

Spatial Analysis and Decision Assistance (SADA) Version 4 Introduction & Schedule (1 day)

Environmental Assessment Methods in SADA
University of Tennessee



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Introductions:

- Participant introductions
 - Name, where from
 - Environmental assessment background
 - Goal, or reason, for taking the SADA course
 - Experience with SADA?



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Schedule (Part 1)

- 8:00 - 8:30 Introductions, Training Overview
- 8:30-9:30 Create SADA File
- 9:30-10:30 Initial Sample Designs
- 10:30-10:45 Break
- 10:45-11:30 Importing Data Into SADA
- 11:30-12:00 Exploration Tools/Statistics
- 12:00-1:00 Lunch
- 1:00-1:45 Human Health/Ecological Risk
- 1:45-2:00 Custom Analysis
- 2:00-2:15 Break
- 2:15-2:45 Basic Spatial Analysis
- 2:45-3:15 Advanced Spatial Analysis
- 3:15-3:45 Decision Analysis
- 3:45-4:15 Secondary Sampling Designs
- 4:15-4:45 3d Visualization
- 4:45-5:00 Wrapup

SADA[™]
Spatial Analysis and Decision Assistance

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Spatial Analysis and Decision Assistance (SADA) Version 4 Overview

Environmental Assessment Methods in SADA
University of Tennessee, Knoxville

username = Student

password = sady

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SADA General Information

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

- Visualization/GIS
- Statistical Analysis
- Geospatial Interpolation
- Geospatial Uncertainty Analysis
- Human Health Risk Assessment
- Ecological Risk Assessment
- Custom Analysis
- MARSSIM Module
- Area of Concern Frameworks
- Cost Benefit Analysis
- Sampling Designs
- Export to Arcview/Earthvision

SADA has been supported by DOE, EPA, and the NRC. SADA Version 3.0 had about 11000 downloads. Version 4.0/4.1 has had 8000+ since January, 2005.

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SADA General Information (cont.)

Free stand-alone package for Windows 98, 98SE, NT SP4 or higher, 2000, ME, and XP.

Contact information, updates, documentation, and downloads are available on-line at <http://www.tiem.utk.edu/~sada/Student/index.shtml>

A SADA user's group, email, annual conferences, and on-site training.

A substantial help file is included.

Conduct "black and white box" testing internally as well as an external beta release period.

Publish verification document on the website.

username = student
password = sada
sada users group.

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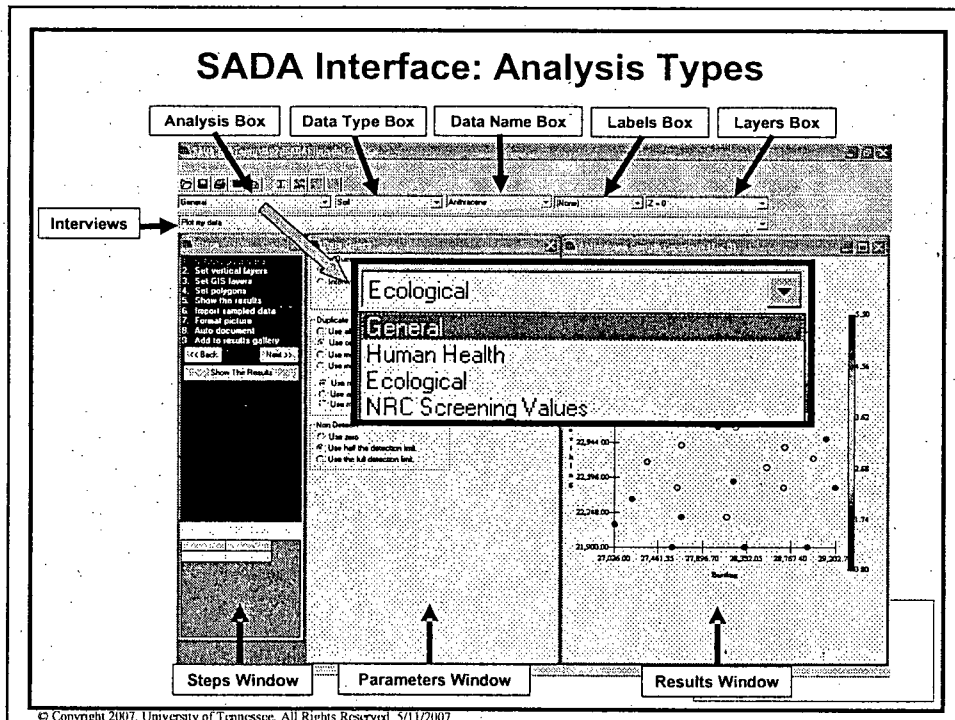
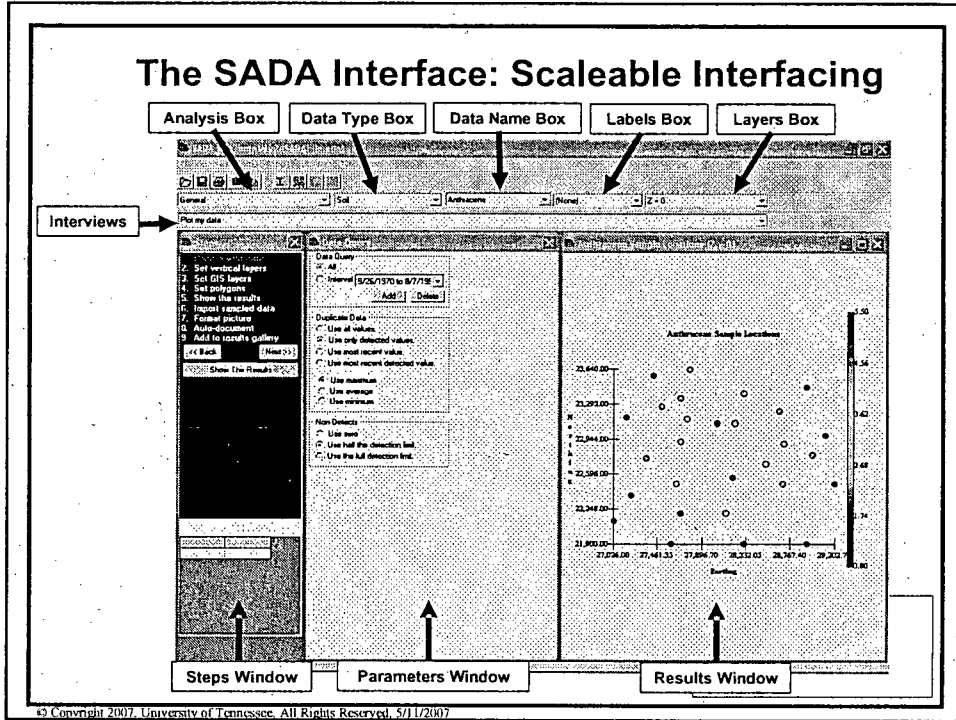
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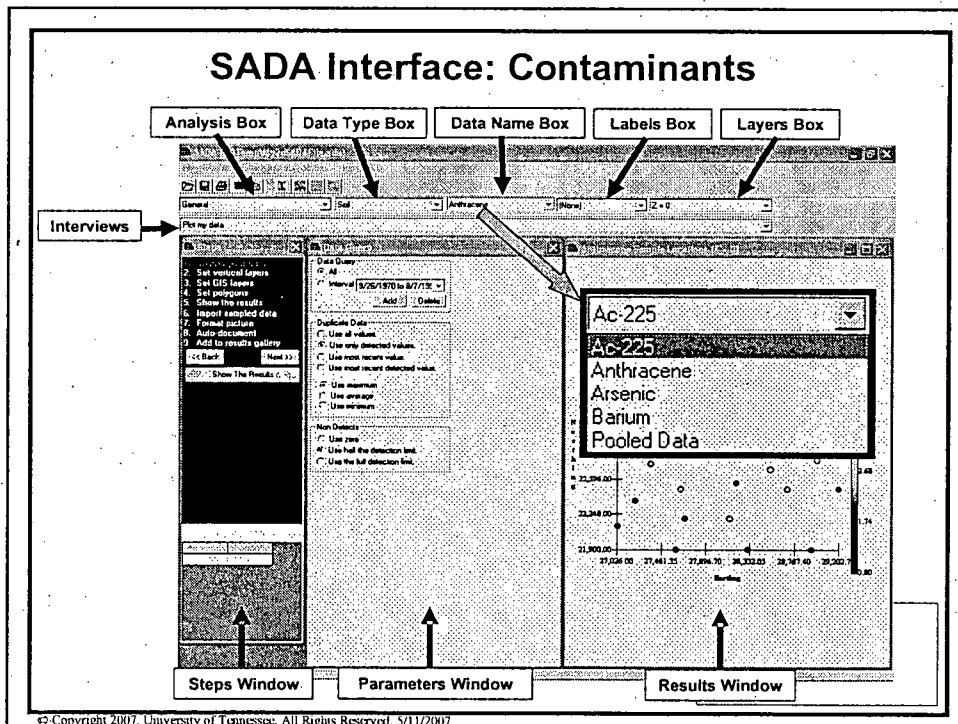
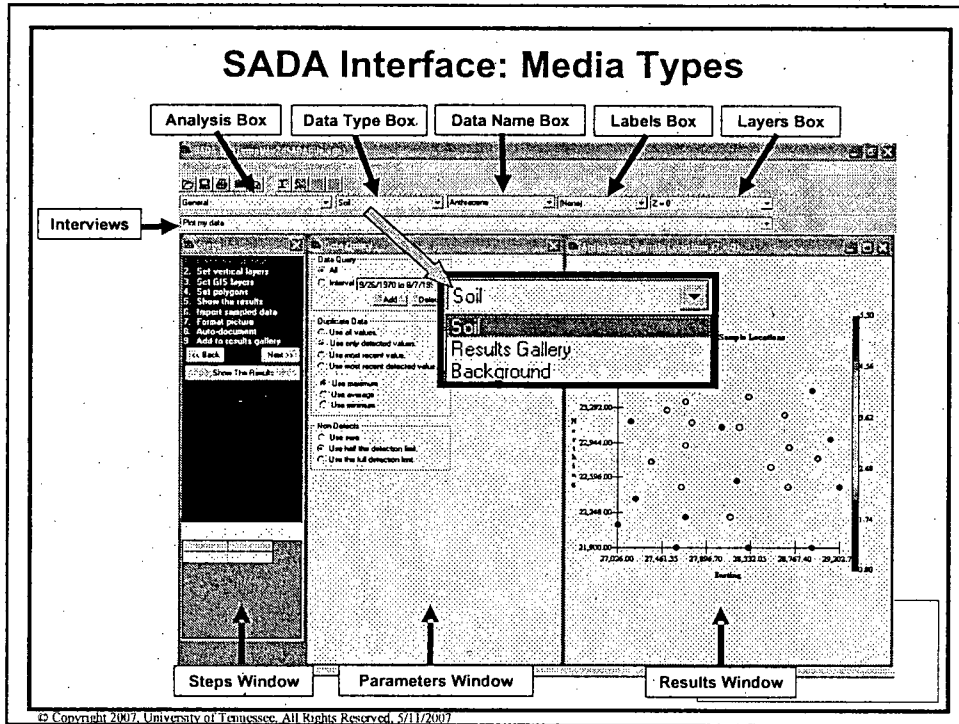
Accomplishments In Version 4

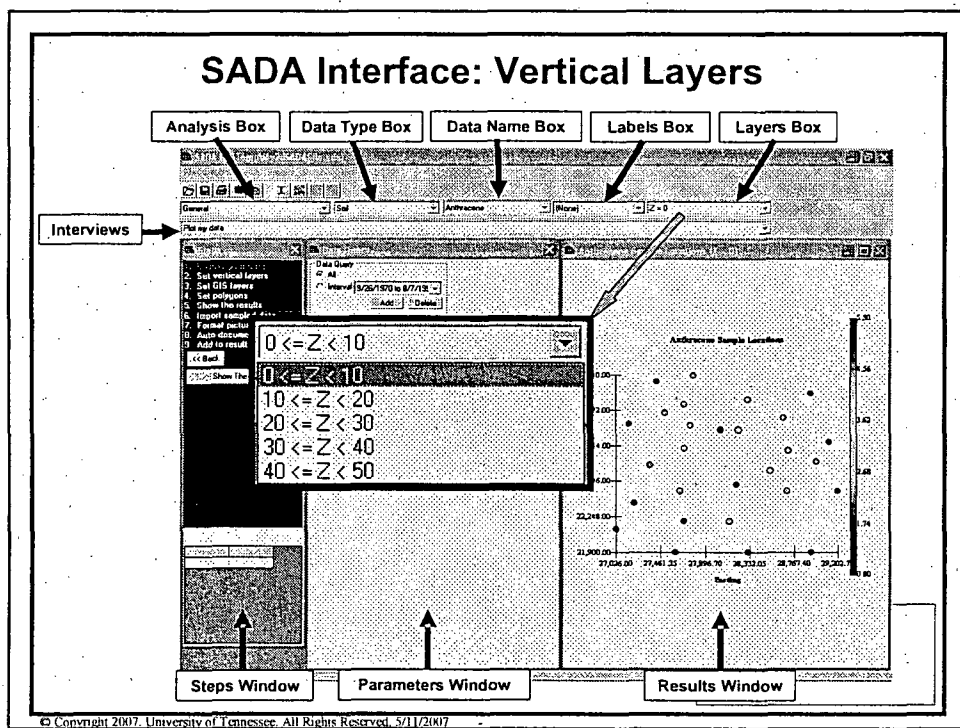
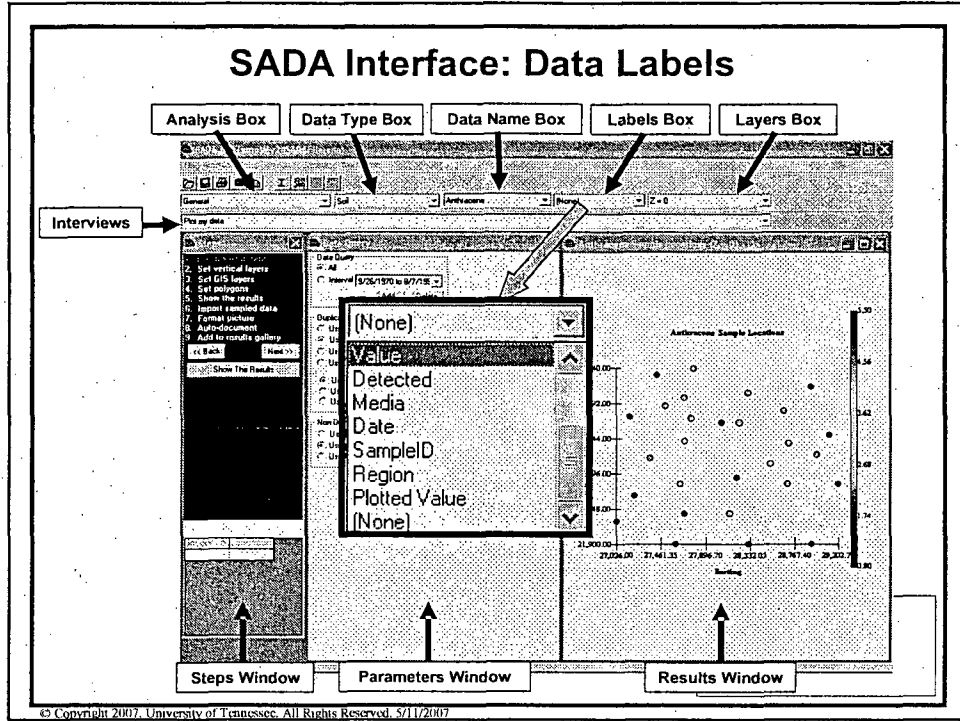
- A More Friendly Interface with Interviews and Process Steps/Reduced User Fatigue
- Initial Sample Design Strategies
- Additional Secondary Sampling Strategies
- Geobayesian Modeling
- New Polygon Tools (circle, square, multiple polygons, 3d slicing)
- Better Vertical Layering Framework
- Improved 3D Viewer
- MARSSIM Module
- Empty SADA Files
- Improved Statistics
- Improved Correlation Modeling
- Results Gallery
- ESRI Shape File Import
- Export to ESRI and EarthVision

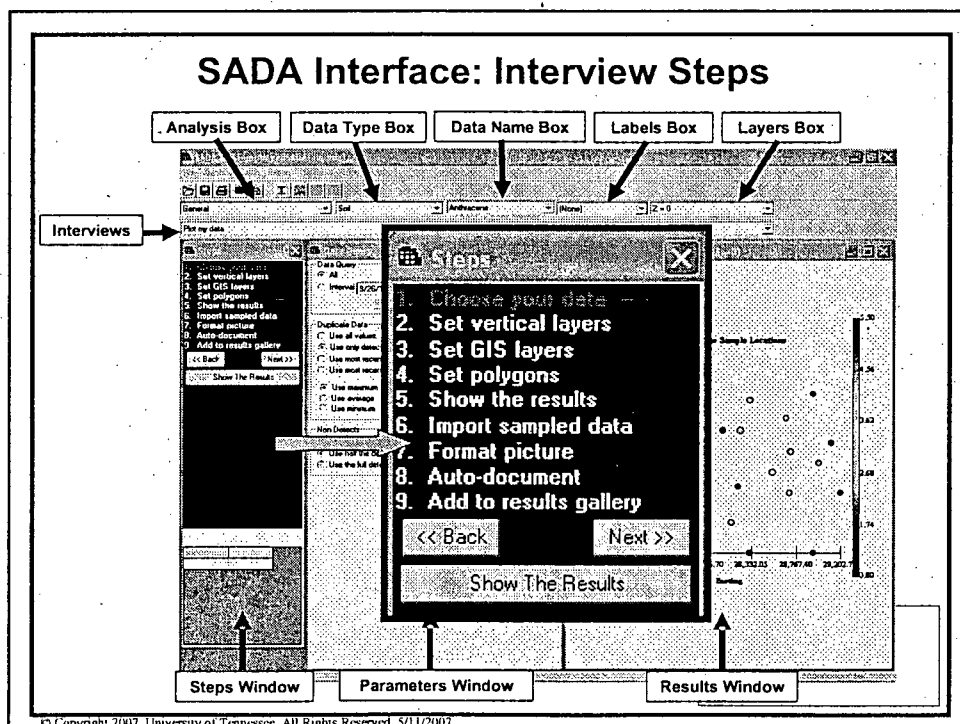
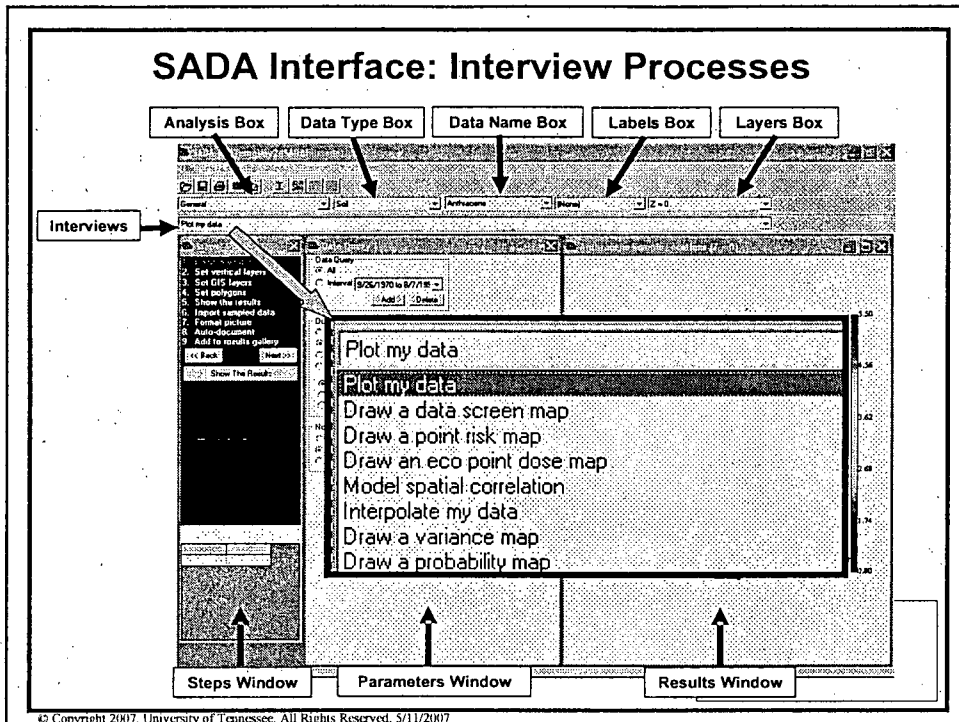
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SADA Interface: Input Parameters

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SADA Interface: GIS Display

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What exactly can you do in SADA?

- | | |
|---|--|
| <ul style="list-style-type: none"> Create initial sample designs Import data Plot data Import GIS layers Aggregate sections of the site Calculate statistics (univariate) Model spatial correlation Create contour maps Create a kriging variance map Perform traditional HH and Eco risk assessments (tabular risk, screens, prgs, benchmarks) Create a HH or Eco contoured risk map Create a HH or Eco point risk map Create a data screen map for HH, Eco, Custom Create an eco point dose map Create an contoured eco dose map | <ul style="list-style-type: none"> Create probability maps Define areas of concern Calculate cost vs cleanup Draw a LISA Map Develop secondary sample designs Perform a MARSSIM data analysis Detect and Define MARSSIM elevated area Visualize results in 3d Autodocument results Create a geobayesian site conceptual model Draw area of concern maps based on conceptual model Calculate cost vs cleanup based on conceptual model Update the site conceptual model Export to ESRI or Earthvision or common window applications |
|---|--|

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Sample Laboratory Data

PROJECT NAME	PROJECT #	SAMPLE I	SAMPLE ID	DATE COLL.	DATE RECD	ANALYZED AT	LAB #	ANALYTE	RESULT	POI	UNITS	METHOD
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	Alethin	< 0.00005	5E-05	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	a-BHC	< 0.00005	5E-05	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	4-BHC	< 0.00005	5E-05	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	4-BHC	< 0.00005	5E-05	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	g-BHC, Lindane	< 0.00005	5E-05	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	4,4'-DDD	< 0.00010	0.0001	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	4,4'-DDE	< 0.00010	0.0001	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	4,4'-DDT	< 0.00010	0.0001	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	Dieldrin	< 0.00010	0.0001	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	Endosulfan I	< 0.00005	5E-05	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	Endosulfan II	< 0.00010	0.0001	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	Endosulfan Sulfate	< 0.00010	0.0001	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	Endrin	< 0.00010	0.0001	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	Endrin Aldehyde	< 0.00010	0.0001	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	Endrin Ketone	< 0.00010	0.0001	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	Heptachlor	< 0.00005	5E-05	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	Heptachlor Epoxide	< 0.00005	5E-05	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	Methoxychlor	< 0.00010	0.0001	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	Toxaphene	< 0.00500	0.005	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	alpha-Chlordane	< 0.00005	5E-05	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/7/2002	02-A162603	gamma-Chlordane	< 0.00005	5E-05	mg/l	8081A
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/6/2002	02-A162603	Aroclor 1016	< 0.00050	0.0005	mg/l	8082
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/6/2002	02-A162603	Aroclor 1221	< 0.00100	0.001	mg/l	8082
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/6/2002	02-A162603	Aroclor 1232	< 0.00050	0.0005	mg/l	8082
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/6/2002	02-A162603	Aroclor 1242	< 0.00050	0.0005	mg/l	8082
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/6/2002	02-A162603	Aroclor 1248	< 0.00050	0.0005	mg/l	8082
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/6/2002	02-A162603	Aroclor 1254	< 0.00050	0.0005	mg/l	8082
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/6/2002	02-A162603	Aroclor 1260	< 0.00050	0.0005	mg/l	8082
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/6/2002	02-A162603	Aroclor 1260	< 0.00050	0.0005	mg/l	8082
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/5/2002	02-A162603	Banum	< 0.0050	0.005	mg/l	8010B
400-640 SINKHOLE	4969 013	BW/JQ	HSSW1	10/1/2002	10/3/2002	10/5/2002	02-A162603	Banum	< 0.0050	0.005	mg/l	8010B

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Data Formats

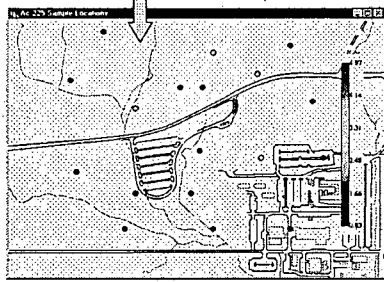
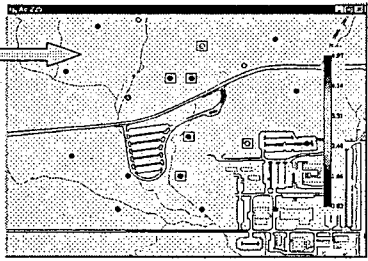
- SADA can accept data in two formats: comma delimited files (csv) and Microsoft Access.
- SADA requires the presence of certain fields in the data set.
 - Easting
 - Northing
 - Depth
 - Value
 - Name
- SADA can use other forms of information as well
 - Media
 - Detection
 - Date
 - CAS Number
- Any other form of meta data can be imported as well. User can plot and retrieve this meta data during an analysis.
- SADA recognizes soil, sediment, surfacewater, groundwater, air, biota, and background, and the "basic" media type. Basic is assigned to data that have no media type.

