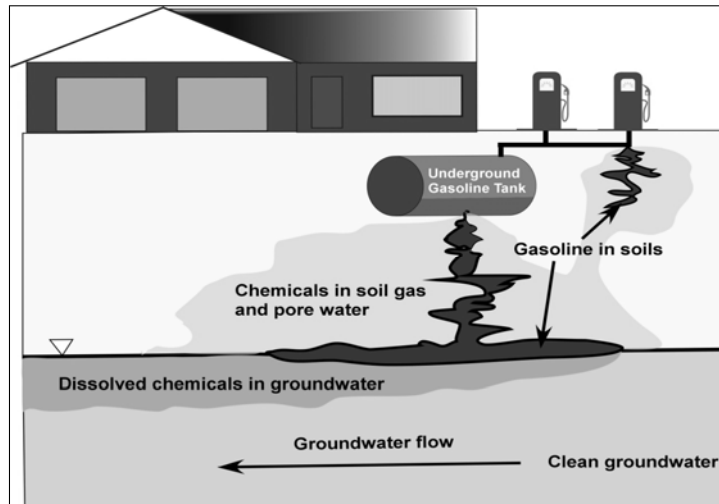
Select Existing Component: Benzene, Toluene, Ethyl Benzene, o-Xylene, MTBE

Name: **Benzene_1**

[Copy Benzene Values](#)

OK **Cancel**

Example: 10,000 gallons of gasoline released in 1997, (unleaded regular with high MTBE). Groundwater pore velocity is 94 ft/yr, moderate degradation in plume





Hands-On Computer Exercise



NUMBER 2

Now You Try Using REMFuel For a Site



Questions answered:

*What will happen if no action taken?
Will source and plume remediation meet
site goals?*

Enter Source and Plume Parameters

REMFuel - [REMFuel Model Parameters]

File Model Help

REMFuel Project

- Project: sflois_no_remediation
- Model Parameters
- View Model Results
- View File Output
- View Graphical Output
- Output vs. Distance

Source Zone Parameters

Source Parameters

Gamma

Source Dimensions

Source Width (m)

Source Height (m)

Source Length (m)

Flow Parameters

Darcy Velocity (m/yr)

Porosity

Source Remediation

Fraction Removed

Source Remediation Time

(Years)

Start Time (T1) End Time (T2)

Transport Parameters

Velocity

Sigmav vMin vMax

Number of Stream Tubes

alpha (m) alphas (m)

Component Name

Decay Rate (per year)

Time, Years

Time -->

Period 1

Period 2

Period 3

Decay Rate (per year)

Zone 1 Zone 2 Zone 3

Period 1 (1,1) (2,1) (3,1)

Period 2 (1,2) (2,2) (3,2)

Period 3 (1,3) (2,3) (3,3)

Daughter Name

Decay Rate (per year)

Zone 1 Zone 2 Zone 3

Period 1 (1,1) (2,1) (3,1)

Period 2 (1,2) (2,2) (3,2)

Period 3 (1,3) (2,3) (3,3)

