Spatial Analysis and Decision Assistance Version 3.0

Windows based freeware designed to integrate scientific models with decision and cost analysis frameworks in a seamless, easy to use environment.

- Visualization
- Statistical Analysis
- Geospatial Interpolation
- Geospatial Uncertainty Analysis
- Human Health Risk Assessment

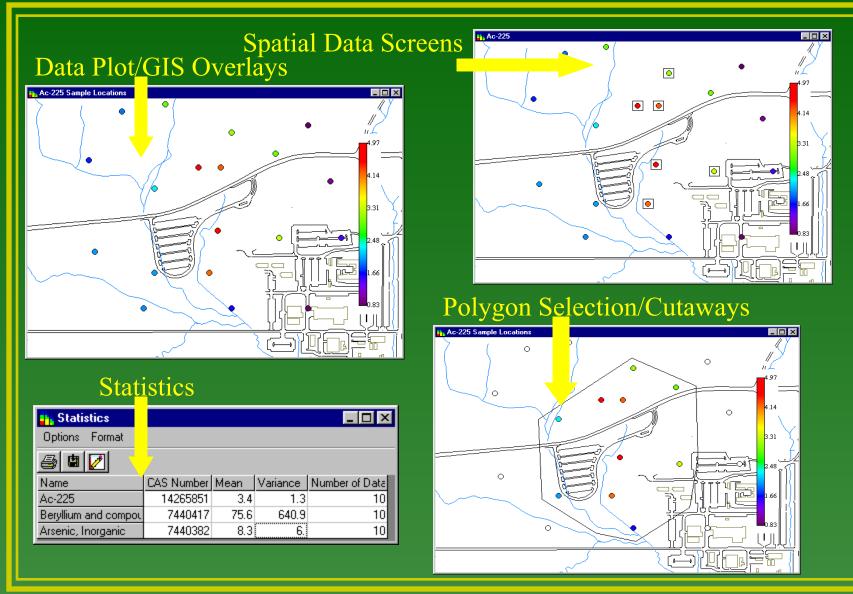
- Ecological Risk Assessment
- Custom Analysis
- Area of Concern Frameworks
- Cost Benefit Analysis
- Secondary Sampling Design

SADA has been supported by both the DOE and EPA and recently the NRC. SADA has had about 4000 downloads from the website.

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For more information contact Robert Stewart, Oak Ridge National Laboratory, 1060 Commerce Park, Oak Ridge, TN 37887. Email u74@ornl.gov.