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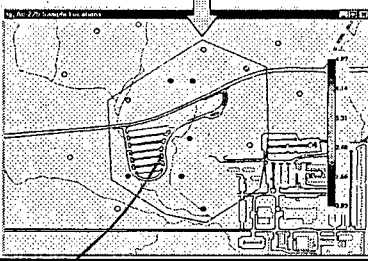
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Data Exploration

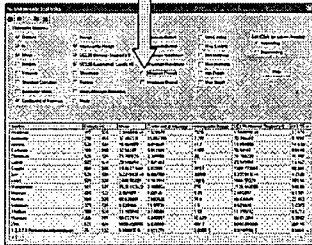
Data Plot/GIS Overlays Spatial Data Screens

Polygon Selection/Cutaways



Statistics

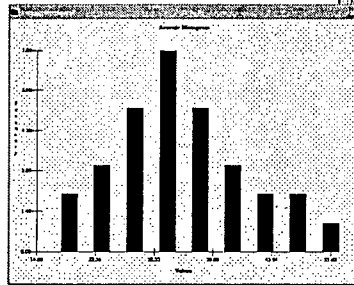


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Analysis inside boundary

Statistics

- Numerous univariate statistics
- Non-parametric hypothesis testing
- Power curve based sample sizes
- Histogram and cdf



Univariate Statistics

Variable	Median	Mean	Coefficient of Variance	Interquartile Range	1st.25 Percentile	Skewness	Kurtosis
Aluminum	437	524	1.544896	11,32373	7970	1.544896	-1.2471
Arsenic	218	414	27.407371	10,807366	3.275	70.346028	5.2894
Cadmium	524	524	18.894829	0.819547	11.7	18.894829	14.823
Copper	524	518	32.54157	0.811541	0.005	72.111	13.519
Lead	524	524	74.702229	2.342259	0.005	0.005	0.005
Nickel	524	524	23.542294	2.8771852	0.005	0.005	0.005
Selenium	524	524	1.02877264	16.822618	0.005	0.005	0.005
Vanadium	524	524	2.271316	0.005	0.005	0.005	0.005
Zinc	524	524	2.271316	0.005	0.005	0.005	0.005

High Test Sample Size and Power

Univariate Statistics

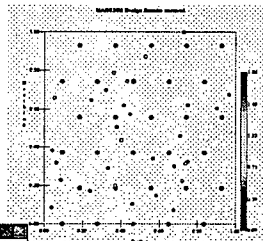
One-Sided Sign Test

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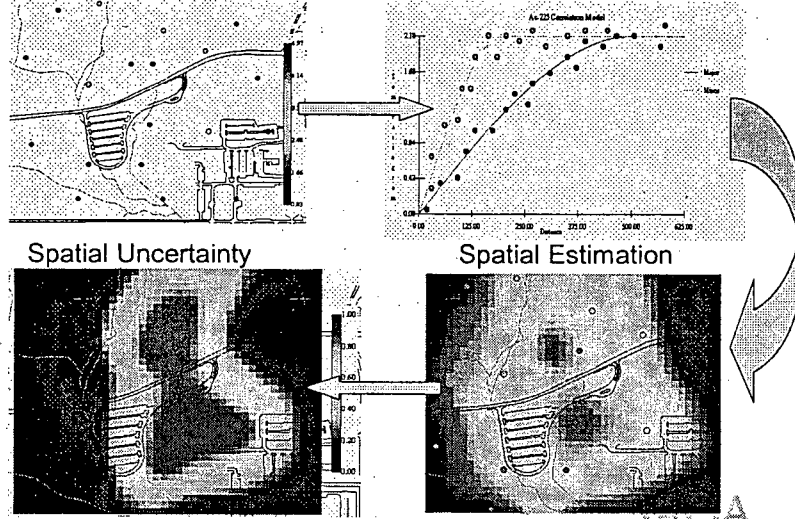
MARSSIM Functionality

- Calculate sample size based on Sign Test and WRS Test
- Develop initial sample design incorporating DCGLS, Area Factors, Instrument sensitivity
- Post sampling analysis (A site passes or fails)
- Detecting and Defining Elevated Areas



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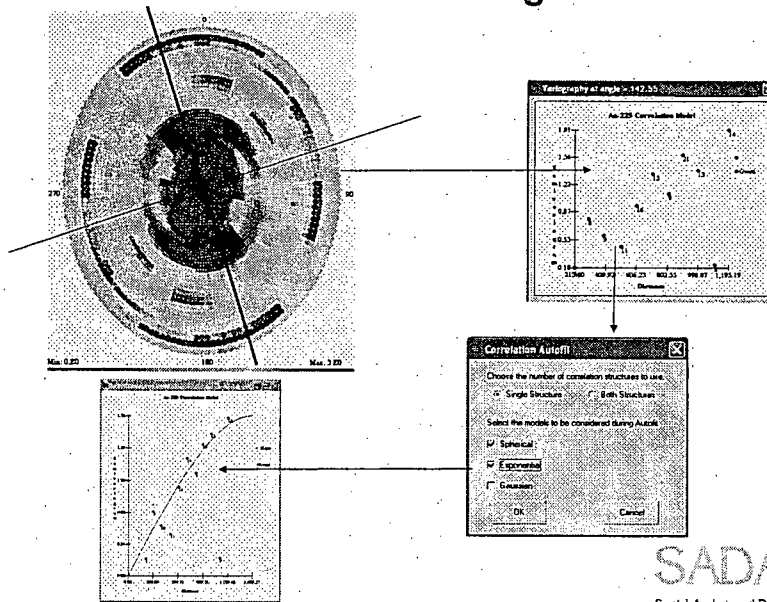
Spatial Analysis



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Correlation Modeling Tools



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Human Health and Ecological Risk

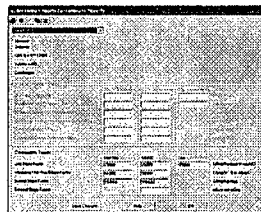
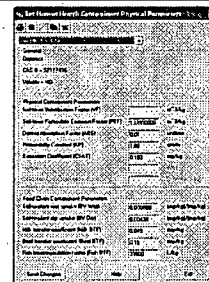
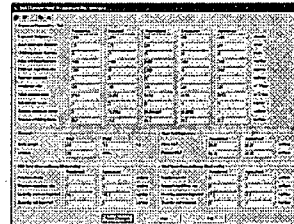
- SADA implements EPA methods for conducting ecological and human health risk assessments
- Calculation of site-specific preliminary remediation goals
- Benchmark database for contaminant effects on ecological receptors
- Exposure modeling for humans and over 20 other terrestrial species
- Contains IRIS/HEAST toxicity databases for calculating risk from exposure
- Contains EPA default exposure parameters for the risk models
- Tabular screening and risk results
- Point screens
- Risk and dose mapping

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Human Health Risk Calculations

- For each media
 - Soil, Sediment, Surface Water, Groundwater
- Exposure Scenarios
 - Residential, Industrial, Recreational, Agricultural, Excavation
- Exposure Pathways
 - Ingestion, Inhalation, Dermal Contact, Food Chain (Beef, Milk, and Vegetable Ingestion)
- IRIS and HEAST Toxicity Databases for Carcinogenic and Noncarcinogenic Effects
- Physical Parameters for Modeling
 - Bioaccumulation Factors
 - Volatilization, Particulate Emission Factors
 - Permeability Constants, Absorption Factors
 - Saturation Coefficients, Radionuclide Half-Lives



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Human Health Risk

- PRG Calculation
- PRG Screens
- Human Health Risk

Risk Based Screening Goals: Target risk = 0.0001...

Pathway:
 Ingestion Dermal Fish Beef All
 Inhalation External Vegetables Dairy

Rads and Nonrads/Soil/Residential/Carcinogenic

Name	CAS	Ingestion	Inhalation	External	All
Ac-226	14265651	5.6E+2	1.5E+5	5.6E+2	
Arsenic, Incl	7440382	4.3E+1	7.4E+4	4.3E+1	

Human Health Risk Results

Pathway:
 Ingestion Dermal Fish Beef All
 Inhalation External Vegetables Dairy

Rads and Nonrads/Soil/Residential/Carcinogenic

Name	CAS	Ingestion	Inhalation	External	All
Ac-226	14265651	5.6E-7	2.1E-9	5.6E-7	1.1E-6
Arsenic, Incl	7440382	1.8E-5	1.1E-9	1.8E-5	1.8E-5
Total		1.8E-5	1.2E-9	5.6E-7	1.9E-5

Screening Results: Target risk = 0.0001/Target ...

Pathway:
 Ingestion Dermal Fish Beef All
 Inhalation External Vegetables Dairy

Rads and Nonrads/Soil/Residential/Carcinogenic

Name	CAS	Ingestion	Vegetables	All
Ac-226	14265651	Yes	Yes	
Arsenic, Incl	7440382	Yes	Yes	

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Spatial Implementation of Risk Assessment

- Conventional Risk Assessment Limitations
 - Typically regulatory exposure assessment guidance recommends a summary statistic for the exposure concentration
 - Spatial information is lost when a summary statistic is used in the RA-exposure is assumed to be continuous in space and time
 - Often this lost info not recovered in the rest of the remediation process
- Reasons for incorporating spatial statistics into risk assessment
 - Maximize the use of limited resources
 - Efficiently collect data
 - Retain collected spatial info in the risk assessment
 - Use all types of available data, including expert judgment
 - To more adequately characterize the exposure distribution
 - Extrapolate from known data to cover data gaps
 - Account for spatial processes related to exposure
 - Better understand uncertainties in the exposure assessment

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Ecological Dose Exposures

- SADA calculates dose (mg/kg BW d) from food ingestion, soil ingestion, dermal contact, and inhalation for terrestrial exposures
- SSL, Female, Male, or Juvenile
- Over 20 different species



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Custom Criteria

- View or Edit Criteria
- Data Screens

Viewing Example Custom Analysis values

Analysis	Caesium	Regional Lvl	State Level	Background
Ac-225	14265851	3	35	24
Arsenic	7440382	121	57	12
Barium	7440383	80	90	20

Custom Analysis

Caesium	Arsenic	Regional Lvl	State Level	Background
14265851	Ac-225	Yes	Yes	Yes
7440383	Barium	Yes	Yes	Yes
7440382	Arsenic	Yes		Yes

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Decision Analysis

- Spatial Screens
- Sampling Strategies

- Spatial Risk
- Area of Concern
- Cost Benefit

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3D Visualization

True 3d Views: Points, Blocks, and Isosurfaces

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Visual Sample Plan

VSP - Initial Sample Design determine # of samples

Sample Designs

SADA has a number of sample design strategies in Version 4.0. These strategies include initial and secondary designs. Some are based on data alone while others are based on modeling results. With the exception of a couple of exclusively 2d designs all are available in 3d dimensions.

Initial Sample Designs

- Judgmental
- Simple Random
- Simple Grid
- Simple Unaligned Grid
- Standard Grid
- Standard Unaligned Grid
- MARSSIM Design
- 2d and 3d Hot Spot search designs

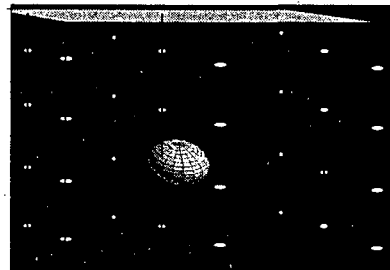
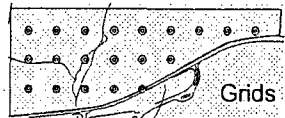
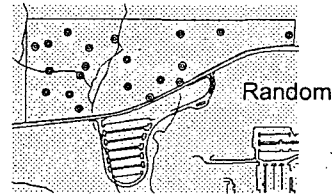
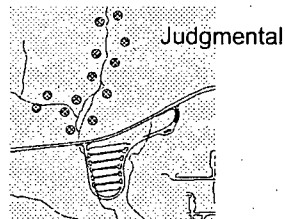
Secondary Sample Designs

- Threshold Radial
- Adaptive Fill
- High Value
 - (soft, simulated & unsimulated)
- High Variance
 - (soft, simulated & unsimulated)
- Extreme Value
 - (soft, simulated & unsimulated)
- Area of Concern Boundary Design
 - (soft, simulated & unsimulated)
- Minimize/Maximize Area of Concern
- LISA Designs
 - (Ripley's K, Moran's I, Geary's C)

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Some Example Initial Designs

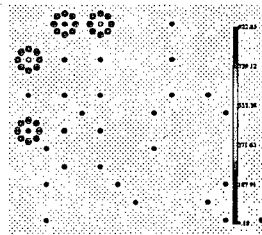


3d hotspotTM
search
Spatial Analysis and Decision Assistance

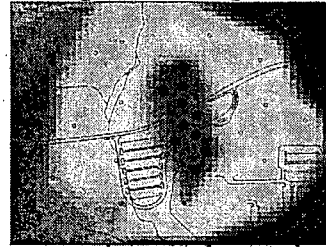
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Some Example Secondary Designs

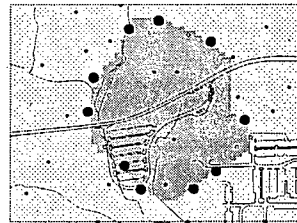
Threshold Radial



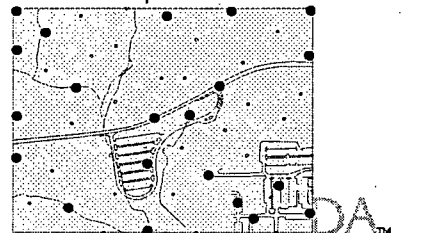
High Value Design



AOC Boundary Design



Adaptive Fill



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SADA Overview: Autodocumentation

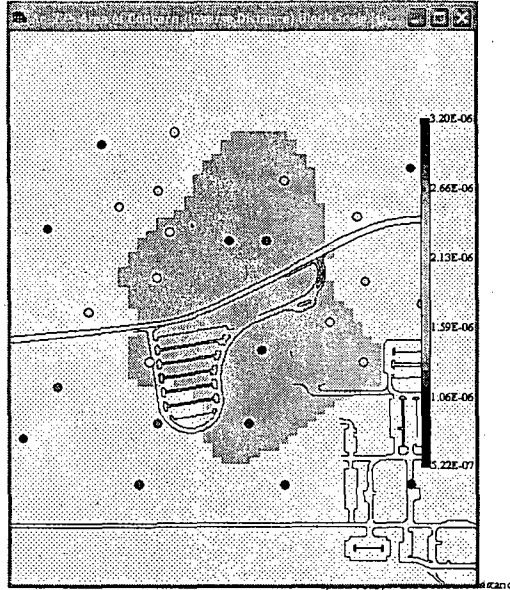
- Provides transparency in the modeling process and facilitates reproducibility of results.
- SADA automatically analyzes any current result and determines what the "ingredients" of that result are. These ingredients are presented to the user, who can choose the level of documentation to create.
- Self-documentation of all parameters, models, and other relevant information.
 - Exposure concentrations
 - Risk models
 - Exposure variables
 - Geospatial parameters
 - Toxicity data
 - Images as bitmaps
- HTML format, can be exported to popular word processors

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SADA Overview: Autodocumentation

- Area of concern map
- Based on HH Risk
- Utilized inverse distance as geospatial model
- Block based area of concern framework.



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SADA Overview: Autodocumentation

Step

1. Choose your data
2. Set vertical layers
3. Set GIS layers
4. Set polygons
5. Set grid specs
6. Interpolation method
7. Search neighborhood
8. Specify decision criteria
9. Show the results
10. Cross validation
11. Format picture
12. Auto-documentation
13. Add to results gallery

« Back Next »

Show The Results

Report Wizard

Auto Documentation

Active Report
Name: test

Change Active Report

Current Information to Add to the Report

- Picture
- GIS Files
- Data Files
- Layering Design
- Grid Dimensions
- Geospatial Parameters
- Geospatial Framework
- Decision Framework
- Human Health Risk Model
- Decision Criteria
- Decision Criteria
- ASCII Results
- Media Data

Layer

Layer Extents

Min Z: 0

Max Z: 10

Grid Information

Dir	Start	Size	Num
East	26900	46.055	50
North	21900	34.8	50

Spatial Parameters

Name	Value
Major Search Radius	1151.375
Minor Search Radius	1151.375
Vertical Search Radius	1
Horizontal Angle	0
Vertical Angle	0
Rotation Angle	0
Min Number of Data Values	2
Max Number of Data Values	20

Step

Analysis of Model Elements

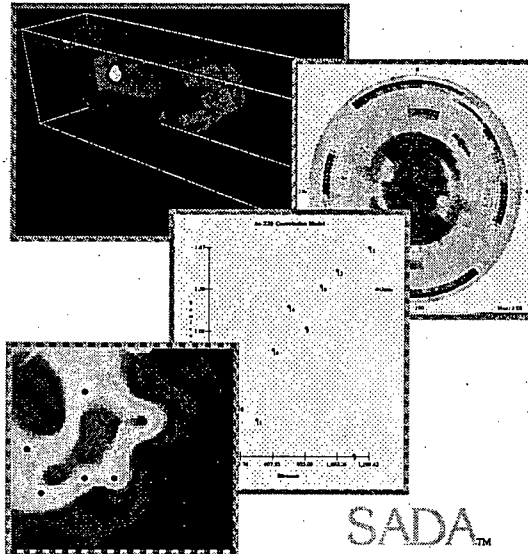
Documentation Output

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Results Gallery

- Users can now save "static" results to the results gallery
- Users can view them, format them, and change various viewing properties
- Prevents users from having to regenerate a picture each time they want to see it
- Version 5.0 will allow dynamic results to be saved for further modeling

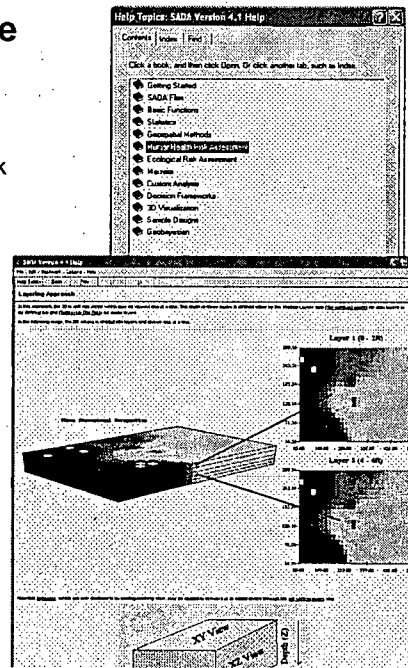
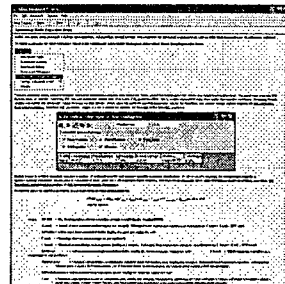


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Comprehensive Help File

- 14 MB help file
- Close to 400 different help file topics
- Number of external links for benchmark sources, etc.
- Help file topics online:
<http://www.tiem.utk.edu/~sada/helpv4/>
- Context-sensitive help on all forms and functions in SADA (press F1 or Help button)



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Goals of Training

- Know how to “get around” in SADA.
 - How is the interface organized?
 - What are all those buttons for?
 - How do I switch between contaminants?
 - Learn about auto-documentation
 - Why are some things disabled at times and available at other times?
 - How do I get information out of SADA?
- Be able to import data into a SADA file.
- Be able to perform a geospatial analysis.
- Use the decision analysis and cost benefit frameworks.
- Understand and use the sample design strategies.
- Setup and perform human health, ecological, and custom analysis.
- Integrate human health, ecological, and custom analysis with geospatial analysis, decision frameworks, and sample design.

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Training Format

We will divide training sessions into two components:

“Follow the leader”

Proceed through each section of SADA from front to back with an example data set. At each major point we'll provide some background information, show you how to use the tool, and then give you a chance to check it out for yourself.

Practice Session

Provide a second example data set for you to work through from scratch.

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Questions?

Comments?

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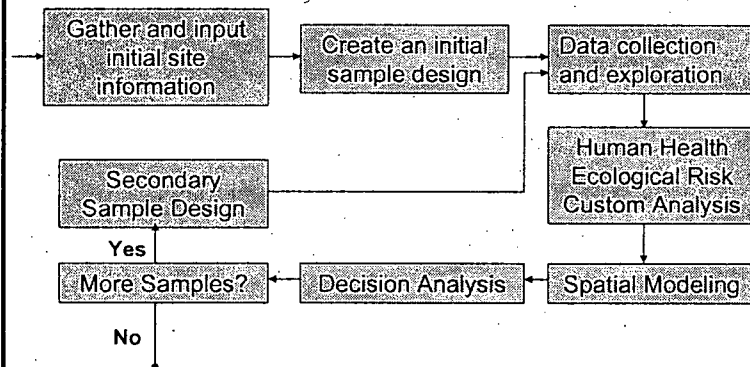
Spatial Analysis and Decision Assistance (SADA) Version 4 Create SADA File

Environmental Assessment Methods in SADA
University of Tennessee, Knoxville



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General Flow of SADA (and the Training Course)



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Empty SADA Files

An empty SADA file contains no sampled data values. It is created for the purpose of laying out a site and deriving an initial sample design.

With an empty SADA file you can set horizontal and vertical extents of your site.

You can overlay the site with ArcGIS Shape Files (.shp) or Data eXchange Files (.dxf).

You can refine the boundaries of your site with the polygon tools.

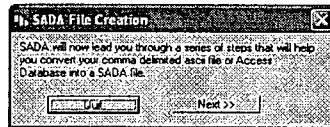
You can develop an initial sample design that can be exported and submitted to the sampling team.

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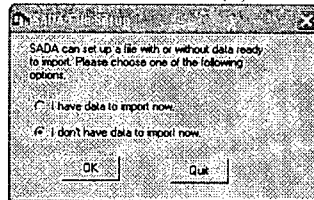
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SADA File Setup

To begin the creation sequence, open SADA, select File, and from the menu bar choose New. The following window will appear.



Press Next >> to continue. The following window will appear.



Select the second option and press OK. (We'll see how to create SADA files when you have data later.)

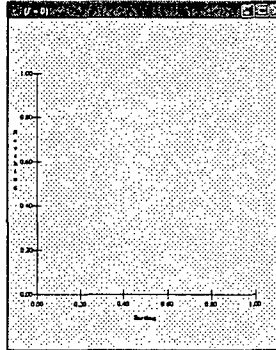
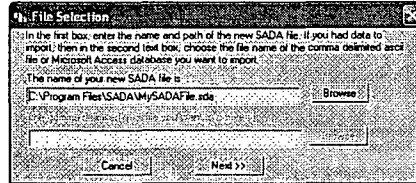
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Create an Empty SADA File

At the file selection window, enter the name of the SADA File. (*Note: the second line is disabled since there is no data to import.*)

Then press **Next >>**, and SADA will open a blank graphics window.