X1 X2

Distance From Source, Meters

Select Component

Benzene
Toluene
Ethyl Benzene
o-Xylene
MTBE

Add Component Delete Component

Component Specific Parameters

Reaction Type

☐ Zero Order Reaction

☒ First Order Reaction

☐ Monod Reaction

Daughter Yield From Parent

Initial Source

Concentration (g/L) Calculate

Mass (Kg) Calculate

Retardation Factor Calculate

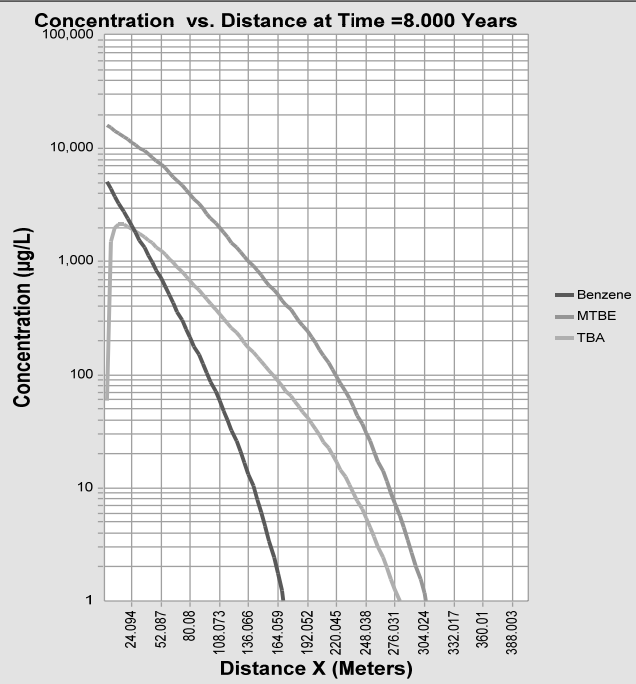
Source Decay (1/yr)

Simulation Parameters

	Intervals	Min Value	Max Value	Units
X - Direction	101	0.1	400	Meter
Y - Direction	1	-100	100	Meter
Z - Direction	1	0	0	Meter
Time	50	0	50	Year