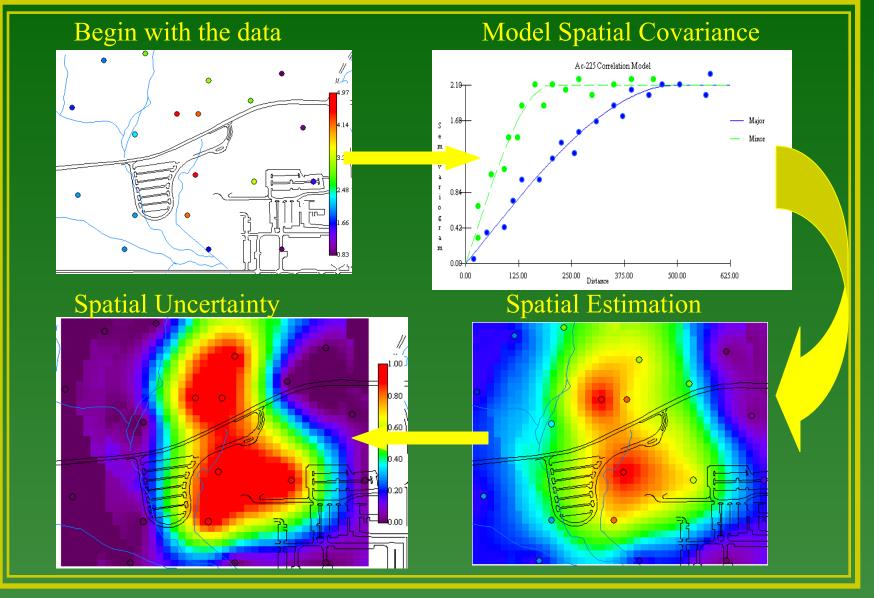
Basic Data Exploration/Visualization



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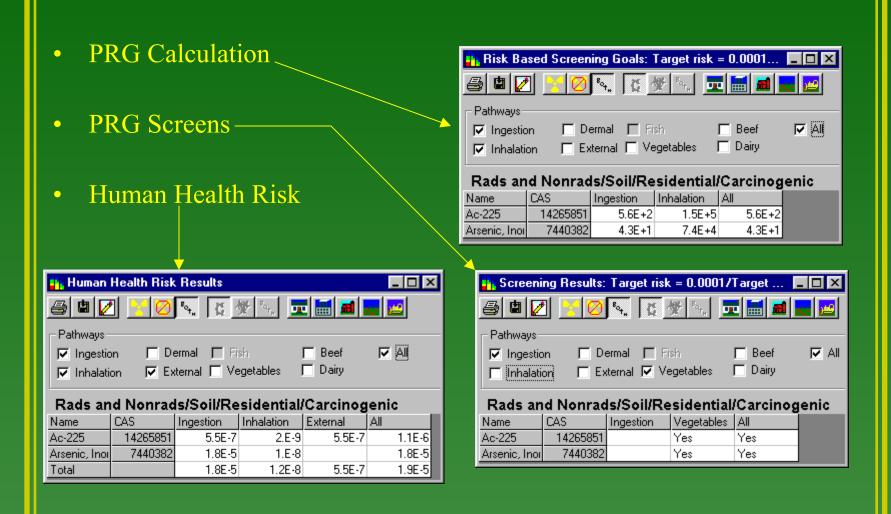
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Spatial Analysis



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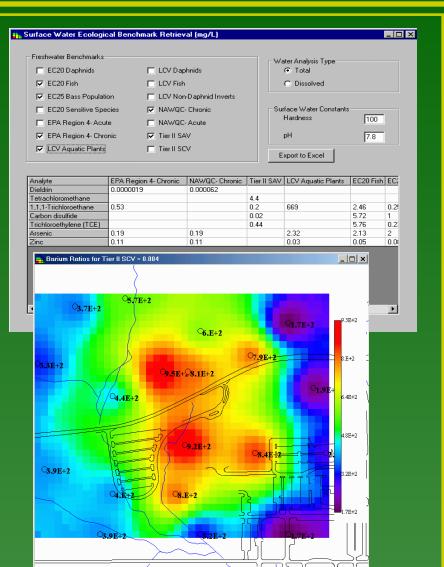
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Ecological Risk Capabilities

Ecological Risk Benchmarks

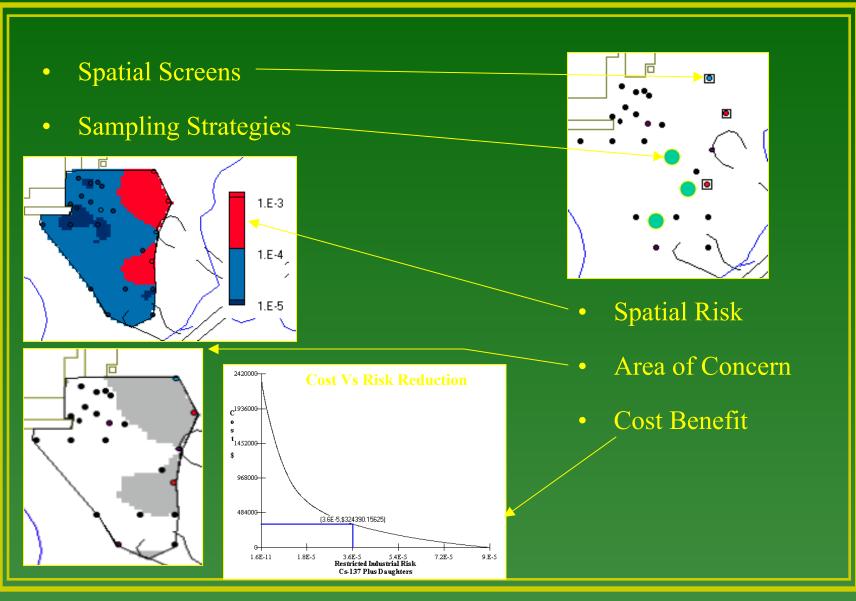
- Suitable for screening ERAs
- Compilation of ecological benchmarks for surface water, soil, and sediment
- Benchmarks a function of environmental variables where appropriate