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GIS Layers

SADA permits users to incorporate Geographic Information System (GIS) layers. GIS tools dynamically map and permit spatial queries to visualize and summarize various features about their area of interest. Larger commercial GIS systems include

- ESRI's ArcGis
- MapInfo
- AutoCad

GIS layers are mapped objects with a common theme. For example, one layer may show all roads and another may show all buildings. Users can control which layers are turned on and what color they are drawn with.

SADA can import Shape files and Data Exchange Formats (.shp, dxf). Data exchange formats (DXFs) are the text files of GIS systems. Originally developed by AutoCad, most GIS systems can export to DXF format. Shape files are generated by ARCGIS.

SADA does not allow users to edit or query the GIS layers within SADA. They serve strictly as maps to provide reference. Work in improving this area is ongoing.

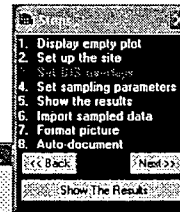
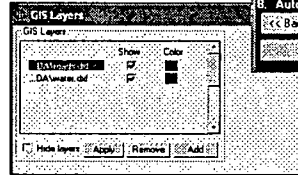
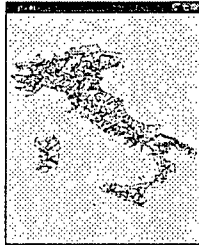
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Import GIS Overlays

To add an overlay to your data or modeling results, select **Set GIS Overlays** from the **Steps Window**. The **GIS Layers** box will appear in the **Parameters Window**.

Select **Add** to add a layer. SADA can import Data eXchange Format (.dxf) or Arc View Shape (.shp) files. To make a layer visible, check the box next to the name under the **Show** column. To change the layer color, click the corresponding **Color** box and choose a color from the palette window.



To view your changes, press the **Apply** button. To turn off the GIS overlay system, click in the box next to **Hide Layers**.

Note that if your GIS layer does not cover the current extent of your site, SADA will warn you. If you choose to continue, SADA will give you the option of using the extent of the layer as your site extents.



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Zooming, Shifting, Restoring

Zooming In

Click the **Zoom In** button to magnify the site. Using the left mouse button, select the region to zoom in on. Releasing the mouse button produces the zoom.

Zooming Out

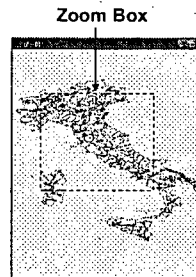
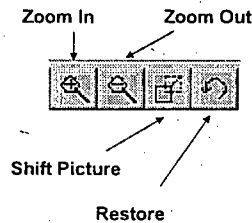
Click the **Zoom Out** button to reduce the magnification. Select the zoom area with the mouse, and the portion of the image that is visible is placed in the zoom box to cause the zoom out effect.

Shifting

Click **Shift Picture** to shift the view. After selecting this option, click your mouse at any point in the picture and pull the mouse in the direction you wish to move the image. A line will appear demonstrating how far the picture will move. Release the mouse button and the picture will redraw.

Restoring

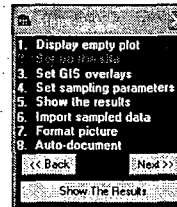
Click the **Restore** button to return the picture to its original scaling and position.



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Adjust Area Boundaries

When an empty SADA file is created, SADA sets default min and max values for easting, northing. To adjust these boundaries, select **Setup the Site** on the **Steps Window**. The site boundary frame allows one to determine the boundaries of the site.

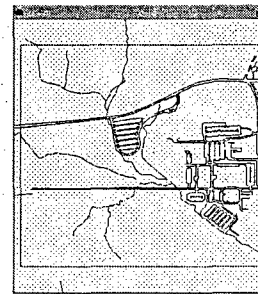


Manually enter values and click the **Apply** button or click the **Draw** button and use the mouse to select an area on the graphics map. All data points outside of the boundary will be eliminated from future analyses.

Site Boundary

	Minimum	Maximum	Apply
Easting	0	1	Draw
Northing	0	1	Snap

The site boundary is always denoted by a brown box on the GIS map.

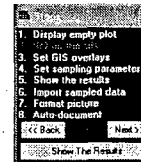


Note: If GIS layers were imported, SADA will ask the user if boundaries should be adjusted to incorporate the layers during their import. These boundaries may then be further adjusted.

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Set Vertical Layers

Select the **Setup the site** step from the **Steps window**. The second frame is the **Set Vertical Layers** frame.



In the middle of the **Parameters window**, the vertical layers dropdown list contains all available Layer designs. Use the drop-down menu to select a design from the list. The definition of each layer in the current layer design will then be visible in the box below.

Set Vertical Layers

All Add

Layers (Double click to edit) Delete

0-0 (Active with no polygons)

Interpolate and Place New Samples

At the top In the middle

To add a layer design, press the **Add** button. In the next window, enter a name for the new Layering design. (The new layering design can be based on a previously developed layering design, the default, or a new design.) Press **Create**.

Create New

Name of the New Layering Scheme

test layer

Based On

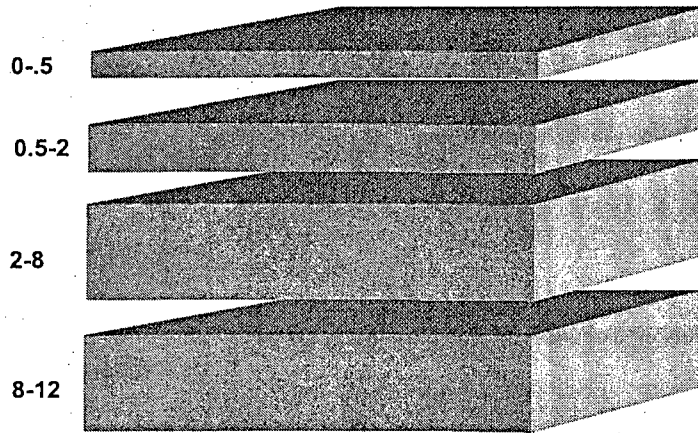
New Layer Design

Create Cancel

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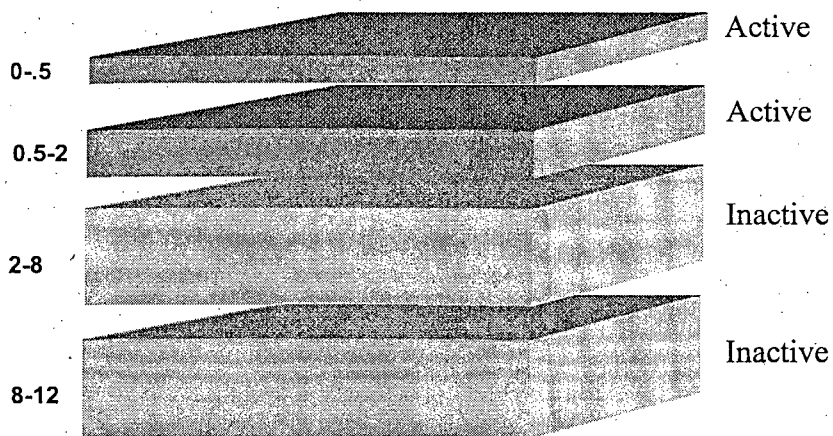
Vertical Layers: Dividing the Subsurface



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Vertical Layers: Dividing the Subsurface



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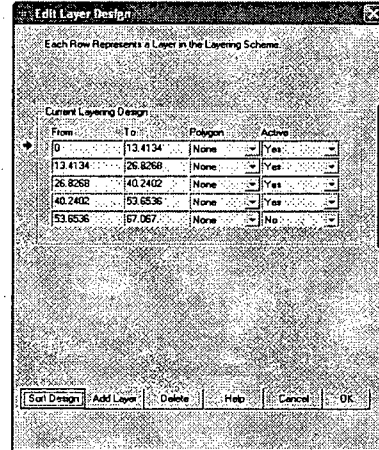
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Set Vertical Layers

Enter values in the **From** and **To** columns to define each layer depth. Press **Add Layer** to add a blank layer to the layer scheme. If polygons have already been created, select the applicable polygon layer to display in each vertical layer. If you would like the data included in a layer to be used when creating a Geospatial Model, select **Yes** for the interpolation option (default). To exclude a layer from a Geospatial Model, set this option to **No**.

Note: All layers must be contiguous and non overlapping. A layer can be a single value.

To delete a layer, select that layer and press **Delete**. To sort the layers by depth, press **Sort Design**. To cancel the layering scheme, press **Cancel**. Otherwise, once all the layers are entered, press **OK**.

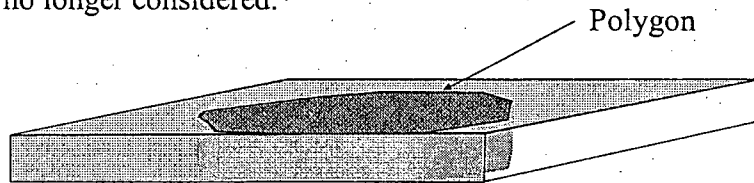


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Subsetting the site: Polygons

Polygons allow you to zero in on sub areas of interest or to better refine your site boundary when you have irregular boundary lines. Anything inside a polygon is included in the analysis. Everything outside the polygon is no longer considered.*



* The exception is geospatial modeling which gives the user the option to allow points outside the polygon to influence modeling inside the polygon

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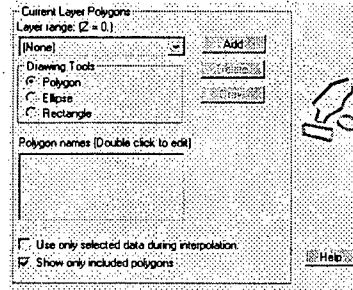
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Create Polygons

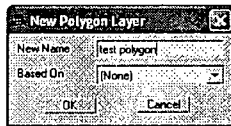
SADA allows users to subset an area or define a specific space by enclosing it in a polygon.

To create a polygon, select **Setup the Site** on the **Steps Window**. The user can create and modify polygon designs in the **Current Layers Polygon Frame**.

Polygon layers will appear in the **Parameters Window**. Click **Add** to create a new polygon collection or **Draw** to modify an existing collection.



Enter the name for the new polygon collection and select, if applicable, what prior collection to base them on.



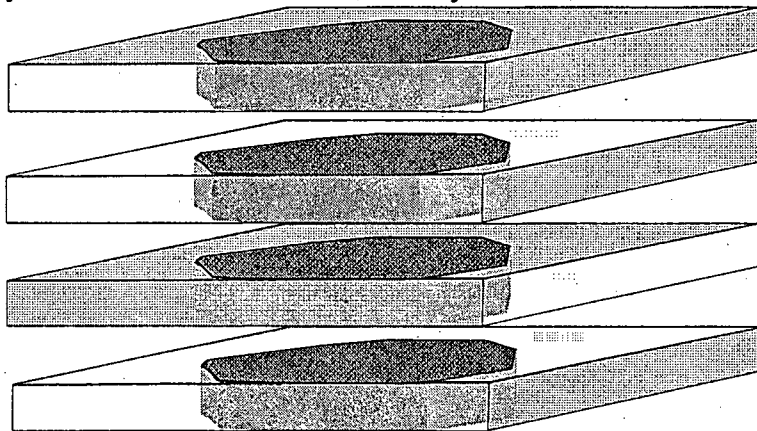
Select that collection in the **Parameters** window and press **Draw**. Use the activated polygon buttons on the main toolbar to create polygons for this collection. After all polygons have been created, select **Done**.

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Cookie Cutter Polygons

SADA asks if you would like to apply the polygon layer to every vertical layer. If yes, then the polygon “cookie cuts” through every layer above and below the current layer.

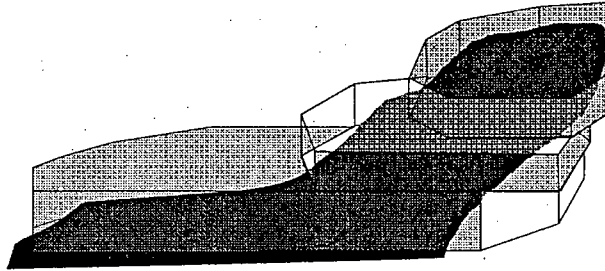


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Polygons Varying by Layer

By varying the polygons for each layer you can trap three dimensional events that vary as a function of depth.

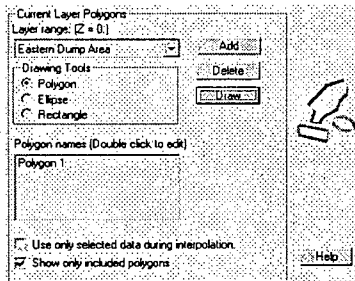


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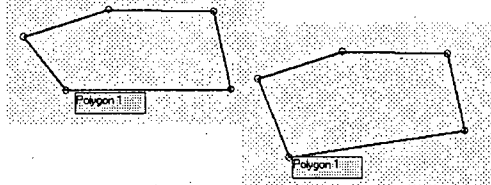
Edit Existing Polygons

Multiple polygons are allowed at a time. In 3d Space, polygons can slice through all layers or only selected layers.



To edit existing polygons, left click on a polygon to highlight vertices. Then:

- Left click inside a vertex to move or delete that vertex. The polygon will turn blue.
- Left click anywhere on the polygon to add a new vertex.
- Right click inside any vertex to move or delete the entire polygon. The polygon will turn red.
- Right click anywhere on the polygon to copy the polygon.



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Questions?

Comments?

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Spatial Analysis and Decision Assistance (SADA) Version 4 Initial Sample Design

Environmental Assessment Methods in SADA
University of Tennessee, Knoxville

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Initial Sample Designs

- Judgmental
- Simple Random
- Simple Grid
- Simple Unaligned Grid
- Standard Grid
- Standard Unaligned Grid
- MARSSIM Grid
- Hotspot: Minimize Sample Size By Cost
- Hotspot: Minimize Sample Size By Hot Spot Definition
- Hotspot: Unknown Hotspot
- Hotspot: Calculate Probability
- 3D Hot Spot Search

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Optimizing Sample Design

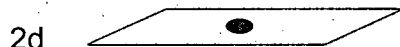
- Last step in Data Quality Objectives Process (DQOP)
- DQOP is a systematic planning approach for data collection that is based on the scientific method that defines the purpose for the data collection, clarify the kind of data needed, and specify the limits on the decision errors needed for the study. Source: "Guidance for the Data Quality Objective Process, EPA QA/G-4, Washington DC 2000" (pdf included on the training CD)
- More references: "Guidance on choosing a Sampling Design for Environmental Data collection, EPA QA/G-5S, Washington DC 2002" (pdf included on the training CD), also Swedish document in preparation "Provtagningstrategier för förorenad mark: Inventering av strategiverktyg för provtagning av jord, SNV 2005 - utkast"

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3 Types of Sample Designs: 2d, 3d, and 3d Core

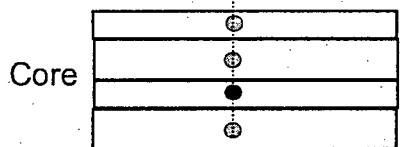
With all designs, SADA first identifies the location of the sample. Then, based on whether there are multiple layers and whether the user wishes to core, the following broad scenarios are possible for a single sample.



In a 2d application, the sample is placed on a single layer.



In a 3d application, the sample is placed on a single layer at the depth required.



In a core application, the sample is placed on a single layer at the depth required. Then all layers above and below are also sampled subject to polygon definitions.

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Determining Number of Samples

You Pick

- User enters number of samples based on some outside decision.

Sign Test

- Sample size is determined using the non-parametric Sign test, user inputs a decision criterion, lower bound of a gray region, and acceptable Type I and II error rates

Wilcoxon Rank Sum

- Sample size is determined using the non-parametric Wilcoxon Rank Sum test, user inputs a decision criterion, a lower bound of a gray region, and acceptable Type I and II error rates

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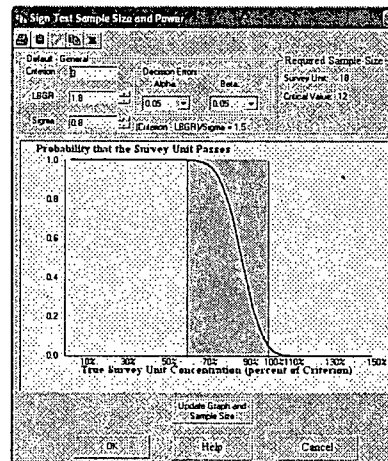
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Determining Number of Samples - Sign Test

- User inputs a decision criterion, a lower bound of a gray region, and acceptable Type I and II error rates

Appropriate for grid designs and simple random sampling

- Used when no background is available

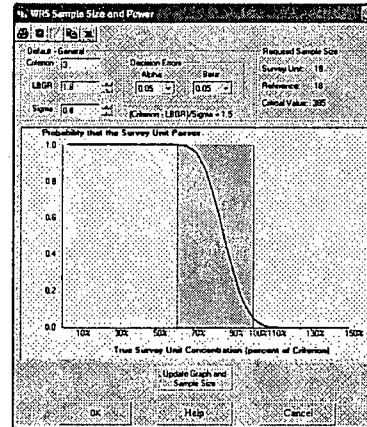


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Determining Number of Samples – Wilcoxon Rank Sum

- User inputs a decision criterion, a lower bound of a gray region, and acceptable Type I and II error rates
- Appropriate for grid designs and simple random sampling
- Used when no background is available



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Judgmental Sampling

Description

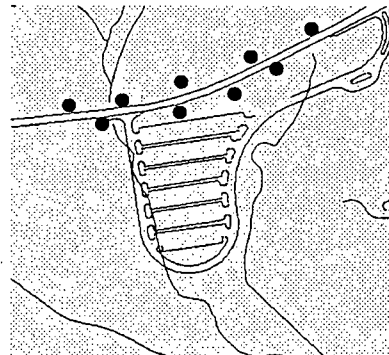
- Selection of sample locations based on expert knowledge or professional judgment

Pros

- Easy to implement
- more efficient (when correct)

Cons

- Introduces bias
- Cannot reliably estimate precision of estimates nor use statistical analyses to draw conclusions



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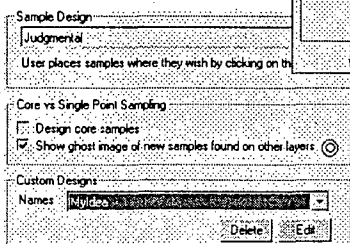
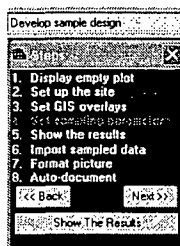
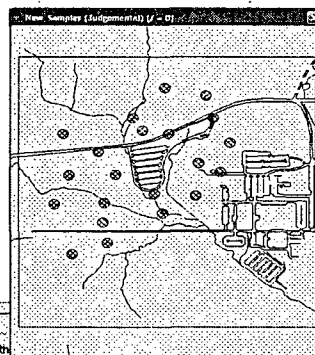
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Judgmental

With Judgmental, the user determines the location of the new samples.

Select **Judgmental** from the drop down list under **Sample Design**. Then press **Show the Results**.

SADA will ask for a name. After entering your name use the mouse to select sample locations on the **Results window**. Press **Done** when through and SADA will prompt for a name for the sample design. The design will now appear in the drop down box under **Custom Designs** on the **Parameters Window**.



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Simple Random

Description

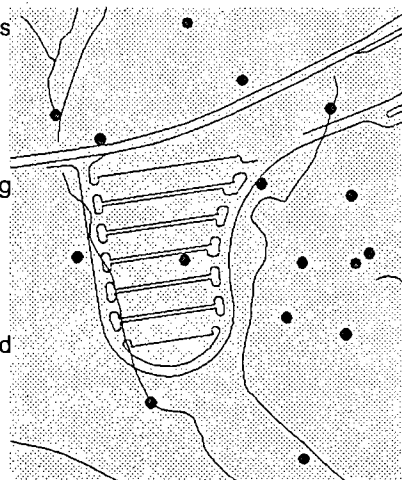
- Samples are distributed randomly across the site.

Pros

- Random sample designs are underlying assumption in most statistical tests.

Cons

- Samples may miss areas of interest and can occasionally be clustered.



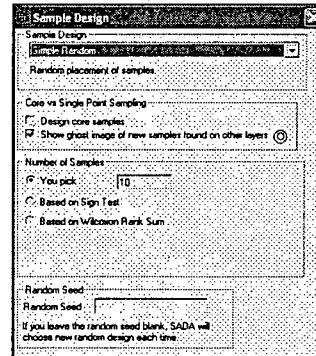
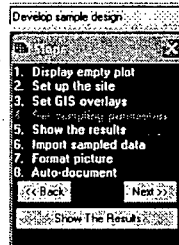
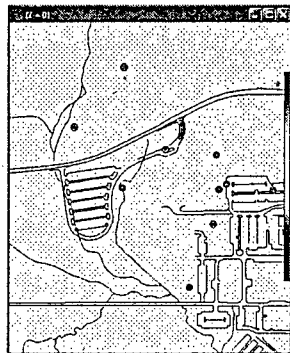
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Simple Random

Simple random is an initial sample design that relies on the generation of coordinate values to create the new samples.

Select **Simple Random** from the drop down list under **Sample Design**. Then enter the desired number of new samples.



Press **Show the Results** and SADA will randomly select your new sample locations.

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Systematic Aligned Grids

Description

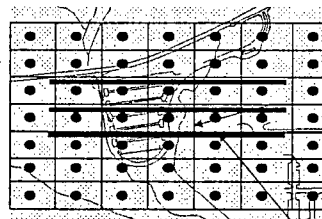
- By specifying a distance between sample points one can generate either a square or triangular grid. Triangular grids provide more information spatially than rectangular grids.

Pros

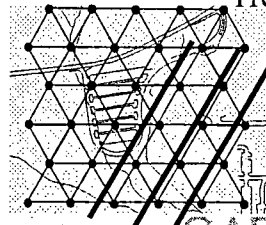
- Better spatial representation than a random placement.
- Supports a geospatial analysis

Cons

- Miss features in a regularized pattern such as piping or ditches.
- Lack of truly random design may have an unknown impact on determining precision of simple statistical values or tests.



Trenches



Triangular

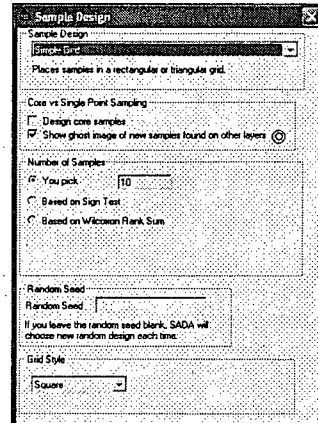
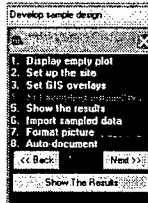
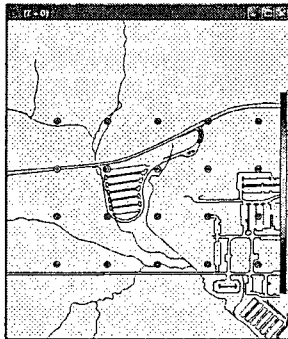
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Simple Grid

Simple grid is an initial sample design that relies on grid style, site boundaries, and number of new samples to generate new samples.

Select **Simple Grid** from the drop down list under **Sample Design**. Then enter the desired number of new samples. Select a square or triangular grid style.



Press **Show the Results** and SADA will select your new sample locations based on the grid selection and place the samples in the center of each grid.

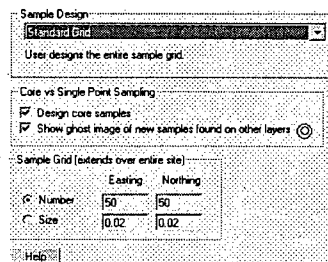
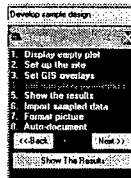
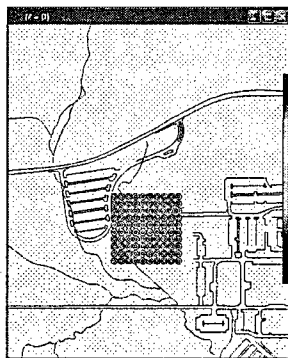
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Standard Grid

Standard grid is an initial sample design that relies on a grid definition and depth classifications to generate new samples.