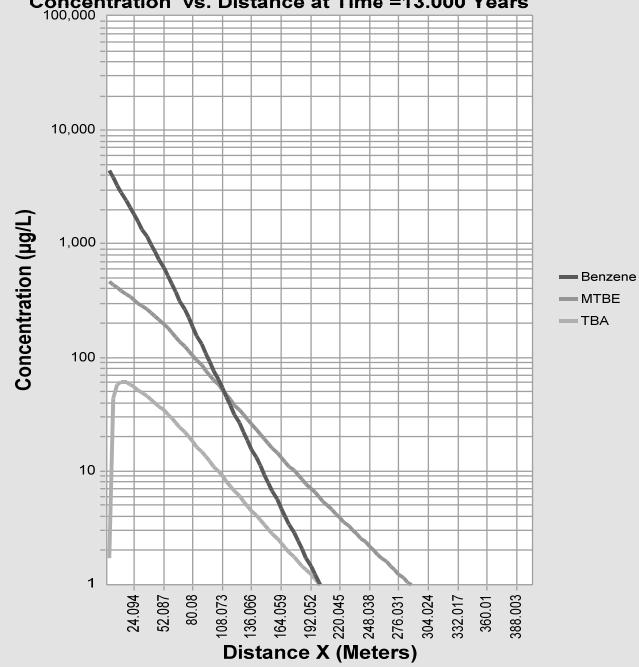
REMFuel

2005 plume



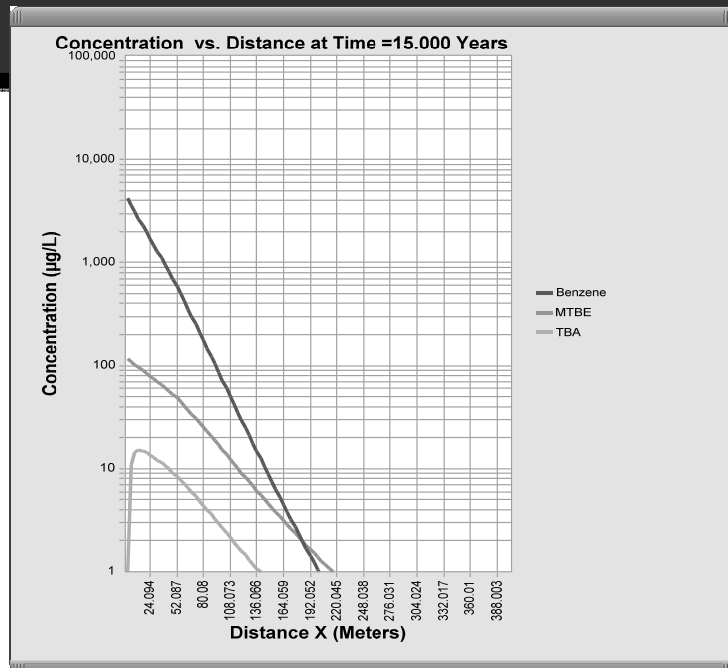
2010 plume

Concentration vs. Distance at Time =13.000 Years



2012 plume

At this site, the MTBE and TBA plumes are shrinking. The benzene plume is stable, and fairly large



Add Source and Plume Remediation

- **Simulate aggressive source remediation in 2012, assume we can remove 90% of LNAPL**
- **Also simulate a plume remediation operation (air sparging, chemical oxidation, etc.) between 20 and 100 m, starting in 2012 and ending in 2017**
- **Assume plume remediation increases benzene and ethylbenzene decay rates by 4X; no effect on MTBE or TBA**

REMFuel Input Page, only need to change a few lines

REMFuel - [REMFuel Model Parameters]

File Model Help

REMProject

Project: sfous_source_remed_plum

Model Parameters

View Model Results

View File Output

View Graphical Output

Output vs. Distance

Source Zone Parameters

Source Dimensions

Gamma 1

Source Width (m) 20

Source Height (m) 2

Source Length (m) 20

Flow Parameters

Darcy Velocity (m/yr) 10

Porosity 0.35

Source Remediation

Fraction Removed 0.9

Source Remediation Time

15 (Years) 15.5

Start Time (T1) End Time (T2)

Transport Parameters

Velocity

0.2 0 2

Sigmav vMin vMax

Number of Stream Tubes 1000

-0.002 -0.0002

alpha (m) alphaz (m)

Component Name Benzene

Decay Rate (per year)

Zone 1 Zone 2 Zone 3

(1,3) (2,3) (3,3)

Period 1 Period 2

1.1 1.1 1.1

(1,2) (2,2) (3,2)

1.1 4.4 1.1

(1,1) (2,1) (3,1)

1.1 1.1 1.1

Time, Years

20 Year

15 Year

Daughter Name Benzene_Daughter

Decay Rate (per year)

Zone 1 Zone 2 Zone 3

(1,3) (2,3) (3,3)

Period 1 Period 2

0 0 0

(1,2) (2,2) (3,2)

0 0 0

(1,1) (2,1) (3,1)

0 0 0

Time, Years

20 Year

15 Year

X1 20 X2 100

Distance From Source, Meters

Simulation Parameters

	Intervals	Min Value	Max Value	Units
X - Direction	101	0.1	400	Meter
Y - Direction	1	-100	100	Meter
Z - Direction	1	0	0	Meter
Time	50	0	50	Year