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Spatial Decision Making



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- Self-documentation of all assumptions
 - Exposure concentrations
 - Risk models
 - Exposure variables
 - Geospatial parameters
 - Toxicity data
 - Images as bitmaps
- HTML format, can be exported to popular word processors

SADA™ Copyright © 2000 University of Tennessee. All Rights Reserved. For more information contact Robert Stewart, Oak Ridge National Laboratory, 1060 Commerce Park, Oak Ridge, TN 37887. Email u74@ornl.g Use of Spatial Analysis and Decision Assistance (SADA) Software to Model Wildlife Exposures

Christopher J.E. Welsh, S. Thomas Purucker, and Robert N. Stewart, The Institute for Environmental Modeling, University of Tennessee, Knoxville

William L. Wilder, Environmental Systems Corporation, Knoxville, TN

I-40/I-640 Site

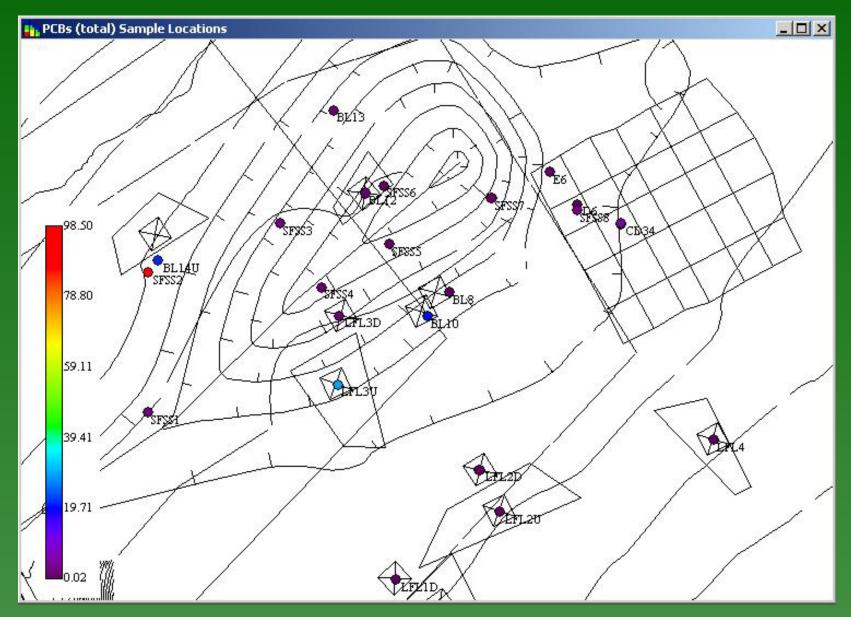


- Knoxville, TN
- Disposal (fluorescent light ballasts)
- Metals, PCBs, Pesticides

I-40/I-640 site



Layout



Polychlorinated Biphenyls (PCBs)

- Persistent
- Bioaccumulative
- Toxic effects

Wildlife Receptors

- Herbivore -- Meadow vole
- Insectivore Short-tailed shrew
- Carnivore Long-tailed weasel

Model for Dose to Wildlife Receptor From Ingestion of Contaminated Food and Soil:

$$Dose_{total} = Dose_{food} + Dose_{soil}$$

Dose $_{total}$ = Total dose in mg/kg BW/d Dose $_{food}$ = Dose from food ingestion Dose $_{soil}$ = Dose from soil ingestion