Select **Standard Grid** from the drop down list under **Sample Design**. Then enter the grid design. Each sample will be placed in the center of the grid block.



Press **Show the Results** and SADA will select your new sample locations based on the grid definition.

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Systematic Unaligned Grids

Description

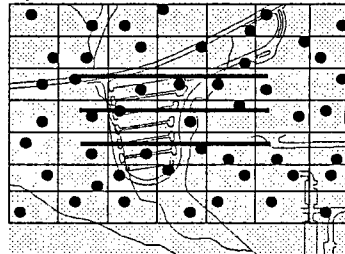
- The same as a standard or simple grid but rather than sampling the center of each cell, we choose a random location in the cell.

Pros

- This approach can help overcome the problem of missing features by randomizing within the cell. This increases the random element of the design while enforcing a regular distribution across the site.

Cons

- Lack of truly random design may have an unknown impact on determining precision of simple statistical values or tests.



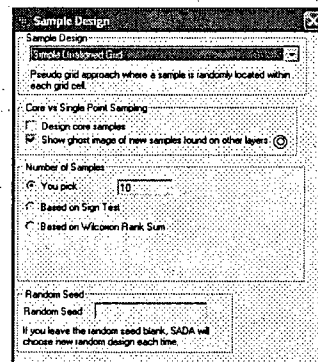
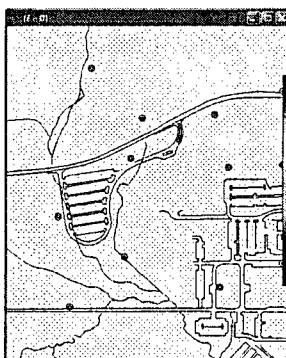
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Simple Unaligned Grid

Simple unaligned grid is an initial sample design that relies on a square grid definition and number of new samples to generate new samples.

Select **Simple Unaligned Grid** from the drop down list under **Sample Design**. Then enter the desired number of new samples.



Press **Show the Results** and SADA will select your new sample locations based on the grid selection and place the samples randomly in each grid.

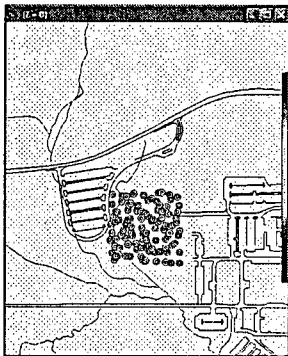
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Standard Unaligned Grid

Standard unaligned grid is an initial sample design that relies on a grid definition and depth classifications to generate new samples.

Select **Standard Unaligned Grid** from the drop down list under **Sample Design**. Then enter the grid design. Each sample will be placed randomly inside the grid block



Sample Design

Standard Unaligned Grid

User designs the entire sample grid. Samples are randomly placed within each cell.

Core vs Single Point Sampling

Design core samples

Show ghost image of new samples found on other layers

Random Seed

Random Seed: []

If you leave the random seed blank, SADA will choose new random design each time.

Sample Grid (extends over entire site)

	Easting	Northing
Number	50	50
Size	0.02	0.02

Press **Show the Results** and SADA will select your new sample locations based on the grid definition.

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Hot Spot Sampling

Hot spot sampling is a 2d initial Ellipgrid model that was originally encoded as Ellipgrid PC by Oak Ridge National Laboratory.

The goals of 2d hot spot sampling are to calculate:

- the probability of hitting or, conversely, missing an elliptical hot spot of a defined size
- The maximum size of a hot spot that would, with a defined probability, be hot by a sample grid definition
- A grid of samples based on finding a hot spot of a defined size with a distinct probability
- A grid of samples based on the cost to sample, the sample area definition, and a limited budget.

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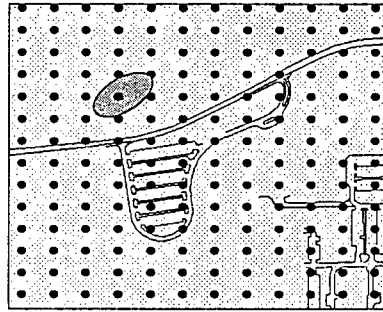
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Two Dimensional Hot Spot Searches

Description

2D Ellipgrid calculates the relationship between hotspot size, grid density, cost, and probability for a variety of circumstances.

- Calculates grid size given desired probability and hot spot size.
- Calculates probability of missing a hot spot of known size with specified grid.
- Calculates smallest hot spot that can be detected with a given probability and grid size.
- Minimize sample design by cost.



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Two Dimensional Hot Spot Searches

If you know any two of the three parameters, SADA calculates the third.

<u>Probability</u>	<u>Size & Shape</u>	<u>??</u>
<u>Probability</u>	<u>??</u>	<u>Grid Specs</u>
<u>??</u>	<u>Size & Shape</u>	<u>Grid Specs</u>

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Two Dimensional Hot Spot Searches

Pros

Useful in determining tradeoffs between cost, size of hot spot, and cost to implement.

Cons

For most applications, sample designs are fairly dense grids and too expensive for many sampling budgets.

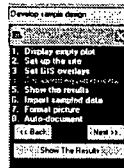
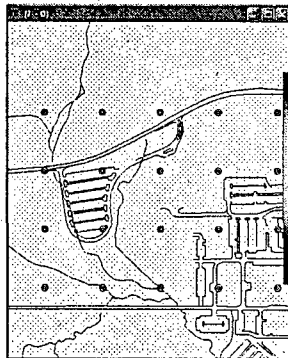
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Hot Spot: Minimize Sample Size by Cost

With Hot Spot: Minimize Sample Size by Cost, the user defines the grid style and cost parameters. This combination yields a possible sample number.

Select Hot Spot: Minimize Sample Size by Cost from the drop down list under Sample Design. Select a square, triangle, or rectangle grid style and enter the cost parameters.



Costs to Sample:	
Planning and Validation One Time Cost:	\$ 1000.00
Sample Collection Cost per Sample:	\$ 50.00
Analytical Cost per Analyte:	\$ 100.00
Budget:	\$ 4000.00

Press Show the Results and SADA will determine the number of new samples and select their locations based on the grid style.

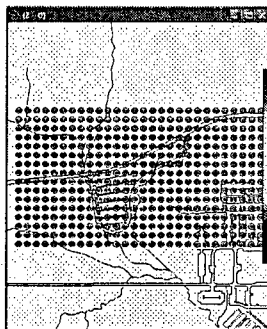
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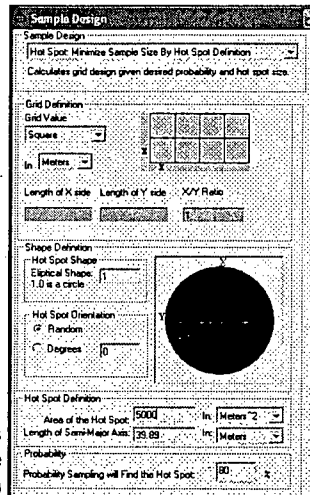
Hot Spot: Minimize Sample Size by Hot Spot Definition

With Hot Spot: Min Sample Size by Hot Spot Definition, the user defines the grid style and the probability of hitting a hot spot of a given size, shape, and orientation. SADA returns the size of each grid cell.

Select **Hot Spot: Minimize Sample Size by Hot Spot Definition** from the drop down list under **Sample Design**. Select a square, triangle, or rectangle grid style and enter the hot spot parameters.



Press **Show the Results** and SADA will determine the length between samples, the number of new samples for your given area, and produce the map.



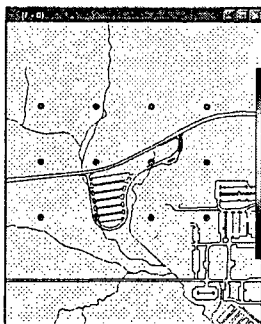
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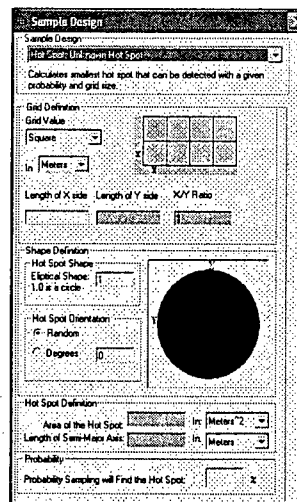
Hot Spot: Unknown Hot Spot

With Hot Spot: Unknown Hot Spot, the user defines the grid style and size, the hot spot shape and orientation, and the probability of detecting a hot spot. SADA determines the hot spot you could detect with the specified probability level.

Select **Hot Spot: Unknown Hot Spot** from the drop down list under **Sample Design**. Select a square, triangle, or rectangle grid style and enter the applicable parameters.



Press **Show the Results** and SADA will determine the number of new samples for your site, determine their locations and report the size of the hotspot you could detect at the specified probability value.



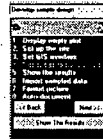
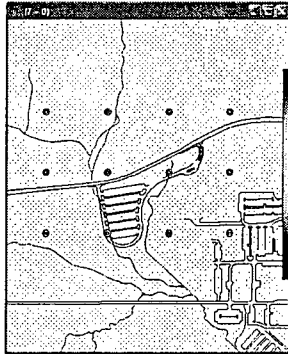
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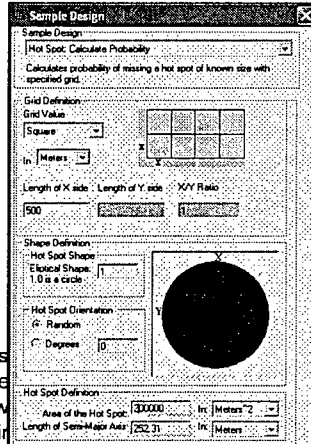
Hot Spot: Calculate Probability

With Hot Spot: Calculate Probability, the user defines the grid and the hot spot size, shape and orientation. SADA returns the probability of hitting such a hotspot with the given grid.

Select **Hot Spot: Calculate Probability** from the drop down list under **Sample Design**. Select a square, triangle, or rectangle grid style and enter the applicable parameters.



Press **Show the Results** and SADA will determine the number of new samples, determine their locations, and report the probability of hitting a hotspot of the specified size.



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Three Dimensional Hot Spot Searches

Description

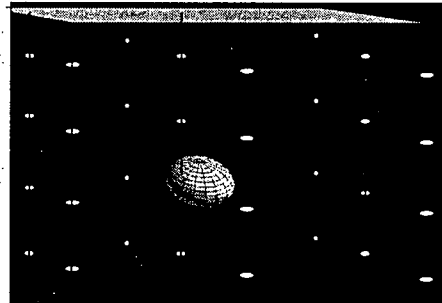
- The concept of hot spot searches in two dimensions can easily be extended into the third dimension through the use of simulation. A grid is specified in three dimensions, and the location of ellipsoids are simulated across the site. The likelihood of hitting such a hot spot is simply the ratio of simulated hits to total simulations.

Pros

- Provides an estimate of how effective a sampling grid will be at finding hot spots in subsurface.

Cons

- As with two dimensional hot spot searches, the grids can be too dense for practical sampling budgets.



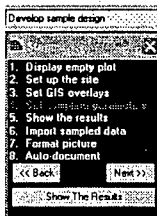
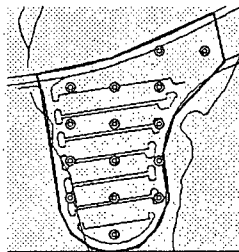
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3D Hot Spot Search

3D Hot Spot Search is a 3d initial sample design that calculates the probability of hitting or missing an elliptical area of interest.

Select 3D Hot Spot Search from the drop down list under **Sample Design**. Enter the hot spot search parameters, number of simulations, and grid design.



Sample Design

3D Hot Spot Search

Calculates likelihood of missing a hot spot of known size in three dimensional space with specified grid.

Three dimensional Hotspot Search Parameters

Ellipse Size

X Radius: 100 Y Radius: 100 Z Radius: 20

Number of Simulations: 10

Sample Grid (extends over entire site)

Number: 50 Easting: 50 Northing: 50

Size: 26.68 22.22

Press **Show the Results** and SADA will determine the probability of hitting the ellipsoid and average number of hits and display the resulting sample design.

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Questions?

Comments?

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Practice Session Creating Files and Setting Up Initial Sample Designs

The objective of this lesson is to be able to create an empty SADA file and then use it to set up a number of initial sample designs.



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Practice Session: Creating Files and Setting Up Initial Sample Designs

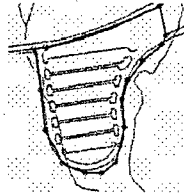
1. Create an empty SADA file called "Lesson1.sda".
2. Go to the "Develop a Sample Design" interview.
3. Set up five vertical layers.
 - a. 0-1
 - b. 1-3
 - c. 3-10
 - d. 10-30
 - e. 30-61
4. Set the boundaries of the site.
 - a. Easting minimum = 26990
 - b. Easting maximum = 28324
 - c. Northing minimum = 22152
 - d. Northing maximum = 23263



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Practice Session: Creating Files and Setting Up Initial Sample Designs

5. Add two GIS layers (Roads.dxf, Water.dxf). Change the color of the water.dxf layer to blue.
6. Add a polygon design called "Parking Lot Area". Make this polygon roughly follow the boundaries of the parking lot in the Roads.dxf layer.



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Practice Session: Creating Files and Setting Up Initial Sample Designs

7. Create a *judgmental* sample design. Make sure to add core hole locations and place your new core holes inside the parking lot. Call the design "MyDesign".
8. Export your sample design to "Lesson1.csv". Open this file in Excel.
9. Open another document in Word. Copy the sample design image into word.
10. Create a *simple random* core design. You only can afford 10 new samples, and leave the random seed value blank. Try this multiple times. Then, try it multiple times with a random seed = 1.

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Practice Session: Creating Files and Setting Up Initial Sample Designs

11. Create a *simple grid* design with 10 new samples. Repeat this for *simple unaligned grid*.
12. Create a *standard grid* design. Set the grid to 20x20. Remove the polygon and reapply the grid.
13. With the polygon still turned off, try an *unaligned standard grid*.
14. Now suppose you are searching for a potential hotspot at the surface. You have \$20,000 available for new samples. Planning and validation will cost about \$5000, the cost per sample to collect it averages about \$200, and the cost to analyze it will be \$400. Use *minimize sample size by cost* to calculate the number of samples you can afford and place them in a square grid.

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Practice Session: Creating Files and Setting Up Initial Sample Designs

15. Suppose now that you want to clean up a site. Regulations stipulate that you cannot leave a contiguous hot spot or elevated area behind greater than 50 feet in diameter (7853 sq feet) on the surface. (This happens often in radiological assessment.) Let's assume that there does exist at least one such hot spot on the site. Use *Minimize sample design by hot spot definition* to lay out a sample design that will find a hot area 50 feet in size with a probability of 90%.
16. Based on available resources, you plan to lay out a 100 foot grid design. What size hot spot would you have a 90% chance of finding on the surface if you use your current grid? Use the *Hot spot: Unknown hot spot* sample design to find out.

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Practice Session: Creating Files and Setting Up Initial Sample Designs

17. Suppose now that you are not permitted to leave behind a hotspot of 50 feet in diameter on the surface. You are proposing to use a 100 foot grid design. What is the probability you would find one if one exists? Use the *Hot Spot: Calculate Probability* sample design.

18. Now suppose that you are dealing with a 3d problem across the entire site. (Turn off your polygon.) You cannot leave behind an area greater than 60 feet across and 60 feet deep (elliptically shaped). You propose to look for this area by using a 20x20 grid and sampling at every layer (0-1, 1-3, 3-10, etc). What is the chance you will find such an object with your grid design? Use *3d Hot spot search*.

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Spatial Analysis and Decision Assistance (SADA) Version 4 Import Data

Environmental Assessment Methods in SADA
University of Tennessee, Knoxville

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Data Formats

- SADA can accept data in two formats: comma delimited files (csv) and Microsoft Access.
- SADA requires the presence of certain numeric fields in the data set (non-numerical values are not permitted for these fields).
 - Easting
 - Northing
 - Depth
 - Value
 - Soil, Sediment, and Biota: mg/kg for nonradionuclides, pCi/g for radionuclides
 - Surface/Groundwater: mg/L for nonradionuclides, pCi/L for radionuclides
- Also required is a name field, which usually corresponds to the contaminant being considered.
 - Name
- SADA can use other forms of information as well
 - Media field required to set up risk assessment (Soil, Sediment, Groundwater, Surface water, Air, Biota, and Background)
 - Detect (1 = detect, 0 = non-detect)
 - Date (mo/da/year)
 - CAS Number (treated as a number and stripped of dashes)
- Any other form of meta data can be imported as well. User can plot and retrieve this auxiliary information during an analysis.

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Pre-Processing Data for SADA

- Title row required.
- Construct media field. SADA recognizes soil (SO), sediment (SD), surface water (SW), groundwater (GW), air (AIR), biota (BIO), and background (Background), and the "basic" media type. Basic is assigned to data that have no media type.
- Create a value field that is always numeric, often involves removing "<" or entering detection limits for non-detected data.
- Evaluate laboratory flags for detect field, assign 1 for detects and 0 for non-detects.
- Ensure that contaminant names are consistently spelled.
- Check that unique sample locations have the exact same x,y,z coordinates when coming from different data sets/sampled at different times.
- Resolve any QA duplicate issues before importing data.

Flag	Meaning	Use for risk?
R	Rejected	No
B	Blanks contaminated	Treat as non-detect
J	Estimated	Yes, treat as detect
UJ	Estimated non-detect	Yes, treat as non-detect
K	Biased high	Yes, treat as detect
L	Biased low	Yes, treat as detect
U	Non-detect	Yes, treat as non-detect

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Pre-Processing Data for SADA

- Choose regional settings that use a period as the decimal symbol instead of a comma (e.g., 1265.034 instead of 1265,034). The comma is the default in a number of Continental European settings.
- When using comma-delimited files, save fields with a comma in them as text fields, (e.g., "1,2-Dichloroethane" instead of 1,2-Dichloroethane)

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Access or csv File Format

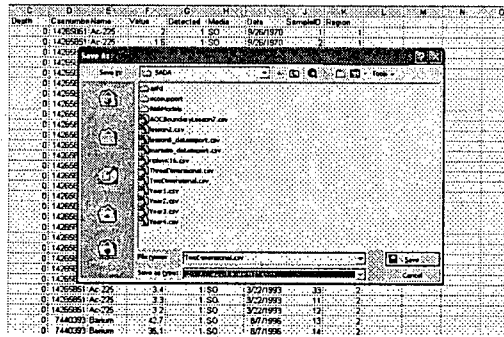
- With pre-processed excel file

x	y	z	Compound	Concentration	Media type	Date
7	8	1	As	44.6	SO	1/1/2006
9	3	3	As	23	SO	1/1/2006
5	4	2	As	11	SO	1/1/2006
9	5	5	Cu	455	SO	1/1/2006
33	3	2	Cu	22	SO	1/1/2006

- Convert to Access file: go to **Data, Convert to Access**, choose New database

- Convert to Comma-delimited file: go to

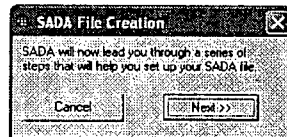
- File,
- Save As
- Select Save As Type: CSV (Comma-delimited)(* .csv)



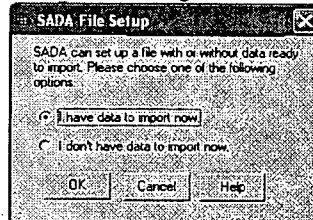
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SADA File Setup- Create File With Data

To begin the creation sequence, open SADA, select File, and from the menu bar choose New. The following window will appear.



Press Next >> to continue. The following window will appear.



If you do not have data to import, select the first option and press OK.

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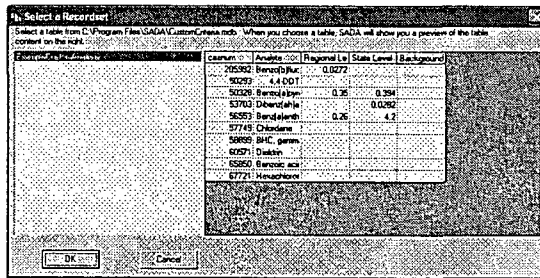
Import Data into Empty File

Data may be imported into an empty file or a file that contains Geobayesian model data.

Select **Import Sampled Data** from the **Steps** window. At the **Data Import** window, select the file to import and press **OK**.



If your input file is an Access database, the following window will appear.



Select the appropriate table from the left pane and press **OK**.

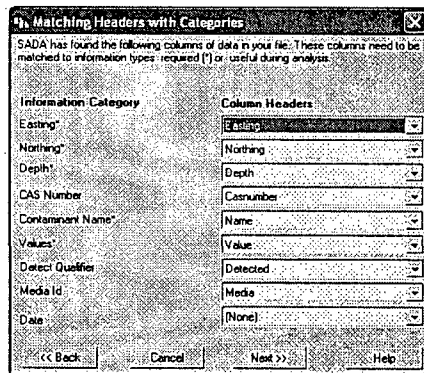
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Importing Data Into SADA

The next step is to match the columns of information in the ascii data file to information categories that are required or may be useful in SADA.

Required information categories are followed by an (*) and must be assigned to a column in the ascii data file. A category is not assigned if the (none) option is selected in the drop down box. The Depth category is required only when data exist at varying depths. If the Detect Qualifier is not assigned, the data are assumed to be all detects.



If Media ID, which denotes the type of media the contaminants are sampled in (e.g. soil or groundwater) is not assigned, SADA adds an artificial media column titled 'Basic' and the human health risk and/or ecological risk modules cannot be setup later.

After the columns have been set, press **Next>>**. SADA begins the conversion process and presents the data as it will be imported into the Data Editor.

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Data Editor

The Data Editor provides a chance to identify errors in the data set and correct them during the import process. It may also be accessed from the Tools Menu at any time later for data corrections or additions.

SADA highlights cells with red if they contain an unacceptable value. To determine the exact error, place the mouse over the red cell and the yellow text box near the top explains the problem. Once there are no red cells, the process continues.

ID	Name	Coordinates	Entry	Number	Depth	Value	Detected	Media
1	Ac-225	1426981	2759.25	21900	0	1.8637	1	SD
2	Ac-225	1426981	2870.25	21900	0	1.8325	1	SD
3	Ac-225	1426981	288.25	21900	0	0.8314	1	DW
4	Ac-225	1426981	2768.5	22200	0	2.0294	1	DW
5	Ac-225	1426981	2813.75	22200	0	1.88278	1	SD
6	Ac-225	1426981	28202.75	22500	0	1.4788	1	SD
7	Ac-225	1426981	271.50	22160	0	1.70781	1	SD
8	Ac-225	1426981	2766.5	22500	0	2.38226	1	SD
9	Ac-225	1426981	2842.3	22100	0	1.93282	1	DW
10	Ac-225	1426981	2821	22100	0	1.23373	1	DW
11	Ac-225	1426981	2887.25	22200	0	2.35146	1	DW
12	Ac-225	1426981	28115.5	22380	0	0.9877	1	SD
13	Ac-225	1426981	2741.75	22580	0	1.3746	1	SD
14	Ac-225	1426981	2777.75	22640	0	2.82544	1	SD
15	Ac-225	1426981	28310.25	22400	0	3.12182	1	SD
16	Ac-225	1426981	28725	22460	0	3.82735	1	SD
17	Ac-225	1426981	28200	22580	0	4.8	1	SD
18	Ac-225	1426981	27500	22500	0	3.3	1	SD
19	Ac-225	1426981	27200	22380	0	2.03	1	SD
20	Station	7440293	2758.25	21900	0	42.77498027	1	SD
21	Station	7440293	28210.25	21900	0	28.1289123	1	DW
22	Station	7440293	28735	21900	0	18.48831343	1	SD
23	Station	7440293	27687.5	22200	0	43.95483395	1	SD

It is recommended that the **Automatic Error Checking** box remain checked so SADA looks for mistakes as you type. When the user is entering or pasting large amounts of data and does not wish the process to be slowed, however, it may be preferable to uncheck the **Automatic Error Checking** box and check errors later with the **Check Errors** button.