Select Component

Benzene

Toluene

Ethyl Benzene

o-Xylene

m-Xylene

p-Xylene

MTBE

Add Component Delete Component

Component Specific Parameters

Reaction Type

☐ Zero Order Reaction

☒ First Order Reaction

☐ Monod Reaction

Daughter Yield From Parent 0

Initial Source

Concentration (g/L) 0.00644 Calculate

Mass (Kg) 164 Calculate

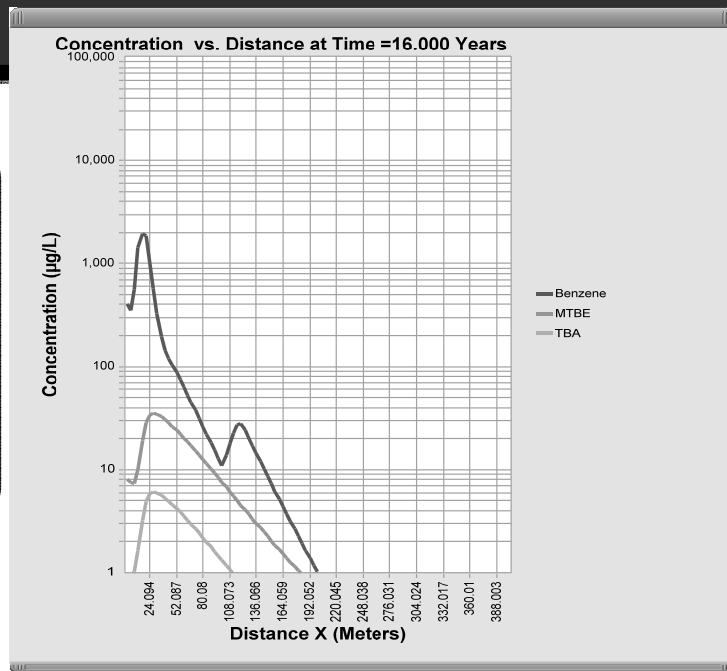
Retardation Factor 1.76 Calculate

Source Decay (1/yr) 1.1

REMFuel

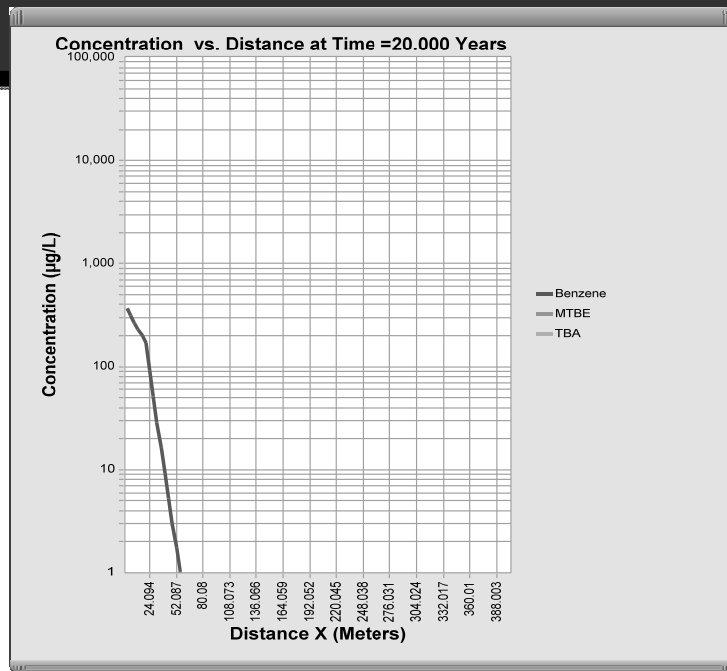
2013 plume

Effect of source remediation seen on benzene and MTBE; plume remediation only affected benzene here (20-100m)