Ingestion of Contaminated Prey



FIR_{BW} = Dry food ingestion rate (kg dry food/kg BW/d)

- C_{plant} = Chemical concentration in plant (mg/kg dry wgt).
 - $C_{plant} = C_{soil} \times BAF_{plant}$
- BAF_{plant} = soil to plant bioaccumulation factor (mg/kg dry plant per mg/kg soil)
- P_{plant} = Plant ingestion as percentage of diet (unitless)
- C_{invert} = Chemical concentration in invertebrate (mg/kg dry wgt).
 - $C_{invert} = C_{soil} \times BAF_{invert}$
- BAF_{invert} = soil to invertebrate bioaccumulation factor (mg/kg dry invertebrate per mg/kg soil)
- P_{invert} = Soil invertebrate ingestion as a percentage of diet (unitless) C _{mamm prey} = Chemical concentration in vertebrate, primarily small mammalian, prey (mg/kg dry weight). If transfer factor is diet-totissue, C _{mamm prey} = C_{diet} x BAF _{diet-to-mamm}.

Ingestion of Contaminated Prey (cont.)

 $DOS_{food} = FIR_{BW} \times [(C_{plant} \times P_{plant}) + (C_{invert} \times P_{invert}) + (C_{mammprey} \times P_{mamm})] \times AF \times AUF$

C mamm prey = Chemical concentration in vertebrate prey (mg/kg dry wgt). C mamm prey = C_{diet} x BAF diet-to-mamm . C_{diet} = Chemical concentration in diet of mammalian prey (mg/kg dry wgt), measured or estimated as C_{diet} = (C_{plant} x P_{plant}) + (C_{invert} x P_{invert}) + (C_{soil} x P_{soil}) with C_{plant}, invert, and P_{plant}, invert, soil referring to mammalian prey parameters

BAF _{diet-to-mamm} = food to mammal bioaccumulation factor (mg/kg dry mammal per mg/kg dry food)

P_{mamm} = Proportion vertebrate prey in diet (unitless)

AF = Fraction of chemical absorbed from food. Assumed = 1. (unitless)

AUF = Area use factor = ratio of animal's home range to area of site. Set to 1, assumes 100% on-site. (unitless)

Ingestion of Contaminated Soil

$$Dose_{soil} = FIR_{BW} \times C_{soil} \times P_{soil} \times AF_{soil} \times AUF$$

FIR_{BW} = Dry food ingestion rate as a function of body weight (kg dry food/kg BW/d)

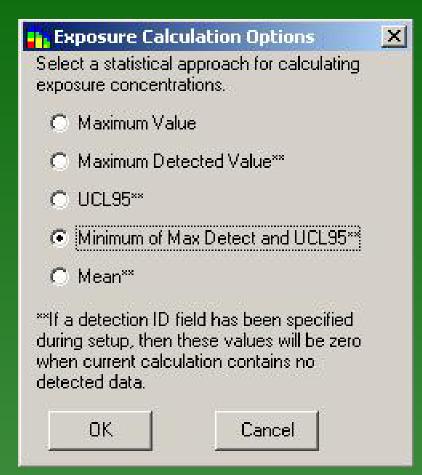
C_{soil} = Chemical concentration in dry soil (mg/kg)

P_{soil} = Soil ingestion as a percentage of diet (unitless)

AF_{soil} = Absorbed fraction of chemical from soil. Assumed = 1. (unitless)

AUF = Area use factor = ratio of animal's home range to area of site. Assumed = 1. (unitless)