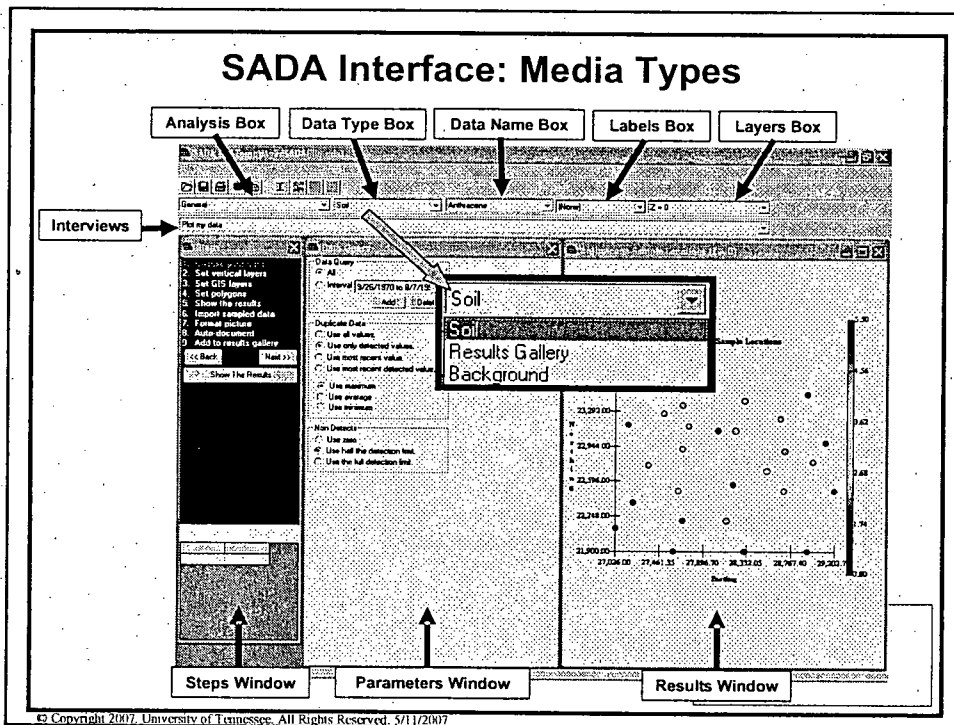
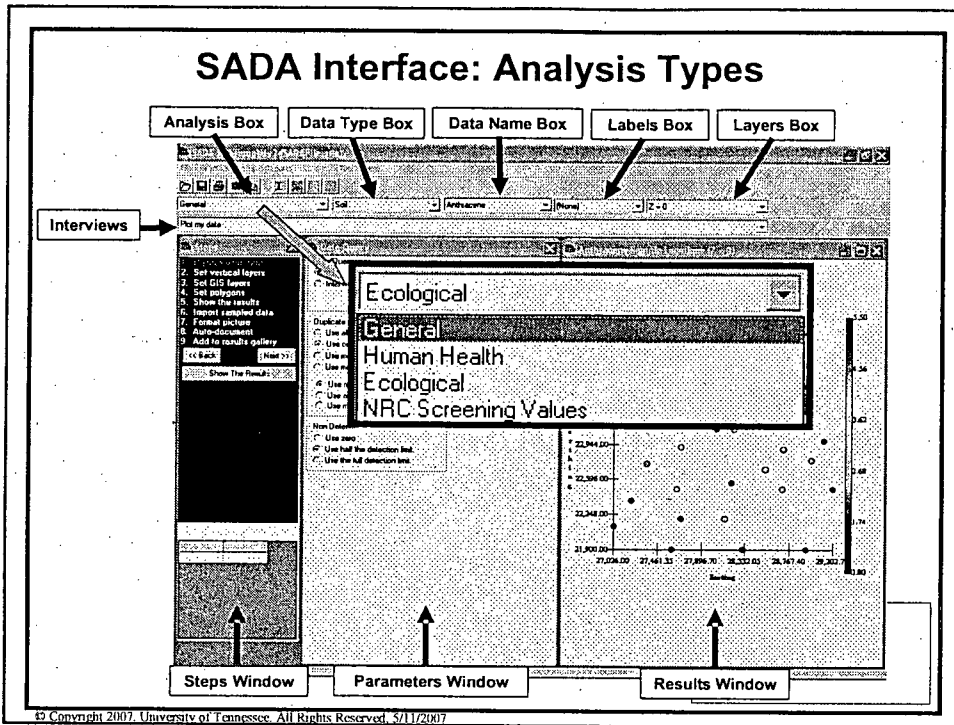
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SADA Interface With Data

The screenshot shows the SADA interface with data. At the top, there is a toolbar with buttons for Analysis Box, Data Type Box, Data Name Box, Labels Box, and Layers Box. Below the toolbar, there is a window titled 'Put my data' with a 'Data Query' section. The 'Data Query' section has a dropdown menu set to 'All' and a text box containing '3/25/1970 to 6/7/19'. Below the 'Data Query' section, there are checkboxes for 'Duplicate Data', 'Use all values', 'Use only detected values', 'Use most recent values', 'Use most recent detected values', 'Use minimum', 'Use average', and 'Use maximum'. Below these checkboxes, there are checkboxes for 'Net Distance', 'Use zero', 'Use half the connection link', and 'Use the full connection link'. On the left side, there is a list of steps: 1. Put my data, 2. Set vertical layers, 3. Set GIS layers, 4. Set polygons, 5. Show the results, 6. Export selected data, 7. Format picture, 8. Auto document, 9. Add to results gallery. Below the list of steps, there are buttons for '<< Back', 'Next >>', and 'Show The Results'. At the bottom, there are three windows: Steps Window, Parameters Window, and Results Window. The Results Window shows a scatter plot titled 'Analytical Sample Locations' with axes for 'Elevation' (ranging from 21,200.00 to 21,640.00) and 'Distance' (ranging from 27,024.00 to 28,302.00). The plot shows several data points scattered across the area.

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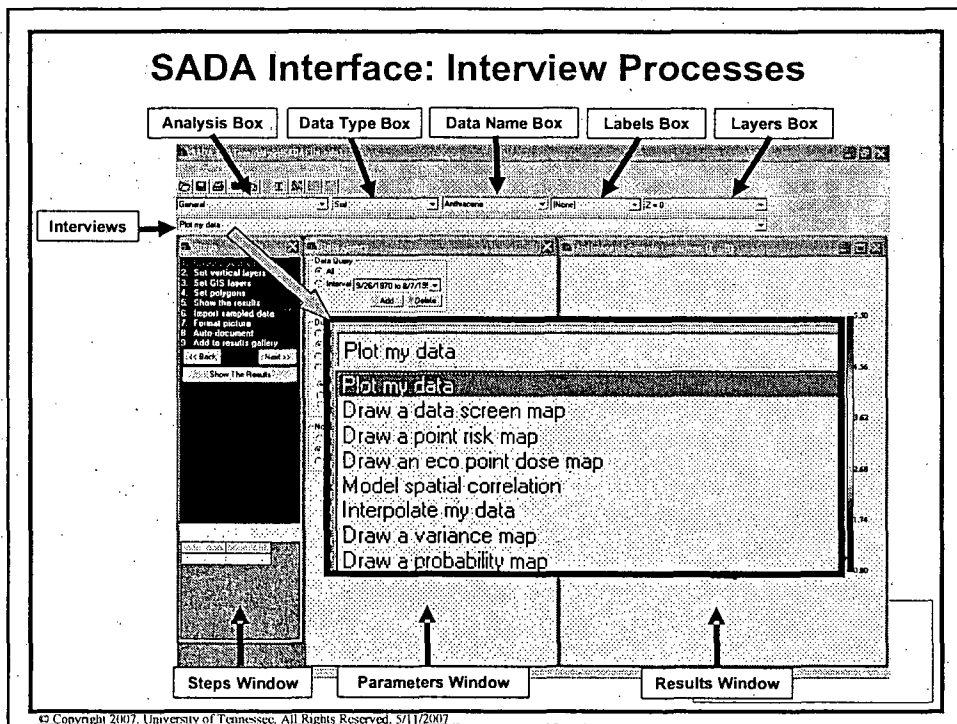
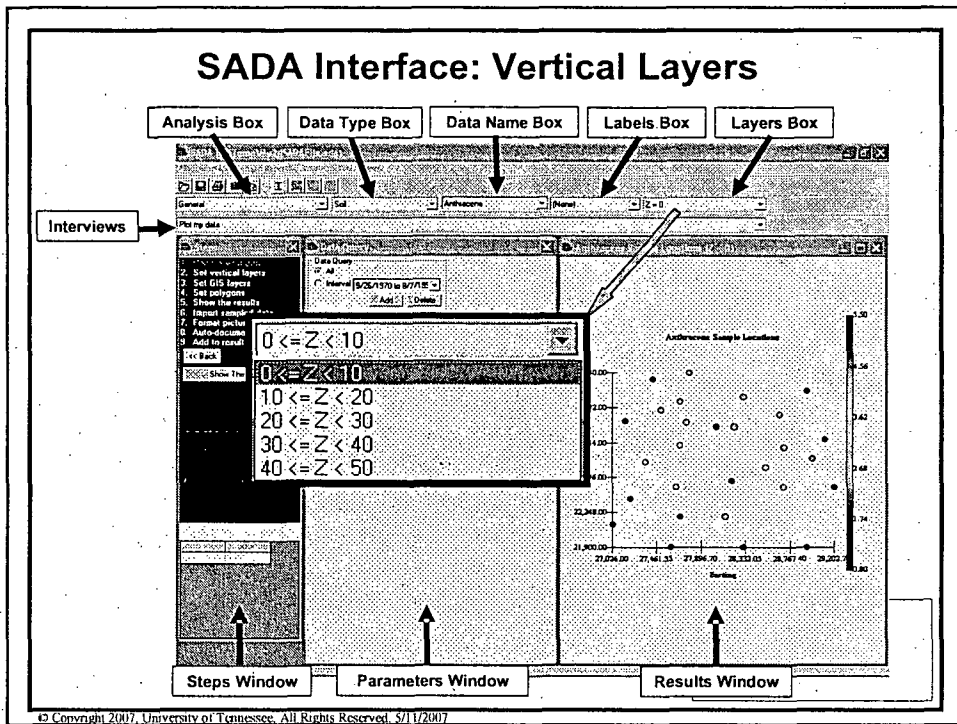


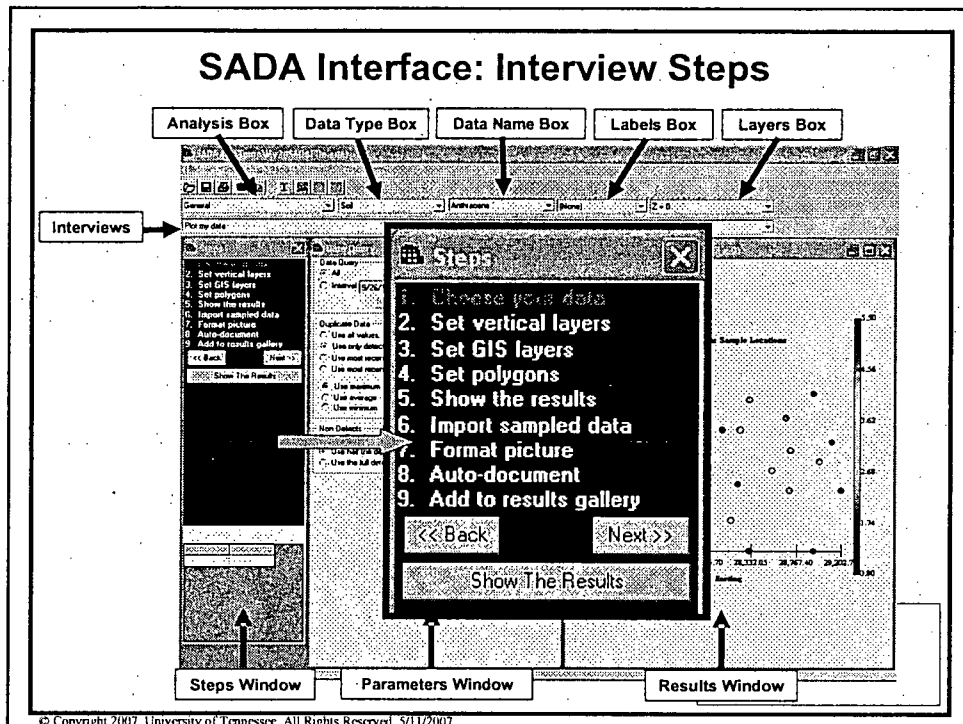
SADA Interface: Contaminants

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SADA Interface: Data Labels

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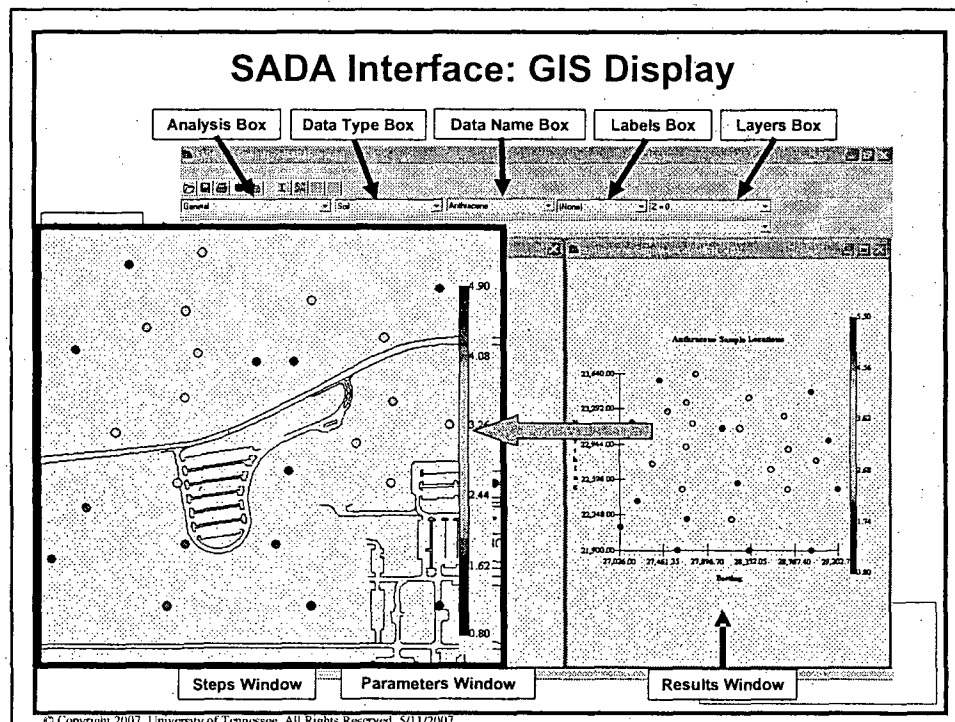
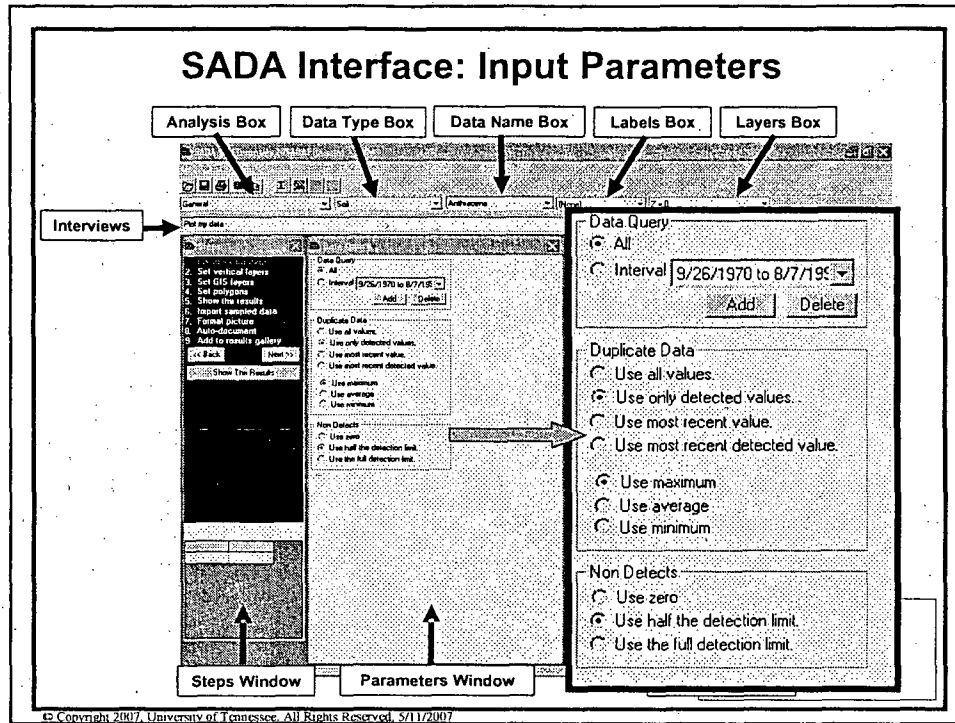




Interview Methods Available with Data

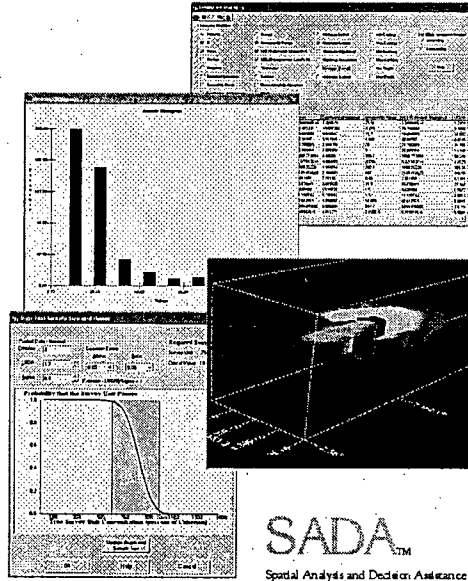
- Plot my data
- Draw a data screen map
- Model spatial correlation
- Interpolate my data
- Draw a variance map
- Draw a probability map
- Draw an area of concern map
- Calculate cost versus cleanup
- Draw a LISA map
- Develop sample design

The screenshot shows the 'Sample Design' dialog box. It includes a 'Sample Design' dropdown menu with 'Synthetic Random' selected. Below it are checkboxes for 'Random placement of samples', 'Cone vs Single Point Sampling', 'Design cone samples', and 'Show ghost image of new samples found on other layers'. There is a 'Number of Samples' field with a value of 0. Under 'If You pick', there are radio buttons for 'Based on Sign Test' and 'Based on Wilcoxon Rank Sum'. A 'Random Seed' field is present with a note: 'If you leave the random seed blank, SADA will choose new random design each time.' The SADA logo and 'Spatial Analysis and Decision Assistance' are visible at the bottom right. A copyright notice at the bottom reads: '© Copyright 2007, University of Tennessee. All Rights Reserved, 5/11/2007'.



Drop-down Menu Items Available with Data

- Show histogram
- View 3-D data
- Setup human health risk, ecological risk, or custom analysis
- Manage autodocumentation reports
- View univariate statistics
- Find number of samples using Sign Test or WRS test
- Query data set
- Add or remove contaminants
- Edit data set



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Questions?

Comments?

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Spatial Analysis and Decision Assistance (SADA) Version 4 Data Exploration

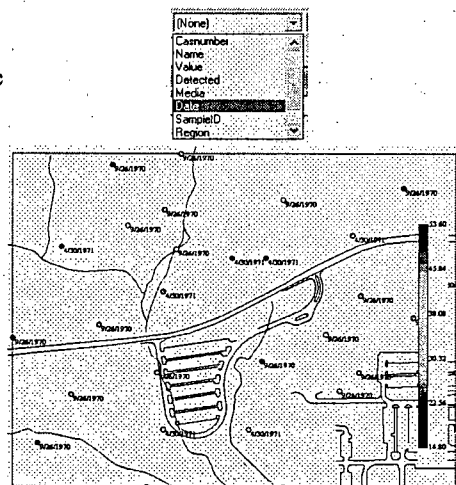
Environmental Assessment Methods in SADA
University of Tennessee, Knoxville

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Showing Meta-Data with Labels

- SADA allows for the import of more fields than the basic required ones. Results for these forms of meta-data can be shown with the label drop-down item.
- Select date from the list of labels to view the date that each sample was collected.



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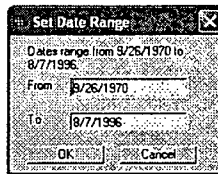
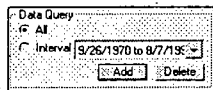
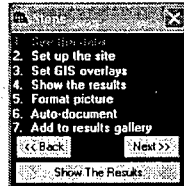
Query By Date

The **See the Data** also permits users to parse the data set by date and perform SADA functions on a portion of the data set (if the date field was specified during data import).

At the top of the **Parameters Window** under **Data Query** are two radio buttons: **All** and **Interval**. (**All** is the default option.) Select '**All**' in order to use all points for a given contaminant. In order to parse the data, select the interval option.

To add date intervals, press the **Add** button and add as many date ranges as necessary in the format mm/dd/yy.

The **Results window** will only display the data points for the specified date range and all SADA functions will be performed on those points only.



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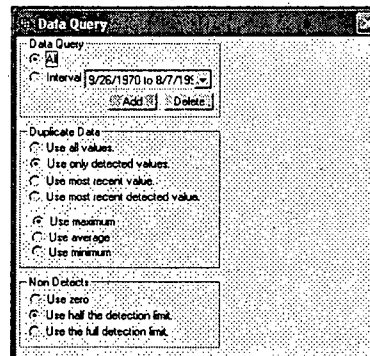
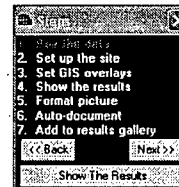
Duplicate Resolution

Duplicates in SADA are multiple analyses for a contaminant. They may be collected for QA purposes

When data is imported, SADA checks for duplicate values. Duplicate values are resolved based on the criteria defined on the **Parameters Window** when you select **See the Data** from the **Steps Window**.

The first four radio buttons under **Duplicate Data** determine what type of duplicates will be used. (Some of the buttons may be disabled depending on the data imported.)

Three more radio buttons further define the duplicate resolution. If more than one point still exists, SADA will use the **Maximum**, **Minimum**, or **Average** value, depending on the user's selection.

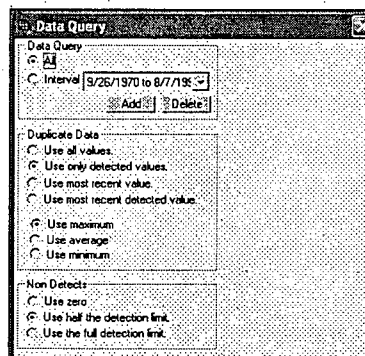
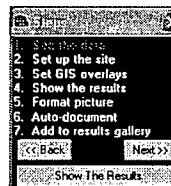


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Proxy Values for Non-detects

- The Data Query window also has non-detect options.
- Data reported as non-detect can have different statistical techniques applied to account for the uncertainty in the concentration (between 0 and the detection limit).
- EPA often recommends using half the detection limit as the proxy value.
- Other methods are possible, such as regression techniques or bootstrapping, but must be implemented before importing data.



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Zooming, Shifting, Restoring

Zooming In

Click the **Zoom In** button to magnify the site. Using the left mouse button, select the region to zoom in on. Releasing the mouse button produces the zoom.

Zooming Out

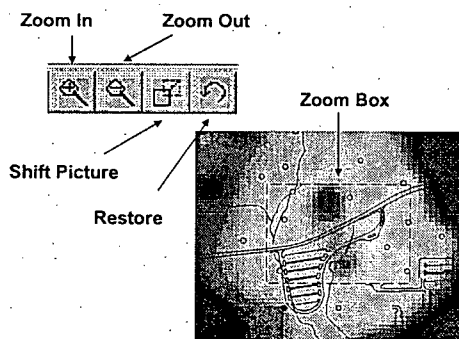
Click the **Zoom Out** button to reduce the magnification. Select the zoom area with the mouse, and the portion of the image that is visible is placed in the zoom box to cause the zoom out effect.