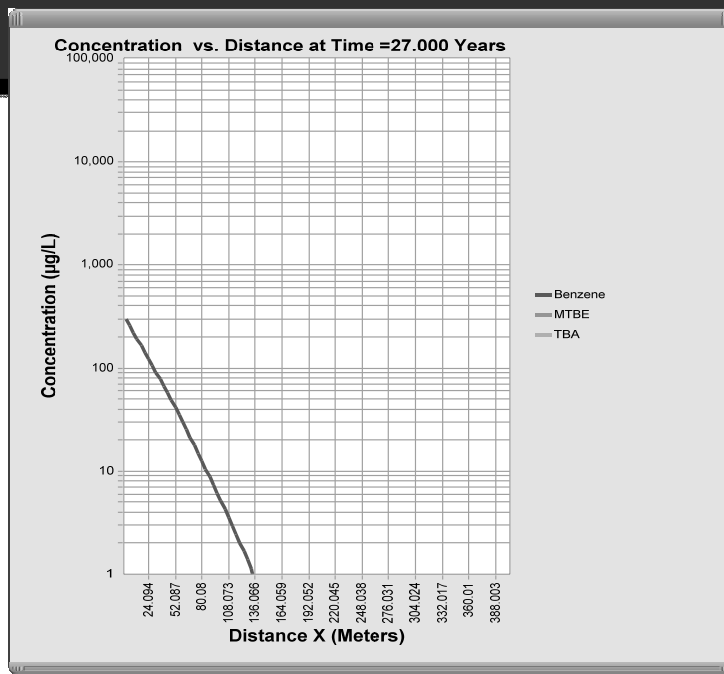
2017 plume

End of plume
remediation
period, only a
short benzene
plume left



2024 plume

Benzene plume rebounds a bit after plume remediation is discontinued, because some LNAPL remained in source zone. MTBE has disappeared.



**BREAK FOR QUESTIONS
FROM
PARTICIPANTS**

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

More Complex Example Model Application – MNA with REMChlor

- **Difficult case where natural attenuation is low**
- **Long-lived PCE source, high discharge to groundwater**
- **Low rates of PCE-TCE-DCE-VC decay**
- **Plume is defined by 1 ppb**



Show Me How It Works

NUMBER 2

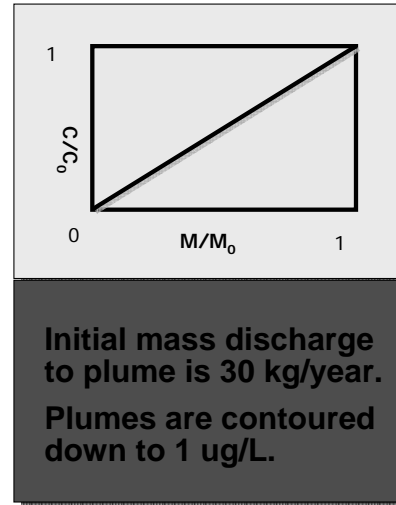
**REMChlor Used to
Evaluate MNA**

(Tutorial 6)