Set Screening Statistics



Set BAFs

Set Terrestrial Modeling Contaminant Parameters	
PCBs (total)	
Chemical Constants Log Octanol-Water Partitioning Coefficient (Log Kow) 7.31 (mg/L)/(mg/L)	Dermal Contact Absorption Fraction 0.06 mg/mg Soil -> Invertebrate Concentration
Inhalation Inhalation Volatile Volatilization Factor (VF) Particulate Emission Factor (PEF) 1316239339 Kg/m3	C Custom BAF (mg/kg)/(mg/kg) Kow-based BAF 33.4187 (mg/kg)/(mg/kg) Tissue Regression Log-linear slope Log-linear intercept
Soil -> Plant Concentration: Foliage C Custom BAF (mg/kg)/(mg/kg) Kow-based BAF 0.0313 Tissue Regression	Soil -> Small Mammal Concentration C Custom BAF (mg/kg)/(mg/kg) Tissue Regression Log-linear slope
Soil -> Plant Concentration: Seed C Custom BAF (mg/kg)/(mg/kg) Kow-based BAF 0.0313 Tissue Regression	Log-linear intercept Diet -> Small Mammal Concentration © Custom BAF 2.63 (mg/kg)/(mg/kg) © Tissue Regression Log-linear slope Log-linear intercept
Save Changes	Exit

$Soil \rightarrow Plant$

K_{ow}-based soil-to-plant BAFs were generated using the following equation from EPA (2000):

$$BAF_{plant} = 10^{1.31 - 0.385 \log K_{ow}}$$

BAF _{plant} = soil to plant foliage bioaccumulation factor (mg/kg dry plant/mg/kg soil)

 K_{ow} = octanol-water partitioning coefficient.

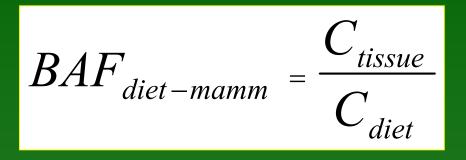
$Soil \rightarrow Invertebrates$

 K_{ow} -based soil-to-invertebrate BAFs were generated using the following equation from EPA (2000):

$$BAF_{worm} = \frac{10^{\log K_{ow} - 0.6}}{f_{oc} \times 10^{0.983 \log K_{ow} + 0.00028}}$$

 BAF_{worm} = soil to earthworm bioaccumulation factor (mg/kg dry invertebrate / mg/kg soil) f_{oc} = fraction organic carbon in soil. Default is set to 1%. K_{ow} = octanol-water partitioning coefficient.

Diet → Small Mammal



BAF _{diet-to-mamm} = food to mammal bioaccumulation factor (mg/kg dry mammal per mg/kg dry food)
C tissue = Chemical concentration in vertebrate tissue (mg/kg dry wgt.)
C diet = Chemical concentration in vertebrate's diet

(mg/kg dry wgt.)

[Using PCB BAF_{diet-mamm} value from Fries et al. (1973)]

Set Exposure Parameters -- vole

Set Species-Specific Terrestrial Exposure Parameters

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Select a species to view (and change if necessary) the default exposure parameters used in determining the daily contaminant dose received from exposure to soil.



Food Ingestion Parame	ters	Mammaliar	n Prey Di	et —
Food ingestion rate 0.8	58 kg dw / 58 kg bw day	Fraction foliage	0	0-1
Fraction foliage	0-1	Fraction seed	0	0-1
Fraction seed	0-1	Fraction	_	
Fraction invert 0	0-1	invert	0	0-1
Fraction mammal 0	0-1	Fraction soil	0	0-1
Soil Ingestion Paramete	ers —	- Soil Inhalat	ion Para	meters —
Soil ingestion	fraction of food IR	Inhalation Rate	0.124	m^3/ day
Dermal Contact Parame	eters	Physical Po	arameter	s
	ka/	Physical Pa Body weight	arameter	s kg

Range:

East to west range is continuous from central Alaska to the Atlantic coast. South of the Canadian border, its western limit is the Rocky mountains. As far south as New Mexico and Georgia

Save Changes

Set Exposure Parameters -- shrew

Set Species-Specific Terrestrial Exposure Parameters



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Select a species to view (and change if necessary) the default exposure parameters used in determining the daily contaminant dose received from exposure to soil.