Shifting

Click **Shift Picture** to shift the view. After selecting this option, click your mouse at any point in the picture and pull the mouse in the direction you wish to move the image. A line will appear demonstrating how far the picture will move. Release the mouse button and the picture will redraw.

Restoring

Click the **Restore** button to return the picture to its original scaling and position.



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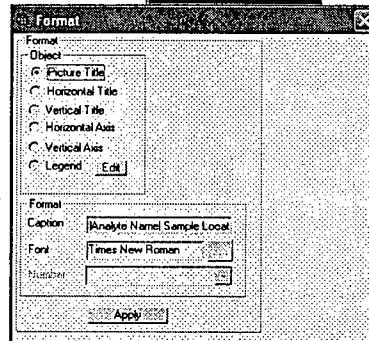
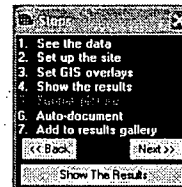
Formatting

To format the picture, select **Format Picture** on the **Steps Window**. Formatting options appear in the **Parameters Window**.

Select the portion of the picture you wish to format under **Object**. The current formatting scheme will appear under **Format**.

After making all the changes, press the **Apply** button.

Press the **Edit** button next to **Legend** to access the **Legend Manager**.



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Managing Legends

SADA allows users to modify the legends that control the color range of data and result output. Two types of legends are permitted.

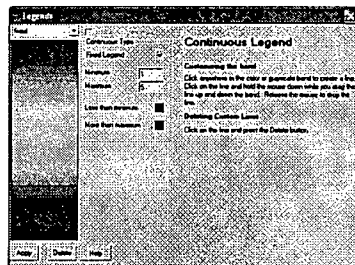
Continuous

An unbroken color band that ranges from dark purple through a spectrum to bright red. Continuous legends can be customized by manually stretching or compressing a subset of the color band.



Categorical

Categorical legends permit the user to break the legend into a series of ranges or categories with set names and colors.



To modify a legend or create a new legend, simply right mouse click over the legend itself or choose **Legend Manager** from the **View** menu.

You can choose from the list of available legend types or build a new one of your own. See the **Help File** for more details.

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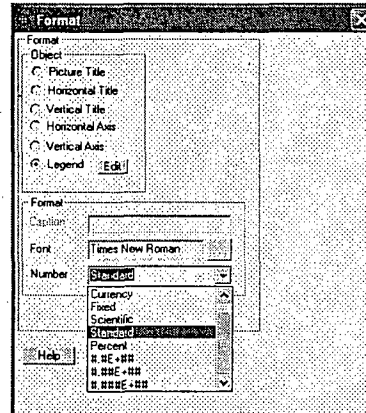
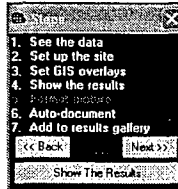
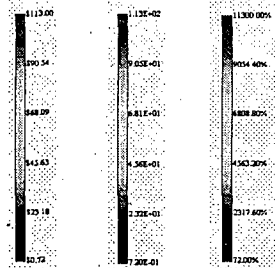
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Formatting Numbers on the Legend

Number Format

A number of different numbering formats are available for the legend.

Click on the Format Picture step, then select Legend from the Object frame, and select from Currency, Scientific, Percent, etc. formats.



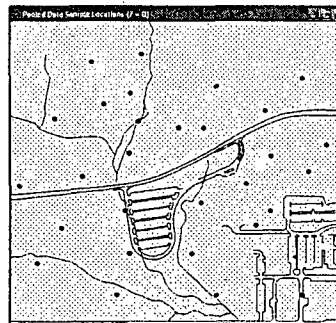
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Pooling Data

Pooling data provides a way for users to apply modeling and summarization applications to all contaminants within a particular data type at once.

Select **Pooled Data** from the **Data Name** box. The data plot demonstrates the distribution of information locations across space. Pooled data sources may extend over rads and nonrads and may be modeled with varying interpolation schemes.



To include or exclude contaminants from the pooled data results, see the **Contaminant Manager**.

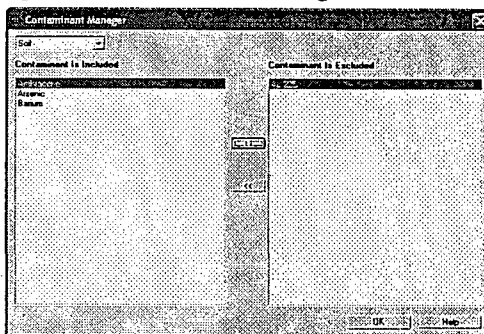
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Contaminant Manager

At any time, you may remove a contaminant from the analysis (or add it back) with the contaminant manager. This is useful for removing non-COCs from further analysis.

To access the manager, select **Contaminant Manager** from the **Tools Menu**.



Select contaminants to remove from the analysis and press the >> button. Similarly, choose contaminants that have been excluded and press the << button.

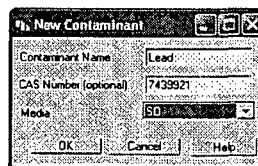
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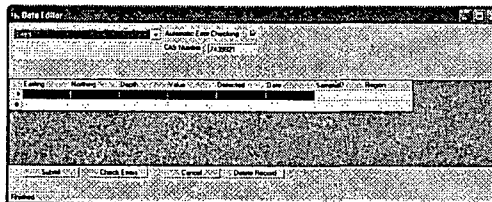
Adding a New Contaminant

To add a new contaminant to an existing SADA file, select **Add a New Contaminant** from the **Tool Menu**.

At the **New Contaminant** window, enter the name of the new contaminant and the CAS number and select the media. Press **OK** for SADA to present the **Data Editor**.



Enter the applicable sample values and press **Submit**.



Note: to add new data for an existing contaminant, use the **Data Editor** from the **Tools Menu**.

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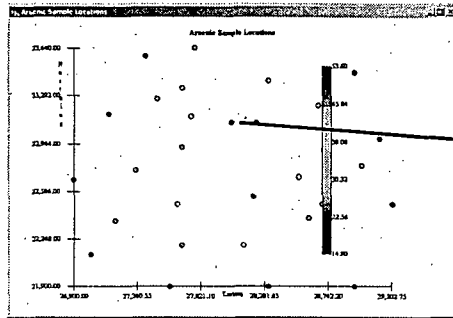
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Getting Information

There are several ways to get basic information from SADA.

Steps Window Information

Click on a data point to retrieve all available information about that data point from the SADA file on the Steps Window.



Field	Value
Name	Ac-Z25
CaseNumber	14255951
Easting	22042.5
Northing	23100
Depth	0
Value	4.9
Detected	
MinValue	0.0

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Getting Information

Basic Information

Use the **Information** button to retrieve all available information on every data point (or modeled value). When a polygon tool is on, this will return only those points found in the polygon.

ID	Name	CaseNumber	Easting	Northing	Depth	Value	Detected
7	Ac-Z25	14255951	27150	23160	0	1.70251	1
19	Ac-Z25	14255951	27280	22390	0	2.03	1
13	Ac-Z25	14255951	27417.75	22590	0	1.92566	1
14	Ac-Z25	14255951	27586.25	21900	0	1.9857	1
14	Ac-Z25	14255951	27625.5	22200	0	2.05229	1
8	Ac-Z25	14255951	27625.5	22520	0	2.305226	1
14	Ac-Z25	14255951	27774.75	23640	0	2.83644	1
9	Ac-Z25	14255951	28042.5	23100	0	4.95262	1
5	Ac-Z25	14255951	28131.75	22200	0	4.185278	1
17	Ac-Z25	14255951	28200	22560	0	4.8	1
10	Ac-Z25	14255951	28221	23100	0	4.232573	1
15	Ac-Z25	14255951	28310.25	23400	0	3.121863	1
11	Ac-Z25	14255951	28667.25	23220	0	2.951485	1
18	Ac-Z25	14255951	28700	22500	0	3.3	1
3	Ac-Z25	14255951	28935	21900	0	0.86314	1
16	Ac-Z25	14255951	28935	23460	0	0.83135	1
12	Ac-Z25	14255951	29113.5	22980	0	0.99677	1
6	Ac-Z25	14255951	29202.75	22500	0	1.49798	1
25	Barium	7440393	27150	23160	0	36.46381467	1

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Viewing Duplicates

- Duplicate values can be accessed from the data query table or from the map.
- Open `twodimensionalwithduplicates.sda`
- Blue lines in the data query window indicate duplicates at that location. Click on it to bring up a table of the duplicate values and how it was resolved.
- Change the data label to "detect" and click on the "Dup" location to view the information in the lower left of the screen.

The screenshot displays the SADA interface with several windows:

- Information Retrieval:** A table with columns: Name, Casrnumber, Easting, Northing, Depth, Value, Detected. It lists multiple entries for 'Ac-225' with various coordinates and values.
- Duplicate Data:** A dialog box titled 'Data checked duplicate values were processed. It means that one was available. The maximum value was chosen.' It shows a table with columns: Name, Casrnumber, Easting, Northing, Depth, Value, Detected, Maska, Date. It lists three entries for 'Ac-225' at coordinates (28310.25, 21300) with values 1.50, 1.50, and 3.1.
- Field Value:** A small table showing the current field value for 'Ac-225' at coordinates (28310.25, 21300) with a value of 3.1.

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Questions?

Comments?

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Spatial Analysis and Decision Assistance (SADA) Version 4 Statistics

Environmental Assessment Methods in SADA
University of Tennessee, Knoxville



Data Quality Objectives

The DQO Process is a seven-step planning approach to develop sampling designs for data collection activities that support decision making. This process uses systematic planning and statistical hypothesis testing to differentiate between two or more clearly defined alternatives.

USEPA 2006. Guidance on Systematic Planning Using the Data Quality Objectives Process. EPA QA/G-4.

<http://www.epa.gov/quality/qs-docs/g4-final.pdf>

Data Quality Assessment

DQA is the scientific and statistical evaluation of data to determine if data obtained from environmental data operations are of the right type, quality, and quantity to support their intended use.

USEPA 2006. Data Quality Assessment: Statistical Methods for Practitioners. EPA QA/G-9S.

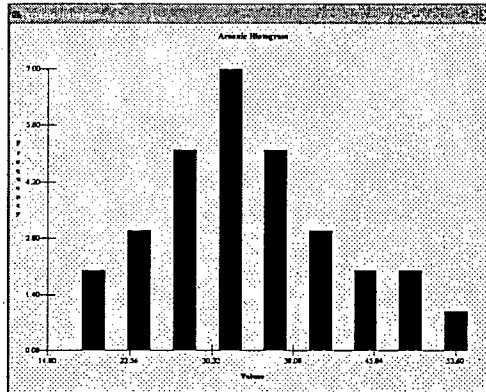
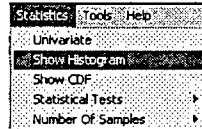
<http://www.epa.gov/quality/qs-docs/g9s-final.pdf>



View Histogram

A histogram is a graphical display of tabulated frequencies. It groups data into bins and plots the number of members for each bin.

Select the **Show Histogram** drop down menu item under Statistics to view a histogram for the selected contaminants.

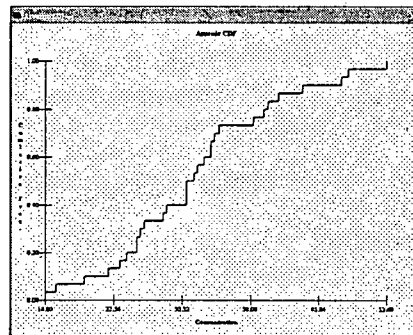
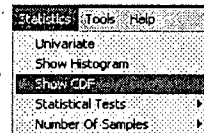


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Ranked Data Plot- Cumulative Distribution Function

A ranked data plot is a plot of the data ranked from smallest to largest plotted along the concentration axis.

Select the **Show CDF** drop down menu item under Statistics to view a cumulative distribution function for the selected contaminants.




Line Query

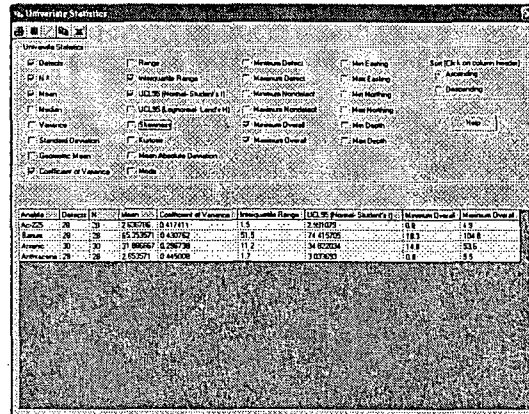
Click the **Line Query** button to pull specific cumulative frequencies off the plot for given concentrations.

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Univariate Statistics

Statistics 

Use the **Statistics** button to calculate univariate statistics on every data point (or modeled value). When a polygon tool is on, this feature will return only those points found in the polygon.



Variable	Count	N	Mean	Std. Deviation	Minimum	Maximum	Minimum Overall	Maximum Overall
Acidity	20	20	1.20000	.4472141	0.5	2.00000	0.5	2.0
Barium	20	20	45.25250	6.432762	31.5	74.41250	31.5	104.8
Arsenic	20	20	37.88026	6.296738	11.2	54.82026	11.2	55.5
Ammonia	20	20	1.02525	0.444008	0.2	1.90000	0.2	1.9

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Univariate Statistics- Detects

- Detections- the number of total samples that were detected
- N- the number of samples collected
- Minimum Detect- the lowest detect value found in the dataset
- Maximum Detect- the highest detected value found in the dataset
- Minimum Non-detect- the lowest detect value found in the dataset
- Maximum Non-detect- the highest detected value found in the dataset
- Minimum Overall- the lowest detect value found in the dataset
- Maximum Overall- the highest detected value found in the dataset

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Univariate Statistics- Central Tendency

- Mean- the sum of the values of a variable divided by the number of values, affected by each value in the data set, including extreme values

$$\bar{X} = \frac{1}{n} \sum_{i=1}^n X_i$$

- Geometric Mean- exponential of the arithmetic mean of the logarithm transformed values, used for lognormally distributed data

$$\exp \left[\frac{1}{n} \sum_{i=1}^n \ln x_i \right]$$

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Univariate Statistics- Central Tendency

- Median- the middle value in an ordered array of numbers, the value below which 50% of the data values fall

odd n $\tilde{X} = X_{([n+1]/2)}$

even n $\tilde{X} = \frac{X_{(n/2)} + X_{([n/2]+1)}}{2}$

- Unaffected by very large or very small values

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Univariate Statistics- Measures of Spread

- Variance- a parameter that measures how dispersed a random variable's probability distribution is, the mean of the squares of the differences between the samples and their mean

$$S^2 = \frac{\sum (X - \bar{X})^2}{n - 1}$$

- Standard Deviation- the positive square root of the variance

$$S = \sqrt{S^2}$$

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Univariate Statistics- Coefficient of Variance

- Coefficient of Variance (CV)- the ratio of the standard deviation over the mean

$$CV = s / \bar{X} = \frac{[\frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X})^2]^{1/2}}{\frac{1}{n} \sum_{i=1}^n X_i}$$

- CV test for normal distribution:
 - There is a simple test based on the CV that can be used to reject the assumption that the data is normally distributed. If the CV > 1, then you can conclude that the data are not normally distributed. Otherwise, the test is inconclusive.

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Univariate Statistics- Measures of Spread

- Range- the difference between the lowest and highest values. Influenced by extreme values.

$$R = \text{maximum} - \text{minimum}$$

- Interquartile Range- the central portion of a distribution, calculated as the difference between the third quartile and the first quartile; this range includes about one-half of the observations in the set. Less influenced by extremes than the overall range.

$$IQR = y(75) - y(25)$$

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Univariate Statistics- Measures of Spread

- Mean Absolute Deviation- the mean of the absolute values of the differences between the respective samples and their mean

$$M.A.D. = \frac{\sum |X - \mu|}{N}$$

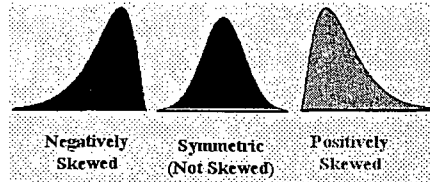
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Univariate Statistics- Measures of Skew

- Skewness- is a measure of symmetry, skewness for a normal distribution is zero, and any symmetric data should have a skewness near zero.

$$b_1 = \frac{1}{N} \sum_{j=1}^N \left(\frac{x_j - \bar{x}}{\sigma} \right)^3$$

- If $S < 0$, the distribution is negatively skewed (skewed to the left).
- If $S = 0$, the distribution is symmetric (not skewed).
- If $S > 0$, the distribution is positively skewed (skewed to the right).



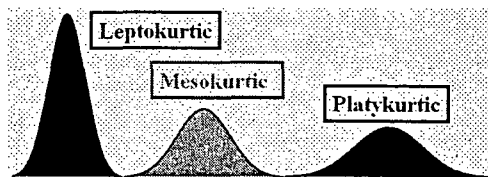
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Univariate Statistics- Measures of Skew

- Kurtosis- Kurtosis is a measure of whether the data are peaked or flat relative to a normal distribution.

$$b_2 = \frac{1}{N} \sum_{j=1}^N \left(\frac{x_j - \bar{x}}{\sigma} \right)^4$$

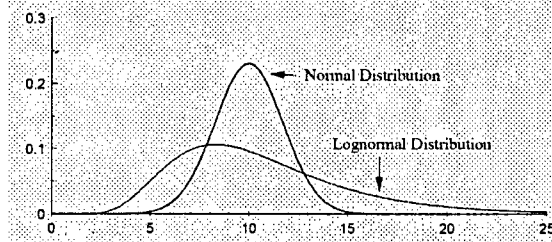
- Leptokurtic: high and thin (high kurtosis values)
- Mesokurtic: normal in shape
- Platykurtic: flat and spread out (low kurtosis values)



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Univariate Statistics- Confidence Limits

- Upper confidence limits primarily used as an exposure concentration for human health and ecological risk assessments
- SADA allows for confidence limits based on normal and lognormal distributions



- Normal distribution- UCL95- upper 95% confidence limit on the mean concentration of a normal distribution
- Lognormal distribution- Geometric UCL95- upper 95% confidence limit on the mean concentration of a lognormal distribution

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Statistical Tests

A statistical test is a procedure for deciding whether a hypothesis about a quantitative feature of a population is true or false.

It is used to determine the statistical significance of a result. Statistical tests separate significant effects from mere luck or random chance.

All hypothesis tests have unavoidable, but quantifiable, risks of making the wrong conclusion. Two main types of error can occur:

1. A type I error occurs when a true hypothesis is rejected (a false negative in terms of the null hypothesis).
2. A type II error occurs when a false hypothesis is accepted (a false positive in terms of the null hypothesis).

Decision Based on Sample Data	True Condition	
	Baseline is True	Alternative is True
Decide baseline is true	Correct Decision	Decision Error (False Acceptance)
Decide alternative is true	Decision Error (False Rejection)	Correct Decision

Guidance for the Data Quality Objectives Process USEPA 2000 QA/G-5, EPA/600/R-96/055 Spatial Analysis and Decision Assistance

Statistical Hypotheses

A null hypothesis is a statistical hypothesis that is tested for possible rejection under the assumption that it is true (usually that observations are the result of chance).

The alternative hypothesis is the hypothesis contrary to the null hypothesis.

The Null Hypothesis, is tested by:

- drawing a random sample from the population
- making a measurement of the feature
- calculating an appropriate function of the data
- comparing this statistic to a critical level

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Non-parametric Tests

A parametric test makes an assumption about the underlying distribution of observed data. A non-parametric test makes no such assumption.

Non-parametric tests:

- Do not assume Normal distributions
- Can handle non-detects
- Not sensitive to outliers
- Work nearly as well as parametric tests when data are normal

SADA currently implements two non-parametric tests used by the DQO and MARSSIM processes: the Sign Test and the Wilcoxon Rank Sum Test.

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One-sided v Two-sided Tests

A two sided hypothesis states that there is a difference between the two groups being tested, but does not specify in advance what direction you think this difference will be.

A one sided hypothesis states a specific direction (e.g., the site concentrations are greater than the reference site concentrations).

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Simple Sign Test Example

SADA implements a one-sided Sign Test for a contaminant data set versus a decision criterion (human health PRG, DCGL, ecological risk benchmark, custom value).

The Sign Test is a simple to implement test that makes the basic assumption that there is information only in the signs of the differences between paired observations, not in the magnitudes of the differences.

- 1) Take the paired observations, calculate the differences, and count the number of positive differences. This is the test statistic B.
- 2) A critical value for a given alpha level or a p-value is derived based on the binomial distribution or simply pulled from a table.
- 3) Null hypothesis is either accepted or rejected.

Arsenic Site Data	Delta for criterion = 10
12	+2
28	+18
8	-2
42	+32
16	+6
23	+13
45	+35
31	+21

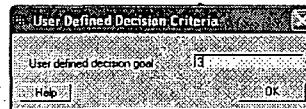
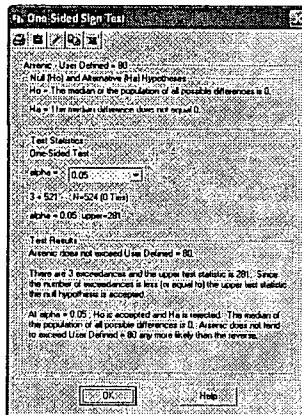
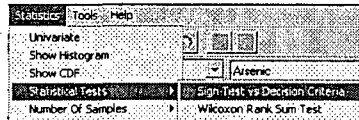
For N=8 and B=7:
p-value = 0.0352
critical value = 7 for
alpha = 0.05

Null is rejected

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Paired Statistics: Sign Test

•Conducts a one-sided Sign Test for a contaminant data set versus a decision criterion (human health PRG, DCGL, ecological risk benchmark, custom value)



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Wilcoxon Rank Sum Test

SADA implements a one-sided and a two-sided Wilcoxon Rank Sum Test (aka Mann-Whitney) for a contaminant data set versus another contaminant data set.

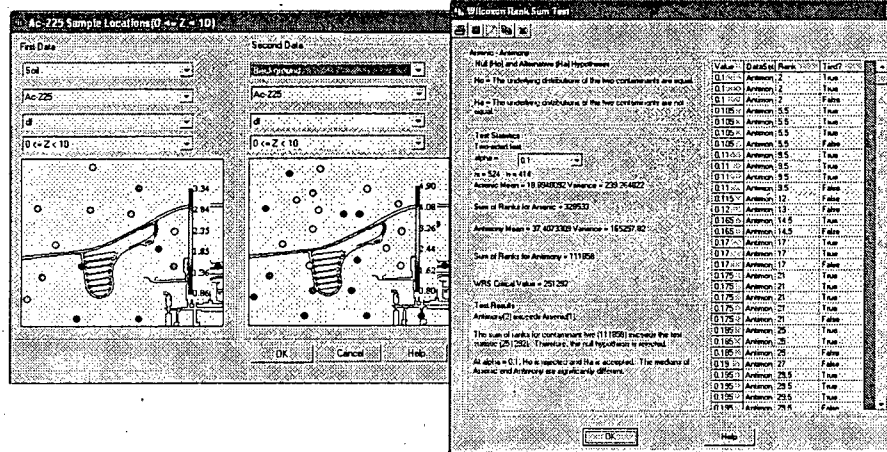
The Wilcoxon Rank Sum test uses a sum of ranks comparison to determine if the two data sets have different means

1. Combine data sets and order from lowest to highest.
2. Sum the ranks for the two different populations.
3. Compute the Wrs test statistic (different forms depending on if there is ties)
4. Compare to critical value for m and n sample sizes
5. Null hypothesis is either accepted or rejected.

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Paired Statistics: Wilcoxon Rank Sum

• Conducts a Wilcoxon Rank Sum Test (Mann-Whitney) for a contaminant data set versus a background data set (or some other data set of your choosing)



Determining Number of Samples

You Pick

- User enters number of samples based on some outside decision.