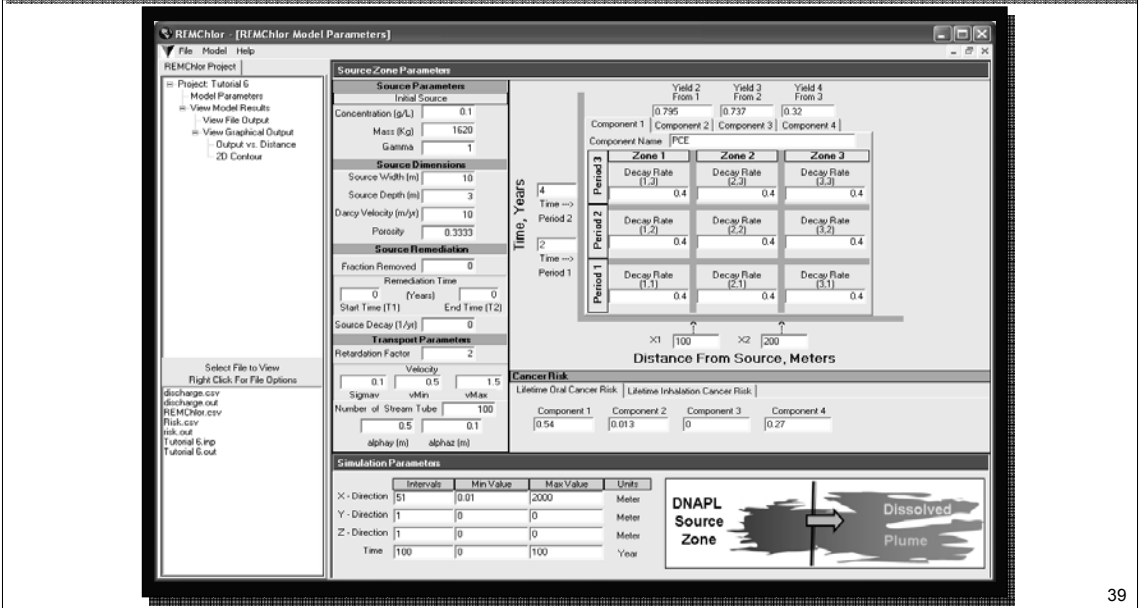
1,620 kg Release of PCE in 1979

- DNAPL source has $\Gamma=1.0$, $C_0=100$ mg/L; water flow through source zone is 300 m^3 per year
- Assume reductive dechlorination from $\text{PCE} \rightarrow \text{TCE} \rightarrow \text{DCE} \rightarrow \text{VC}$
- Assume that only $\frac{1}{2}$ of DCE is converted to vinyl chloride (VC) by reductive dechlorination, the other $\frac{1}{2}$ is destroyed
- Ground water pore velocity is 30 m/yr , $R=2$, decay rates are low: PCE, 0.4 yr^{-1} ; TCE, 0.15 yr^{-1} ; DCE, 0.1 yr^{-1} ; VC, 0.2 yr^{-1}



What Will Happen if No Action is Taken?

Part A: Simulate Natural Attenuation of Source and Plume



What Will Happen if No Action is Taken?

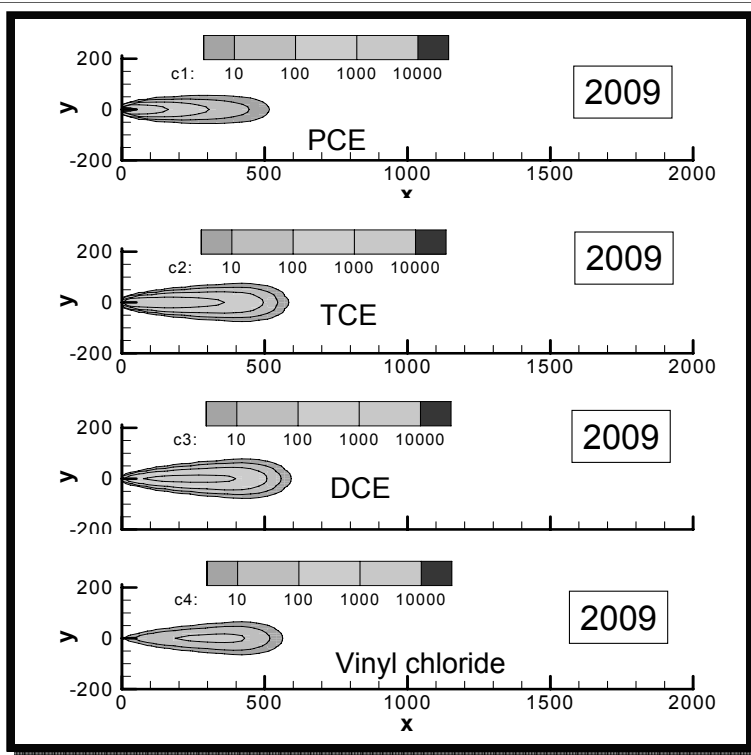
Spill:

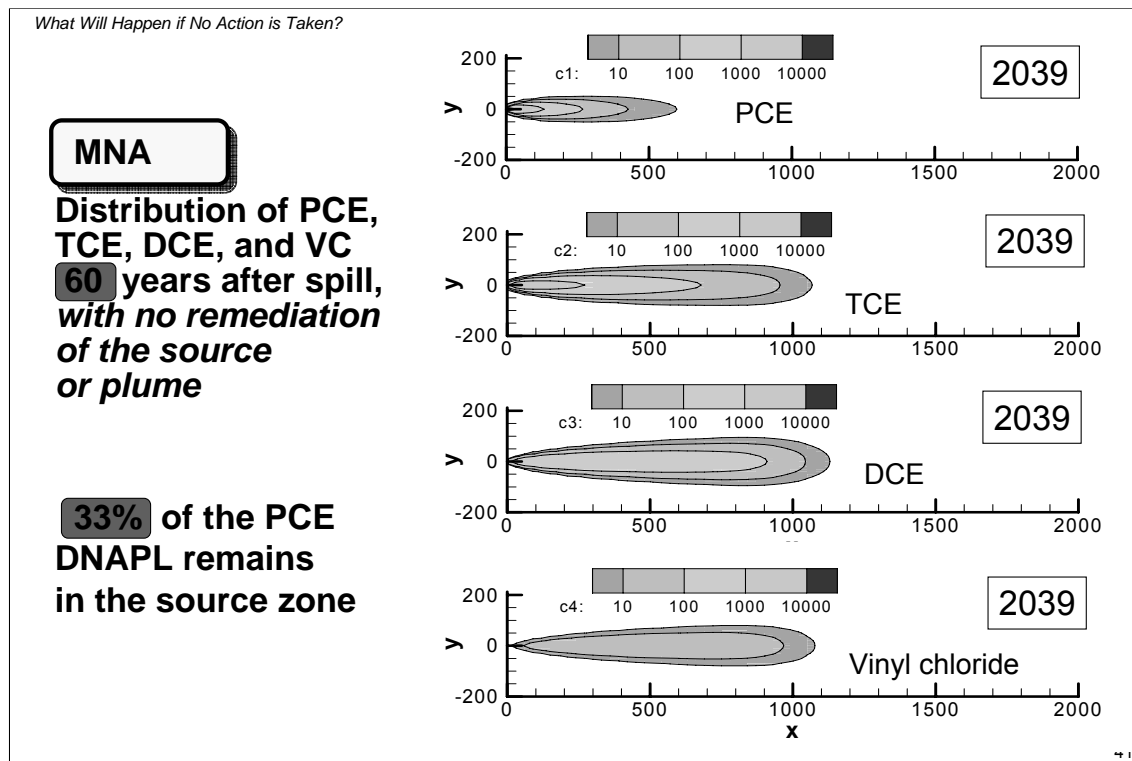
**Release of 1620 kg
PCE in 1979.**

Plume reactions

**PCE → TCE
→ DCE → VC**

**57% of the
PCE DNAPL
remains
in the
source zone**



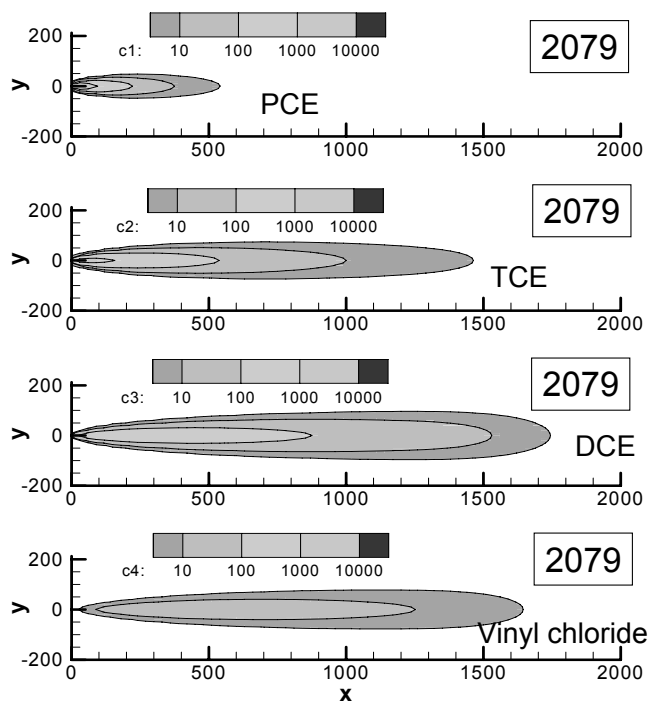


What Will Happen if No Action is Taken?