Food Ingestion Pa	rameters		Mammalia	n Prey Di	et
Food ingestion rate	0.2	kg dw / kg bw day	Fraction foliage	0	0-1
Fraction foliage	0	0-1	Fraction seed	0	0-1
Fraction seed	0	0-1	Fraction		
Fraction invert	1	0-1	invert	0	0-1
Fraction mammal	0	0-1	Fraction soil	0	0-1
Soil Ingestion Para	ameters –		- Soil Inhala	tion Para	meters
Soil ingestion	0.03	fraction of food IR	Inhalation Rate	0.065	m^3/ day
Dermal Contact Pa	arameters		- Physical P	arameter	s
Adherence Factor	000001	kg/ cm^2	Body weight	0.017	kg
A CONTRACTOR OF					

Range:

most of North America from southern Saskatchewan and Nova Scotia to central Nebraska and Georgia.

Save Changes

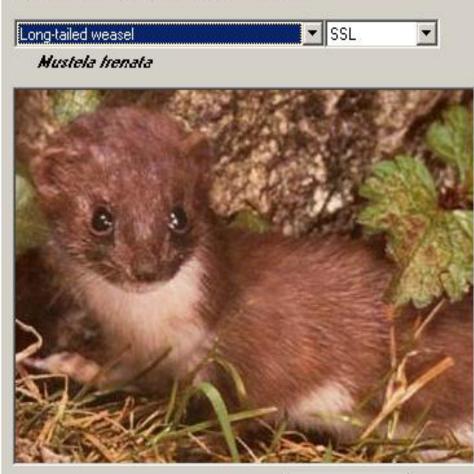
Set Exposure Parameters -- weasel

Set Species-Specific Terrestrial Exposure Parameters

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Select a species to view (and change if necessary) the default exposure parameters used in determining the daily contaminant dose received from exposure to soil.



Food Ingestion Parar	meters-		- Mammaliar	Prey Di	et
Food ingestion rate	0.1	kg dw / kg bw day	Fraction foliage	0.485	0-1
Fraction foliage	0	0-1	Fraction seed	0	0-1
Fraction seed	0	0-1	Fraction		20
Fraction invert	0	0-1	invert	0.485	0-1
2	1	0-1	Fraction soil	0.029	0-1
Soil Ingestion Param	eters —	11	- Soil Inhalat	ion Para	meters —
	0.039	fraction of food IR	Inhalation	0.456	m^3/ dav
jernen j		1000 IN	Rate	10.100	uay
Dermal Contact Para			- Physical Pa		
	meters	kg/ cm^2			

Range:

Extending from just north of the United States-Canadian border through Central America to northern South America.