Sign Test

- Sample size is determined using the non-parametric Sign test, user inputs decision criterion, LBGR, acceptable Type I and II error rates

Wilcoxon Rank Sum

- Sample size is determined using the non-parametric Wilcoxon Rank Sum test, user inputs decision criterion, LBGR, acceptable Type I and II error rates

Determining Number of Samples Sign Test

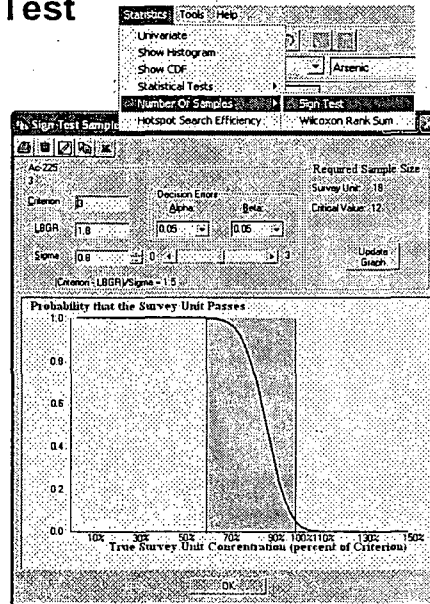
Use if contamination is not present in background and measurements are radionuclide-specific or use if background levels are a small fraction of the decision criterion

Evaluates whether the median of the data is above or below the decision criterion

Survey reference area is not necessary

Compare contaminant levels with decision criterion values

Each measurement below the decision criterion contributes evidence that the survey unit is clean and the null hypothesis should be rejected



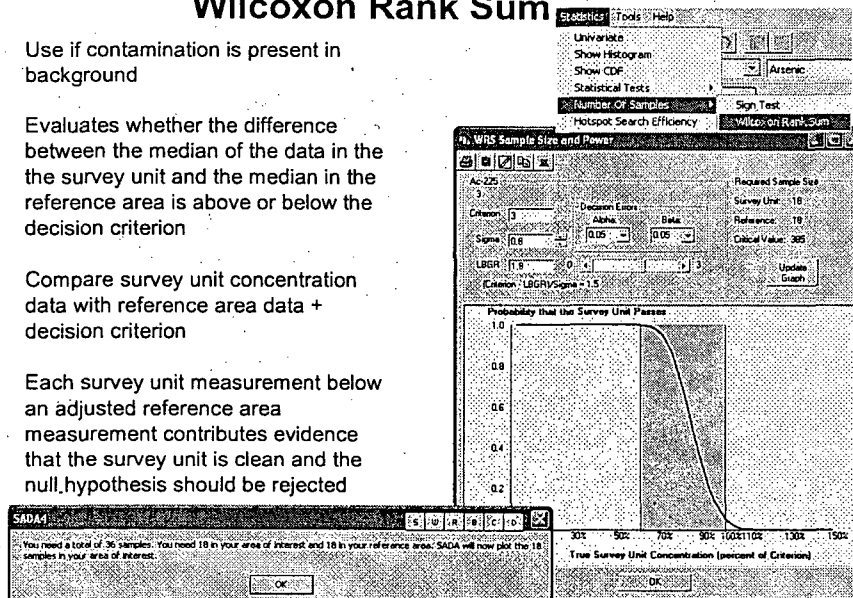
Determining Number of Samples Wilcoxon Rank Sum

Use if contamination is present in background

Evaluates whether the difference between the median of the data in the the survey unit and the median in the reference area is above or below the decision criterion

Compare survey unit concentration data with reference area data + decision criterion

Each survey unit measurement below an adjusted reference area measurement contributes evidence that the survey unit is clean and the null hypothesis should be rejected



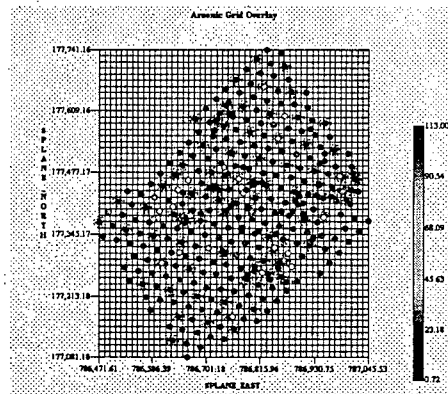
MARSSIM Functionality in SADA 4

- Calculate sample size based on Sign Test and WRS Test; incorporating DCGLs, decision variables, area factors, instrument sensitivity
- Develop initial sample design (MARSSIM grid or simple random)
- Post sampling analysis (A site passes or fails)
- Detecting and Defining Elevated Areas

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Overview of LISA Maps

- Local Index of Spatial Association (LISA) displays show maps of moving window statistics, these statistics are calculated at each grid node and the results displayed
- Ripley's K- sampling intensity with each window
- Moran's I- measure of correlation between all points in each window
- Geary's C- semivariance calculation (average dissimilarity) between points within each window



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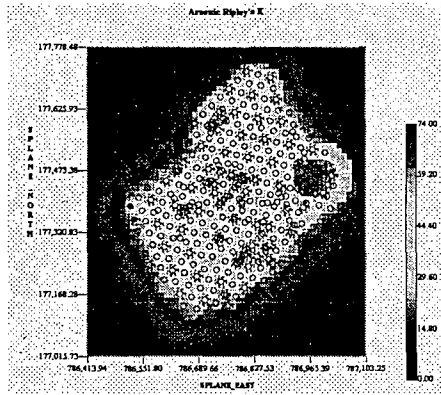
Ripley's K

- Ripley's K- sampling intensity with each window
- Users must first specify a LISA Search Radius
- Quantifies the spatial pattern intensity of points for various sizes of a circular search window
- Computes the overall mean number of points located within a search window of radius t :

$$\hat{K}(t) = \frac{\lambda^{-1} \sum_{i=1}^n \sum_{j=1}^n I_t(e_i, e_j)}{n}$$

for $i \neq j$ and $t > 0$

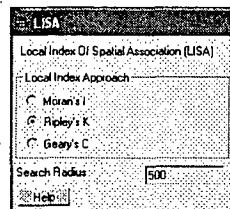
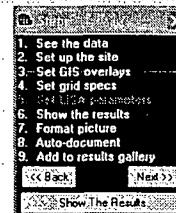
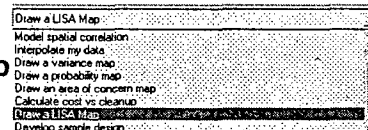
- γ is point intensity (n/A), I_t is an indicator of whether inside search window
- There is an edge correction effect for grid areas on the fringe



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Producing LISA Maps

- Select **Draw a LISA Map** from interview menu
- Click **Set LISA Parameters Step**
- Select a **Local Index Approach**
- Enter a **Circular Search Radius** for the moving window
- Click **Show the Results**



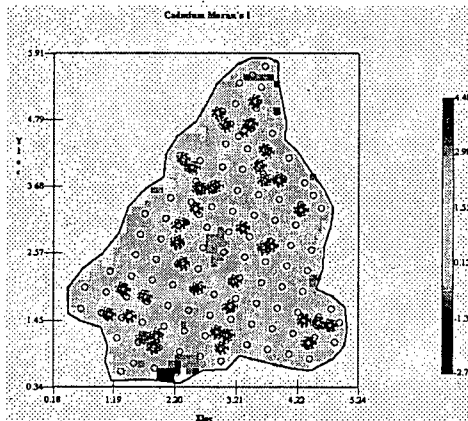
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Moran's I

- Moran's I- measure of correlation between all points in each window
- Users must first specify a LISA search radius
- Computes the degree of correlation between the values of a variable as a function of spatial lags
- Similar to Pearson's correlation coefficient, ranges from -1 (-correlation) to 1 (+ correlation), expected value close to 0

$$I(d) = \frac{\sum \sum w_{ij}(d)(x_i - \bar{x})(x_j - \bar{x})}{\frac{W(d)}{\sum (x_i - \bar{x})^2} n}$$

- $w_{ij}(d)$ indicates whether pairs are in the same distance class, $w(d)$ is the sum of $w_{ij}(d)$

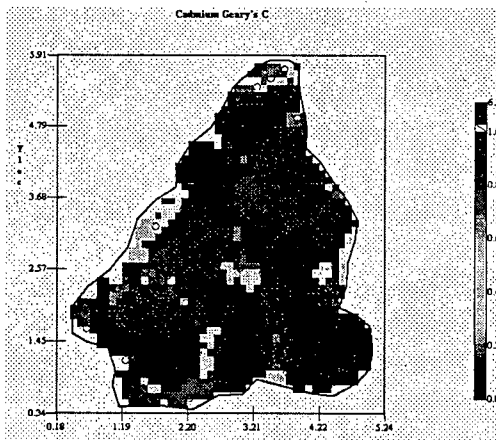


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Geary's C

- Geary's C- semivariance calculation (average dissimilarity) between points within each window
- Needs pretty high sampling densities to be informative
- Users must first specify a LISA Search Radius
- Measures the semivariance (average dissimilarity) among values of a variable at nearby locations

$$c(d) = \frac{\sum \sum w_{ij}(d)(x_i - x_j)^2}{\frac{2W(d)}{\sum (x_i - \bar{x})^2} (n - 1)}$$



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Future Statistics for SADA

- Hypotheses testing (t-test, Wilcoxon Signed Rank test, Quantile test)
- Distribution Fitting (Shapiro-Wilks,)
- Bivariate Statistics (Pearson and correlation coefficients, scatter plots, regression)
- ProUCL
- Additional methods for determining sample size
- Improved histogram and other data plots (ranked data, quantile)
- Cluster (spatial stats, autocorrelation, tests)
- Trend testing (time plots, Mann-Kendall)
- Tests for outliers

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Questions?

Comments?

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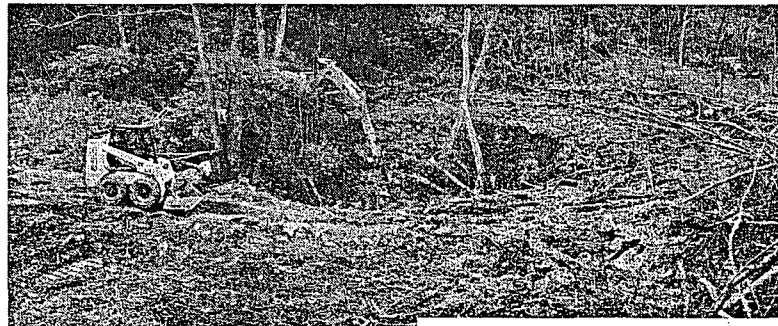
Practice Session Importing Data, Exploration, Statistics

The objective of this lesson is to be able to create a SADA file from a comma-delimited file, then use the SADA interface to explore the data sets and generate basic statistics.

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Practice Session: Importing Data, Exploration, Statistics

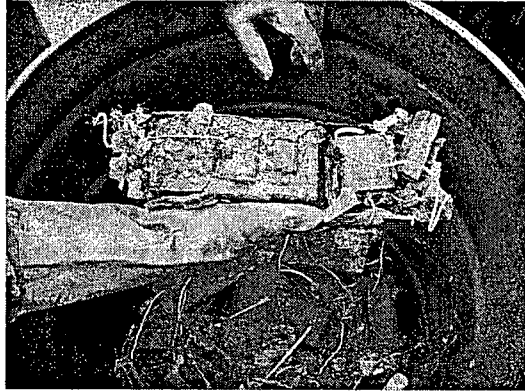


I-40/I-640 Site

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Practice Session: Importing Data, Exploration, Statistics

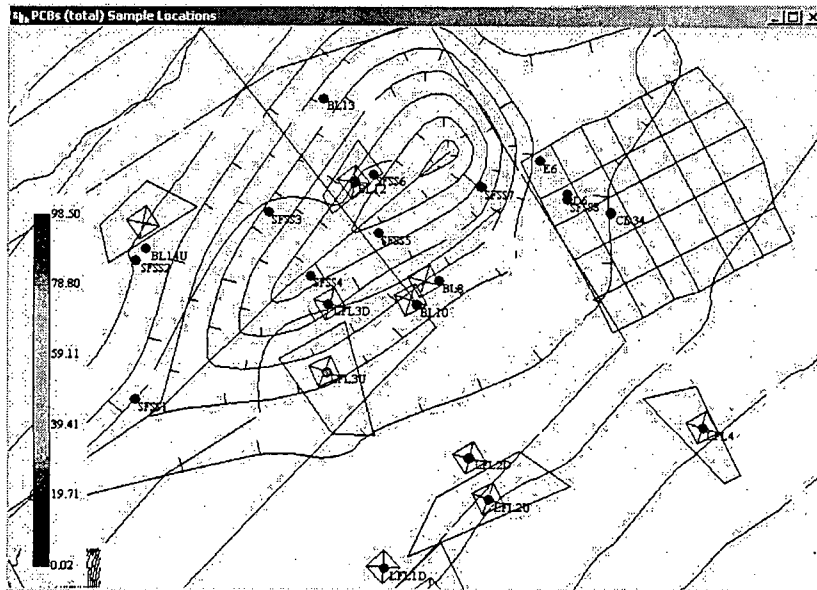


1. Knoxville, TN
2. Disposal (fluorescent light ballasts)
3. Metals, PCBs, Pesticides

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Practice Session: Importing Data, Exploration, Statistics



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Practice Session: Importing Data, Exploration, Statistics

1. Create a new SADA file called "Lesson2.sda" using the comma-delimited file lesson2.csv. Match headers to the appropriate categories:
 - a. Easting-Easting
 - b. Northing-Northing
 - c. Depth-Depth
 - d. CAS Number – CAS #
 - e. Contaminant Name – ANALYTE
 - f. Values – Value
 - g. Detect Qualifier – detect
 - h. Media ID – Media
 - i. Date – DATE COLLECTED
2. Check for errors and submit, then save your SADA file
3. Add the GIS layer called SITE_MAP2.dxf



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Practice Session: Importing Data, Exploration, Statistics

4. Set Contaminants to Pooled Data to see all data locations.
5. Right-click on the map to zoom in on the sinkhole, then restore full view.
6. Press the information button to see how and where duplicates were resolved (blue font in table).
7. Under Step 1. See the Data- change duplicate resolution from Use Only Detected Values to Use All Values. Change Use Maximum value to Use Average Value. For non-detects, change Use half the detection limit to Use the full detection limit.
8. Select Aroclor-1248 and customize the legend using a categorical legend scale.



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Practice Session: Importing Data, Exploration, Statistics

9. Set the Data Labels to "Value" to show the Aroclor-1248 location with a concentration of 29.14. Find the coordinates and sample collected data of this point by clicking on it and viewing the small table on the lower left of the screen.
Northing _____
Easting _____
Date Collected _____
10. Remove Calcium, Magnesium, Potassium, and Sodium from the analysis using the Contaminant Manager.
11. Select Pooled Data and run the Univariate Statistics function. Record the detection frequency and standard deviation for Aroclor-1248
Detection Frequency _____
Standard Deviation _____

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Practice Session: Importing Data, Exploration, Statistics

10. Run the Sign Test Sample Size and Power and set the Criterion to 21, LBGR to 14, alpha to 0.1, beta to 0.1, and the sigma to the value you recorded for the Univariate Statistics in #11. Check the number of samples you have versus what this test shows that you need. Do you have a sufficient sample size to achieve the desired power?

11. Run the one-sided Sign Test with alpha = 0.05 for Aroclor-1248 versus a criterion of 21. Is the null hypothesis (the data does not exceed 21) accepted or rejected?

12. Draw a LISA Ripley's K map with a search radius of 25 to view areas of high and low sampling density.
13. Save file- we will use this file again for practice session 5.

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Spatial Analysis and Decision Assistance (SADA) Version 4 Basic Spatial Analysis

Environmental Assessment Methods in SADA
University of Tennessee, Knoxville

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Basic Spatial Analysis Tools

"All models are wrong; some models are useful."

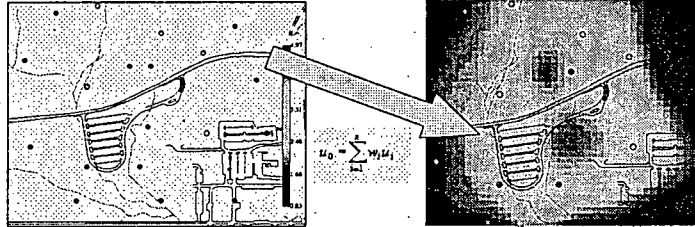
George Box, Professor Emeritus, University of Wisconsin

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Basic Spatial Analysis Tools

Spatial interpolation is used to predict values between sampled locations.



The methods discussed throughout this text estimate the unsampled location as a weighted linear combination:

$$u_0 = \sum_{i=1}^n w_i u_i$$

Where u_0 is the estimate, u_i are the sampled data and w_i are the weights assigned to the data values.

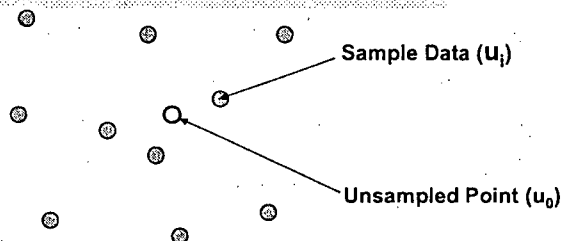
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Basic Spatial Analysis Tools

An easy illustration of how one could use such a system is to assume that all the weights are equal to $1/N$. In this scenario, the value at the unsampled point is simply equal to the average of all the samples surrounding it.

$$u_0 = \sum_{i=1}^n \frac{1}{N} u_i = \frac{1}{N} \sum_{i=1}^n u_i = \frac{\sum_{i=1}^n u_i}{N} = \bar{u}$$



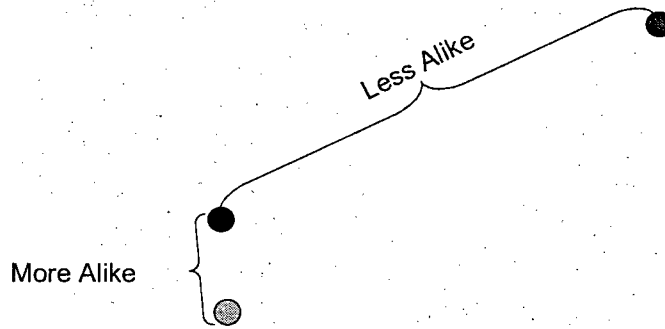
The difference between the methods is how they arrive at the weights for each sampled point.

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Determining Weights

All of the methods presented here generally work on the principle that data points closer are more alike than data points farther away. This plays a key role in all of the approaches to weighting sample values.

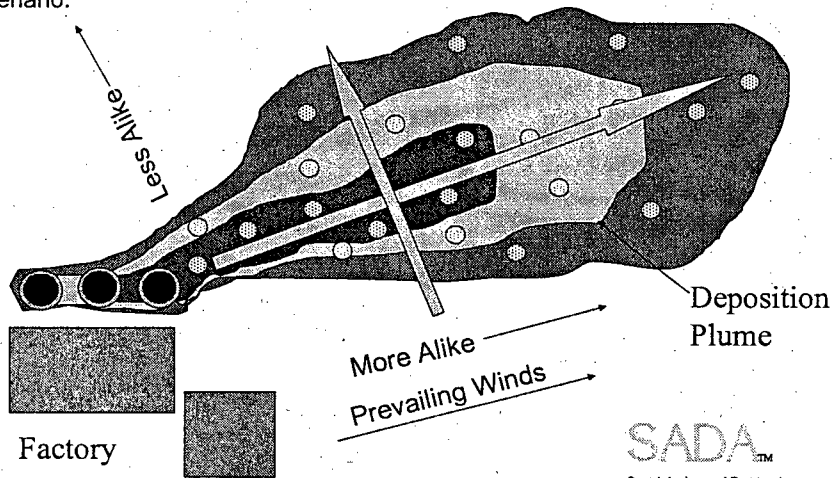


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Spatial Anisotropy

One example of spatial correlation would occur with a plume or deposition scenario.

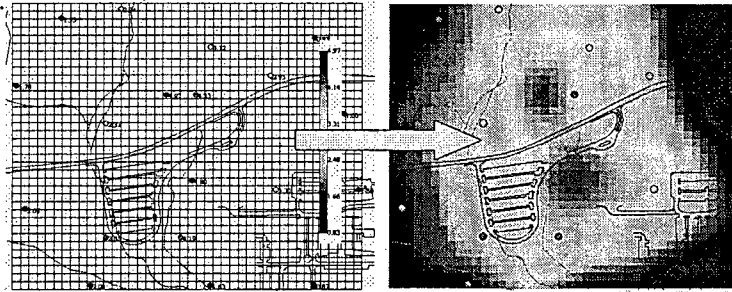


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Grid Definition

Rather than estimate values at only a single point, we wish to estimate them at a number of points in order to fill in the picture of contamination. All spatial interpolators in SADA depend on a grid definition to function. A grid definition simply describes the number, size, and location of a uniform set of blocks. These blocks will be the focus of the interpolation schemes. SADA's interpolation schemes will estimate the concentration value at the center of each block. From the interview list choose **Interpolate My Data**. Select **Set Grid Specs** from the **Steps Window** to define the grid. Press **Show Grid** to see your result.



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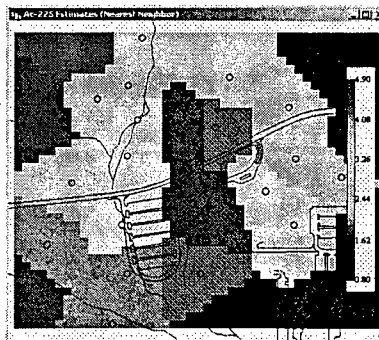
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Nearest Neighbor

This is the simplest of all interpolants in SADA. Any unsampled point is simply equal to the data point closest to it. In our previous notation we would describe Nearest Neighbor as

$$u_0 = \sum_{i=1}^n w_i u_i \quad \text{where } w_i = \begin{cases} 1 & \text{if } u_i \text{ is the nearest value} \\ 0 & \text{otherwise} \end{cases}$$

- Choose **Interpolation methods** and then select **Nearest Neighbor** from the list of available interpolants.
- Press **Show The Results** to see the map.



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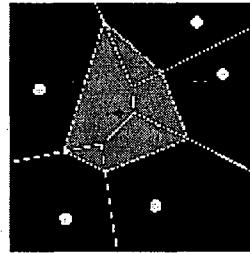
Natural Neighbor

In natural neighbor we allow more than the nearest neighbor to influence the estimation. When data points are distributed in space they are inherently representing a certain area around them. Sample points in sparsely sampled regions must represent a higher region than those in more densely sampled areas. These regions are called *area of influence* and it is possible to draw simple geometries that bound them.

In natural neighbor, the areas of influence are calculated first. Then the area of influence for the point we wish to estimate is overlaid creating regions of overlapping areas of influence. For any given sample point, the portion of the overlap becomes the weight assigned to that sample point.

$$u_0 = \sum_{i=1}^x \frac{a_i}{A} u_i$$

Where A is the area of influence for u_0 and a_i is the area of overlap between u_0 and u_i .

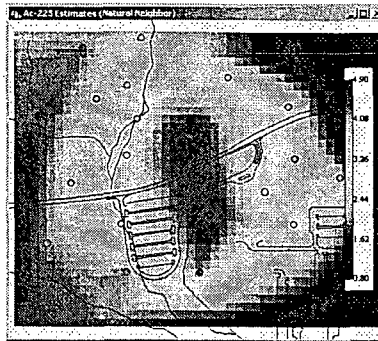


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Natural Neighbor

- Press **Interpolation methods** and then select Natural Neighbor from the list of available interpolants.
- Press **Show The Results** to see the map.