MNA

**Distribution of PCE,
TCE, DCE, and VC
100 years after spill,
with no remediation
of the source
or plume.**

15% of the PCE
DNAPL remains
in the source zone.



What Will Happen if No Action is Taken?

PCE example

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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What Will Happen if No Action is Taken?

Cancer Risk From Drinking Water at a Given Location Over Time (REMChlor Also Includes the Inhalation Risk)

Compute chronic daily intake (CDI) of each carcinogen:

$$CDI_i = \frac{q_w}{m T_{life}} \int_{\max(0, t - T_{ex})}^t C_w^i(t) dt$$

Where

q_w is the daily water intake (2 l/d)
 m is the body mass (70 kg)
 T_{life} is the 70 year lifetime averaging period

t is the Time
 T_{ex} is the length of the exposure period (30 years)
 C_w is the concentration of the carcinogen in the well.

The CDI is essentially the cumulative dose of carcinogen.

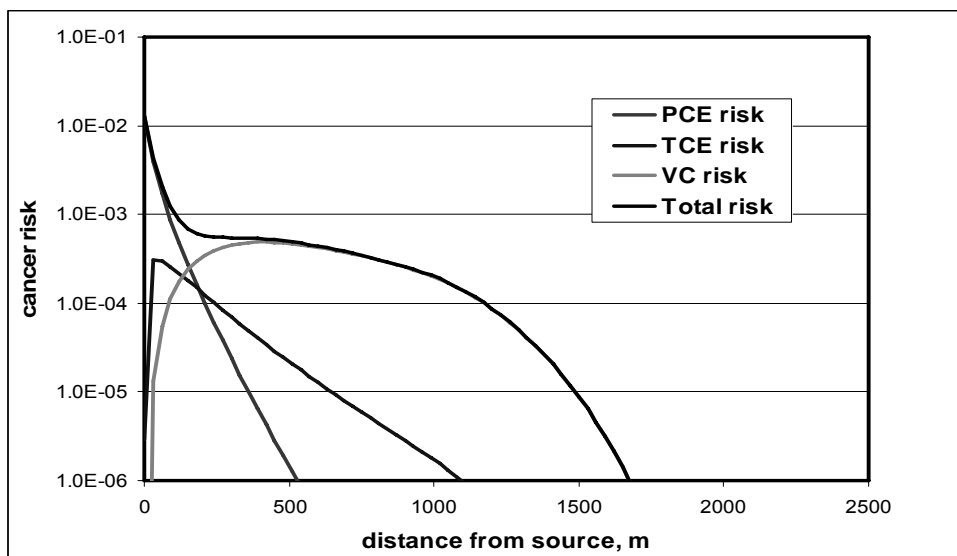
With a cancer risk slope factor, SF, the cancer risk is then:

$$Risk_i = CDI_i \times SF_i \quad Risk_T = \sum Risk_i$$

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What Will Happen if No Action is Taken?

Lifetime Cancer Risks in 2079 (Exposure from 2049-2079)



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**BREAK FOR QUESTIONS
FROM
PARTICIPANTS**

New Ways to stay connected!

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



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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

The screenshot shows a web form titled "U.S. EPA Technical Support Project Engineering Forum Green Remediation: Opening the Door to Field Use Session C (Green Remediation Tools and Examples) Seminar Feedback Form". The form is part of the EPA's Technology Innovation Program. It includes a sidebar with links like "Go to Seminar", "Links", "Feedback", "Home", and "CLU-IN Studio". The main content area contains a message: "We would like to receive any feedback you might have that would make this service more valuable. Please take the time to fill out this form before leaving the site." Below this are input fields for "First Name:", "Last Name:", "Daytime Phone Number:", and "Email Address:". The email field is pre-filled with "bent.jen@epa.gov". At the bottom, there is a checkbox labeled "Please send a copy of my feedback confirmation to a record of my participation to this address" and a "Date of Seminar:" field with the value "December 15, 2009".

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