Save Changes

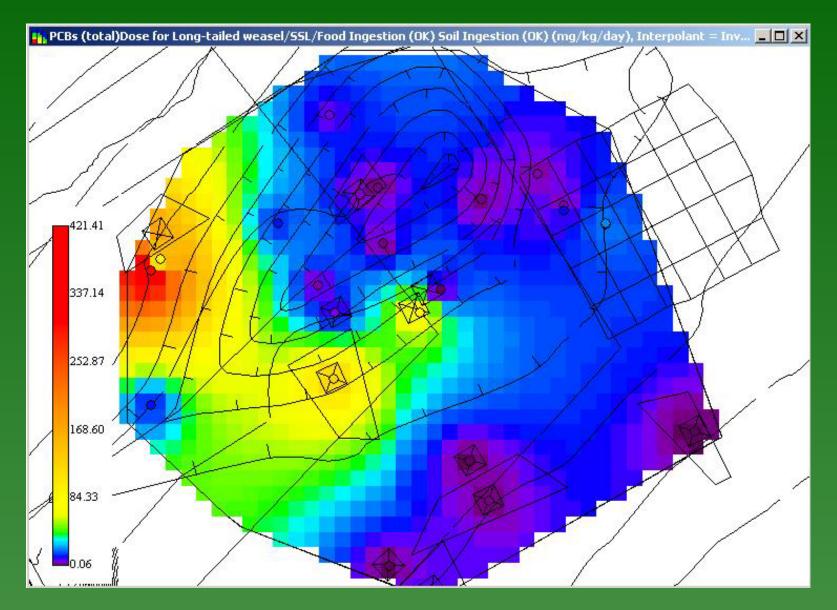
Exposure Dose Results

<mark>hSADA (C:\files\consult\sinkhol</mark> e40 ile View Graphics Maps Setup Ec	the second s	and a reaction of the second				- 8
	I MARK					
cological	▼ Soil	 Pooled Data 	(None)	•		
Pooled Data Sample Locations	and the second	Long-tailed weasel Dermal Contact Inhalation Dod Ingestion Soil Ingestion A177 0.0245 C.3966 0.0215 C.3966 0.0126 C.6972 0.1705	Total Dose	Gener	Atrol Panel	X Info Data Cov Geo Decision Sampling

Estimated Doses (mg PCBs/kg BW/d) From Exposure to Total PCBs

Receptor	Food ingestion	Soil ingestion	Total dose
Meadow vole	0.28	0.27	0.55
Short-tailed shrew	257.71	0.09	102.78
Long-tailed weasel	65.67	0.06	65.73

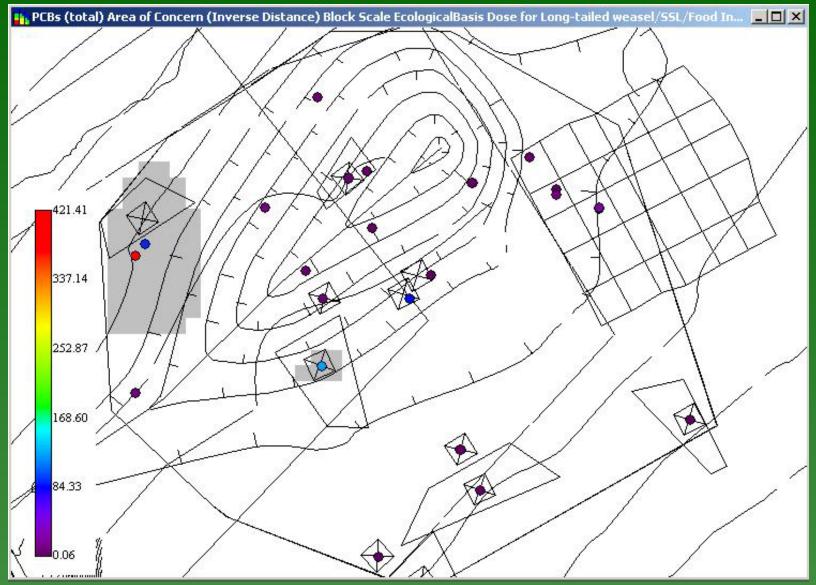
Point Dose map



At Risk?

Receptor	Total dose	NOAEL	LOAEL	NOAEL HQ	LOAEL HQ
Vole	0.55	0.051	0.51	10.8	1.1
Shrew	102.78	0.067	0.668	1534.0	153.9
Weasel	65.73	0.209	1.029	314.5	63.9

Clean Up?



Long term plans for SADA

- 1. Maintain SADA as a free software product.
- 2. Provide training and support to SADA users.
- 3. Continue development of SADA in several key areas.
- 4. Keep current functions and models up to date with latest guidance and scientific advances.
- 5. Provide annual SADA releases.
- 6. Continue exchanging ideas and components with FIELDS.

Future Plans

Maintain SADA as a free software product.

SADA is free to anyone and can be downloaded from the website.

SADA is stand alone software and requires no additional software purchases.

SADA has had over 4000 downloads to date.

Continued Development (currently)

3D Sample Design - expand current 2d and 3d sample capabilities to reflect more realistic 3d sampling scenarios in both initial and secondary designs.

Risk Assessment - add human health risk updates as well as expand ecological modeling functions.

Geospatial Characterization Advances - improve key geostatistical functions that serve as the basis for many SADA models.

Visualization and GIS - improve and add new features to SADA's current 2d and 3d visualization functions.

Statistical Analysis - broaden SADA's repetoire of statistical functions including nonparametric methods, hypothesis testing, etc.

FIELDS Compatability - Continue sharing developed modules with FIELDS.