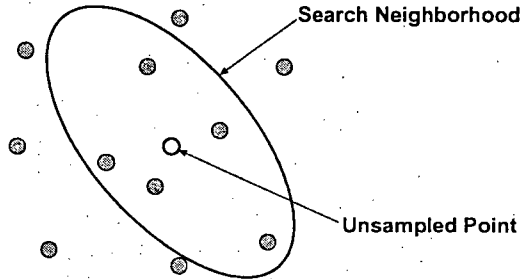
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Inverse Distance

The estimated value V_0 at an unsampled location is estimated as the weighted average of nearby values.

$$V_0 = \sum_{i=1}^N w_i V_i$$



Inverse Distance

$$w_i = \frac{1}{d_i^p \sum_{j=1}^N d_j^{-p}}$$

w_i is the weight for the i th neighbor
 d_i is the distance of the i th neighbor
 p is the power
 N is the number of neighbors within the search neighborhood

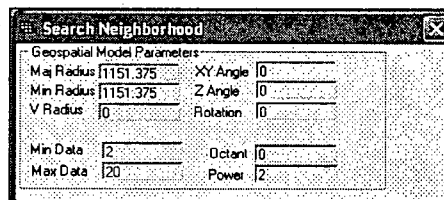
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Search Neighborhoods

Inverse distance requires a neighborhood definition for estimating concentration values at a point. A neighborhood is defined as an area around the point in which data values will be used to estimate the concentration value. Data values outside the neighborhood will be excluded.

The neighborhood is always defined by a search ellipse that can be manipulated in shape and size to include or exclude various data. The parameters which control the shape and size of the search ellipse are entered on the **Parameters Window** when **Search Neighborhood** is selected from the **Steps Window**.



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Search Neighborhoods

The parameters Major Radius, Minor Radius, and XY Angle control the size and shape of the search ellipse.

Major Radius

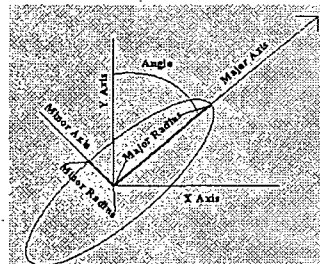
The long radius of the ellipse.

Minor Radius

The short radius of the ellipse.

XY Angle

The angle or direction the long radius points. This angle is measured clockwise from the positive Y axis (0 deg is North). The minor elliptical axis is perpendicular to the major axis.



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Search Neighborhoods

For three-dimensional data, the ellipse becomes an ellipsoid. The following parameters, in addition to those listed above, describe the search ellipsoid in 3D space.

Z Angle

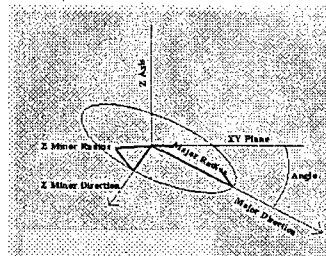
The angle or dip below the XY plane at the point of estimation. This angle is measured as negative degrees below the plane.

V Radius

Also referred to as Z minor radius, it is the radius of the ellipse in the vertical direction.

Rotation

The parameters described to this point fully form the body of the ellipsoid in 3D space. The rotation parameter then rotates this ellipsoid about the major axis the specified number of degrees.



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Search Neighborhoods

The following view shows the effect of the rotation parameter on the ellipsoid body. This view is along the major elliptical axis. The rotation angle rotates two orthogonal directions clockwise relative to the major elliptical axis when looking toward the origin. The following parameters define the search criteria within the search ellipse.

Min Data

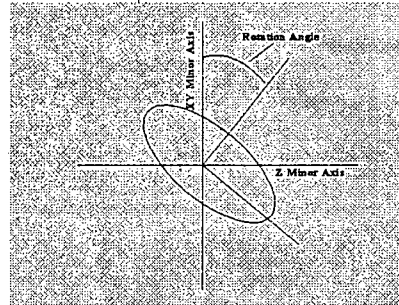
The minimum number of data required before estimating the concentration. If the minimum is not met, SADA returns an unestimated value. These values become empty spaces in the plot.

Max Data

The maximum number of data to use in estimating a point.

Octant

The ellipsoid is divided into quadrants, four if two-dimensional, eight if three-dimensional. If the Octant value is greater than zero and there are fewer data points than the octant value in each quadrant, then the point will not be estimated.

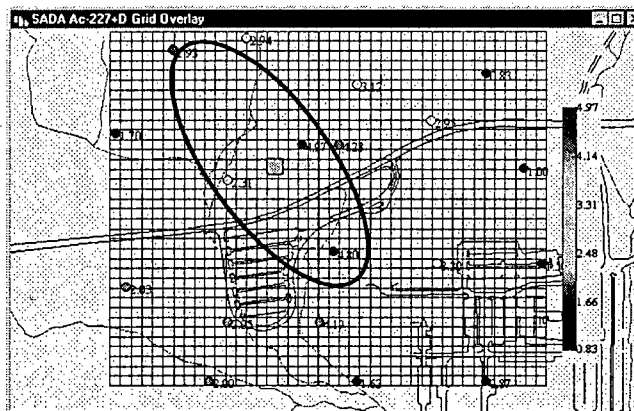


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Search Neighborhoods

Neighborhoods allow the user to search for a single unsampled point.



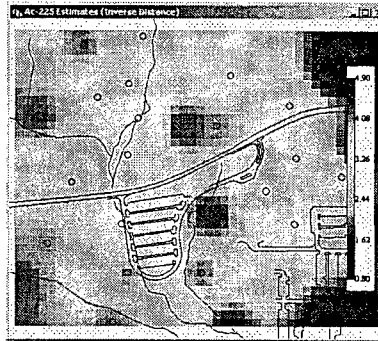
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Inverse Distance in SADA

- Press **Interpolation methods** and then select Inverse Distance from the list of available interpolants.
- Setup an appropriate search neighborhood and specify the power parameters after selecting **Search Neighborhood**.
- Press **Show The Results** to see the map.

Inverse Distance Estimates Map

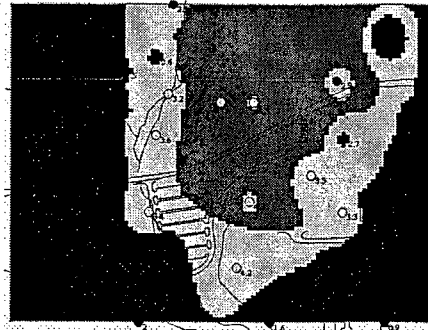
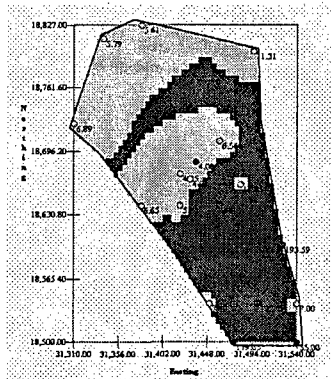


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Extreme Value Effects

Interpolations can be “smeared” by extreme valued points causing an inaccurate elevation of interpolated values for great distances.

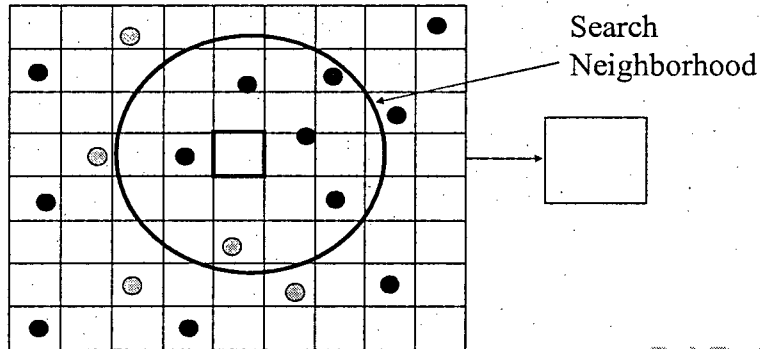


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Extreme Value Effects

Extreme values can have unwanted effects on the interpolation model particularly for those that use search neighborhoods. These extreme values can cause high value "smears" or other artifacts in the result.

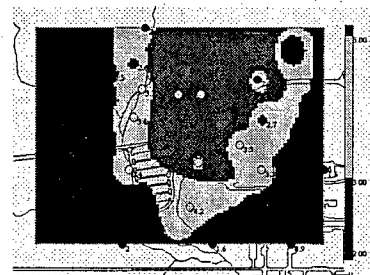
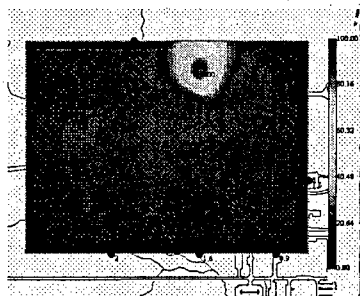


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Extreme Value Effects

Sometimes smearing can go unnoticed because of the designation of the legend. Linear continuous legends tend to mask smearing. Categorical legends often better reveal smearing effects.



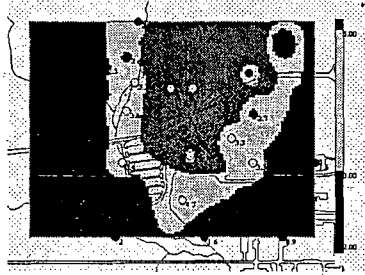
Here we have exactly the same interpolation results displayed in two different ways: with a smooth linear legend and a categorical legend. Notice how the smearing is highlighted in the later plot.

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Addressing Extreme Value Effects

Smearing effects can be dealt with in various ways. In inverse distance, the power value (p) may be increased. By increasing the value of p , data points have very small influences over even short distances. Other methods include decreasing the search radius.



Power = 2



Power = 7

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Cross Validation

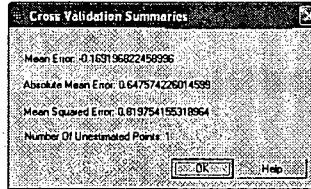
- Cross validation is the process of determining how well our modeling is reflecting reality.
- The truth is that we will almost never know how well it is performing since we will likely never have samples at every point we estimate. If we did we could simply compare them and evaluate the model performance.
- As an approximation to this approach, we can cross validate by removing one at a time each sample that we do have and allow the model to predict its value based on the remaining data
- We can then compare this estimate with the real value and make comparative statements between the different models.
- It is important to remember that cross validation provides evidence (rather than proof) of how a model is performing since in each estimation we have $N-1$ samples rather than N .
- To cross validate click on cross validation and choose a method.
 - Plot Error (Simple subtraction of estimated and real values)
 - Plot Absolute Error (Absolute value of the difference in real and estimated values)
 - Plot Percentage Error (Absolute difference/Real value *100)

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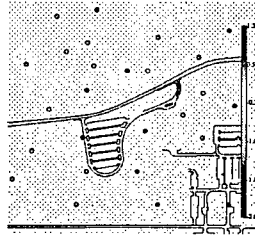
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Cross Validation

- SADA produces a summary of the model's performance. This can be compared across models as form of performance assessment.
 - Mean of errors
 - Absolute mean error
 - Mean squared error
 - Number of unestimated points



- Pressing Ok SADA will show the graphical result. These results can understanding about model performances in regions of the site.



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Questions?

Comments?

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Practice Session Basic Spatial Analysis Tools

The objective of this lesson is to practice setting up and using Nearest Neighbor, Natural Neighbor, and Inverse Distance to create contour maps. Also, each method's performance is compared via cross validation techniques.

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Practice Session: Basic Spatial Analysis Tools

1. Open up "Lesson3.sda". Choose the "Interpolate My Data" interview and turn on the polygon "Boundary".
2. Select set grid specs and view it. Notice the part outside the polygon turns grey. This part of the grid is not used in the analysis.
3. Use the Nearest Neighbor method to contour the area inside the polygon.
4. Add this to the results gallery as "Nearest Neighbor".

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Practice Session: Basic Spatial Analysis Tools

5. Cross validate the Nearest Neighbor method. Add the results here.
Mean Error _____
Absolute Mean Error _____
Mean Squared Error _____
Add the graphical result to the results gallery as "Nearest Validate".
6. Use the Natural Neighbor method to contour the area inside the polygon. Add this to the results gallery as "Natural Neighbor".
7. Cross validate the Natural Neighbor method. Add the results here.
Mean Error _____
Absolute Mean Error _____
Mean Squared Error _____
Add the graphical result to the results gallery as "Natural Validate".

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Practice Session: Basic Spatial Analysis Tools

8. Use the Inverse Distance method to contour the area inside the polygon. Notice now that you need to fill in the Search Neighborhood parameters. Initially, try a major and minor radius of 150. Set the V radius to 1. Min data should be 1, and max data should be 20. For now, xy angle, z angle, rotation, and octant should all be 0. Set the power to 2.
9. Try changing the power to 4. Notice the affect on the map.
10. Try changing the minor radius to 75. What happens? Leaving the minor radius as 75, change the xy angle to 135 and reapply. Notice how preference is now given to the 135 degree angle. The contours now stretch along this 135 line.

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Practice Session: Basic Spatial Analysis Tools

11. Try changing other parameters and see how they affect the final outcome.
12. Now change the parameters back to those found in step 8. Reapply and add it to the results gallery as "Inverse Distance".
13. Cross validate the Inverse Distance method. Add the results here.
Mean Error _____
Absolute Mean Error _____
Mean Squared Error _____
Add the graphical result to your results gallery as "Inverse Validate".

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Practice Session: Basic Spatial Analysis Tools

14. Switch from Soil to Results Gallery and review your results. Which one is doing better? Think about what kinds of criteria could be used for determining which one performs better.
15. Copy these images into PowerPoint or Word, where you can see them side by side.

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Spatial Analysis and Decision Assistance (SADA) Version 4 Advanced Spatial Tools

Environmental Assessment Methods in SADA
University of Tennessee, Knoxville

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Advanced Spatial Tools

“Most people use statistics as a drunkard uses a lamppost, more for support than illumination.”

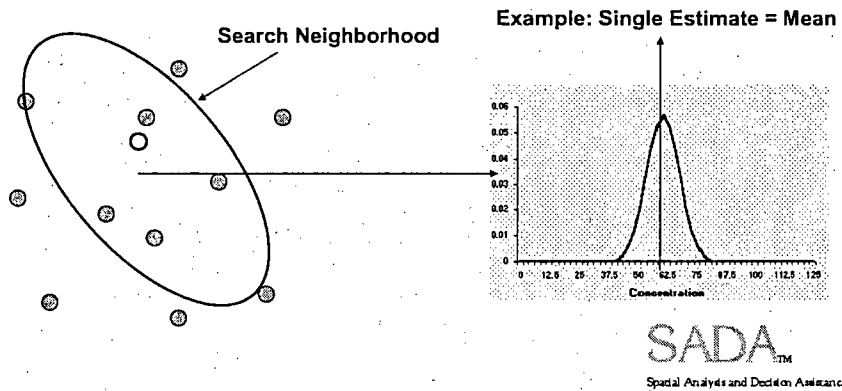
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Part 7: Advanced Spatial Tools (Geostatistics)

With basic spatial analysis tools, each interpolant produced a single estimate for each unsampled point. With a geostatistical approach, a distribution of possible values is constructed and used as a model for the actual unsampled value. Both an estimate and a model of uncertainty can be now obtained. From this distribution of points, a central moment, such as the mean or media, is chosen as a single estimate for contouring purposes.



Geostatistics

SADA provides two kriging (geostatistical) models: Ordinary and Indicator kriging. Ordinary kriging assumes a normal or lognormal distribution for the data. Indicator kriging is a non parametric approach that does not assume any distribution.

Like the methods discussed in Basic Spatial Analysis Tools, both methods are based on a weighted combination of nearby samples. However, the development and expression of these weights is quite complex and beyond the scope of this training guide.

It may be helpful to think of kriging as an advanced form of the inverse distance method. Recall that the inverse distance method weights sampled values by their distance from the unsampled location.

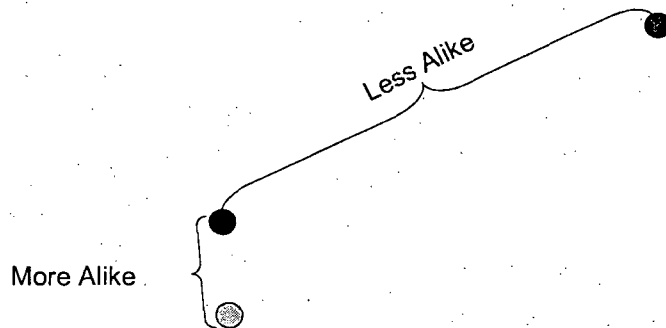
Kriging approaches the problem in much the same way. However, rather than distance (d), the weights are based on the amount of *spatial correlation* or *spatial covariance* that samples exhibit at varying distances $C(d)$.

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Spatial Correlation

If data are spatially correlated, then on average, sample points that are close to each other are more alike than sample points further away. (More complex spatial correlations exist but this type is the most common).

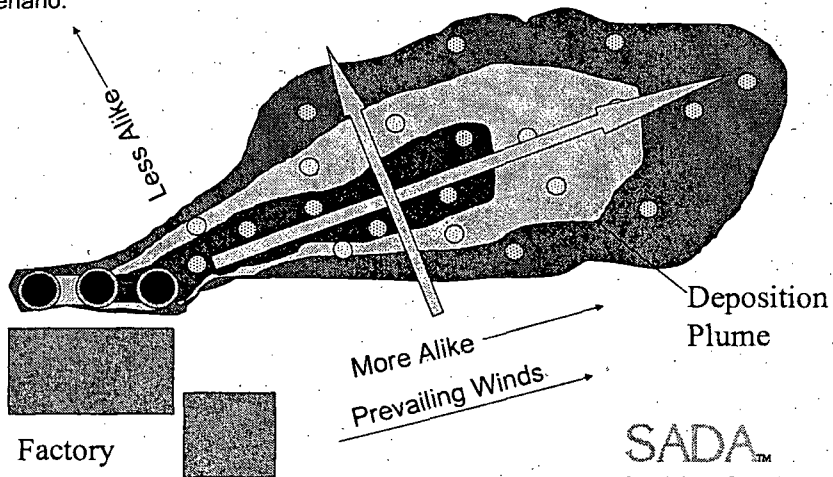


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Spatial Anisotropy

One example of spatial correlation would occur with a plume or deposition scenario.



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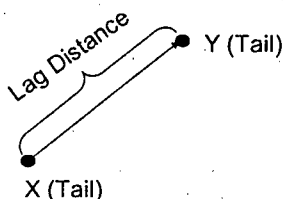
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Spatial Correlation

The degree to which data are more or less "alike" for any given distance can be calculated. SADA uses the *semi-variogram* method, which returns a measure of variance for any given distance of separation. This measure is defined as half of the average squared difference between values separated by distance h. The term h is referred to as the *lag* or *lag distance*.

$$\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} (x_i - y_i)^2$$

where N(h) is the number of pairs separated by distance h, x_i is the starting sample point (tail), and y_i is the ending sample point (head).

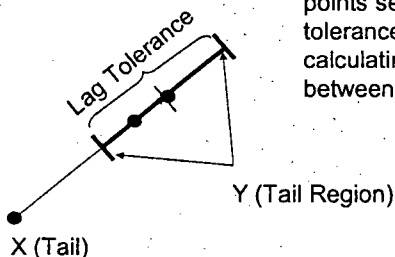


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Spatial Correlation

Rarely in practice, will you ever have any sample points separated by exactly a lag distance h. Therefore, a lag tolerance centered about the lag distance will permit a capture of more data points in the calculation of $\gamma(h)$. In the figure below, all data points within the blue shaded area will be used.



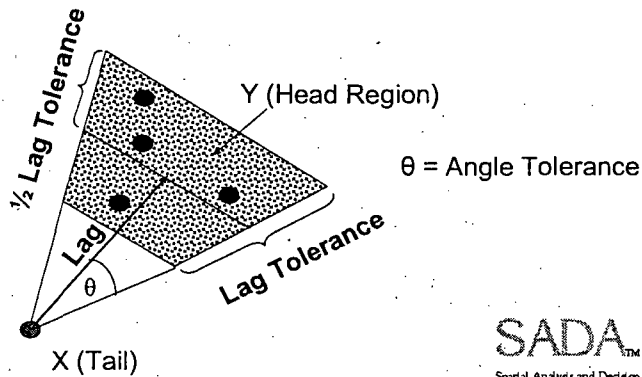
So if we are interested in the variance of all data points separated by 10 feet and we permit a lag tolerance of 2 feet. We will actually be calculating the variance of all pairs of data between 9 and 11 feet apart.

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Spatial Correlation

Although assigning a lag tolerance helps, most cases will never have enough samples separated by a lag - tol/2 to lag + tol/2 along a straight line to calculate the semivariogram value. Therefore, an angle tolerance, θ , is also introduced to expand the region and to include more points in the calculation of the semivariogram value for the specified lag distance. In the figure below, all data points within the blue shaded area will be used.

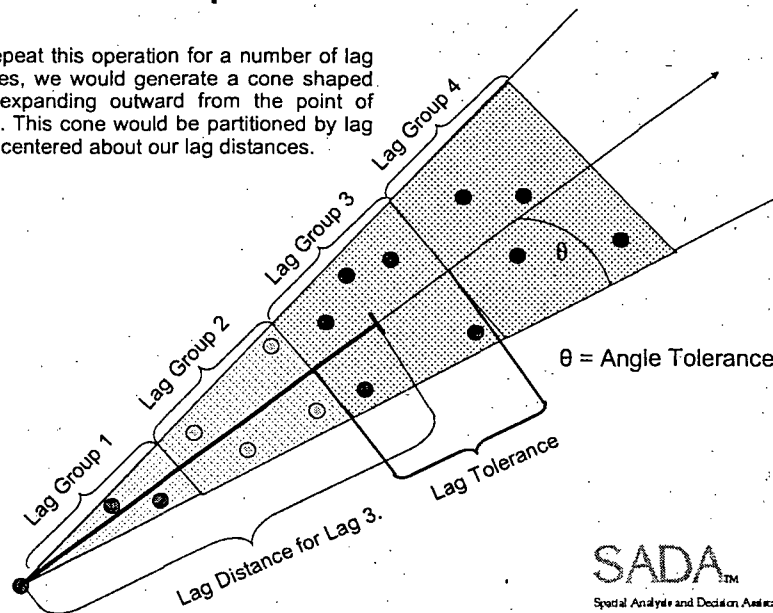


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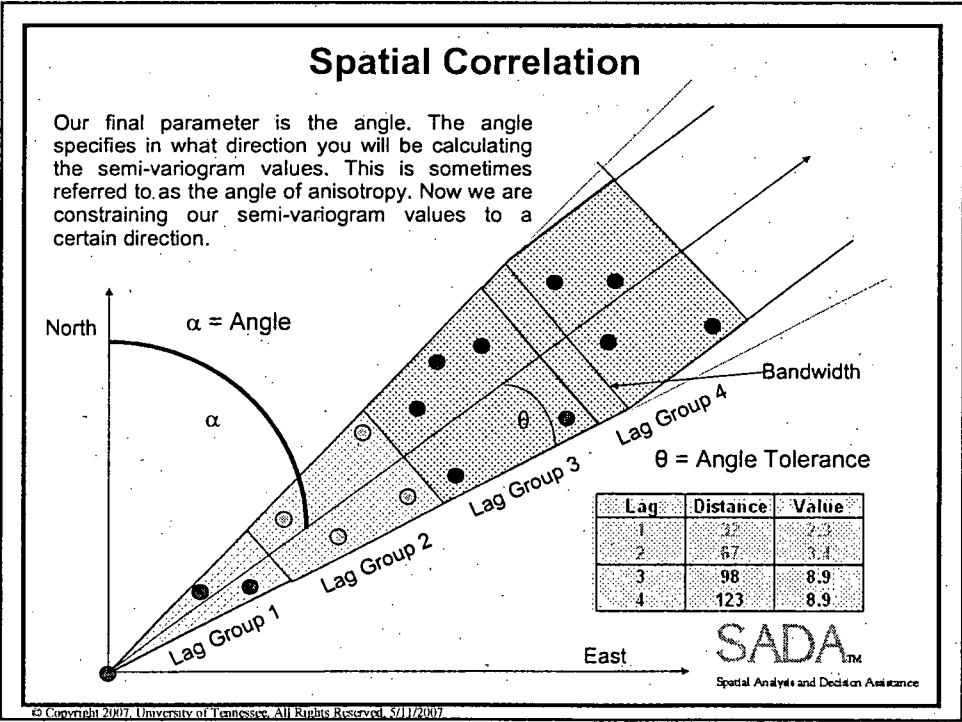
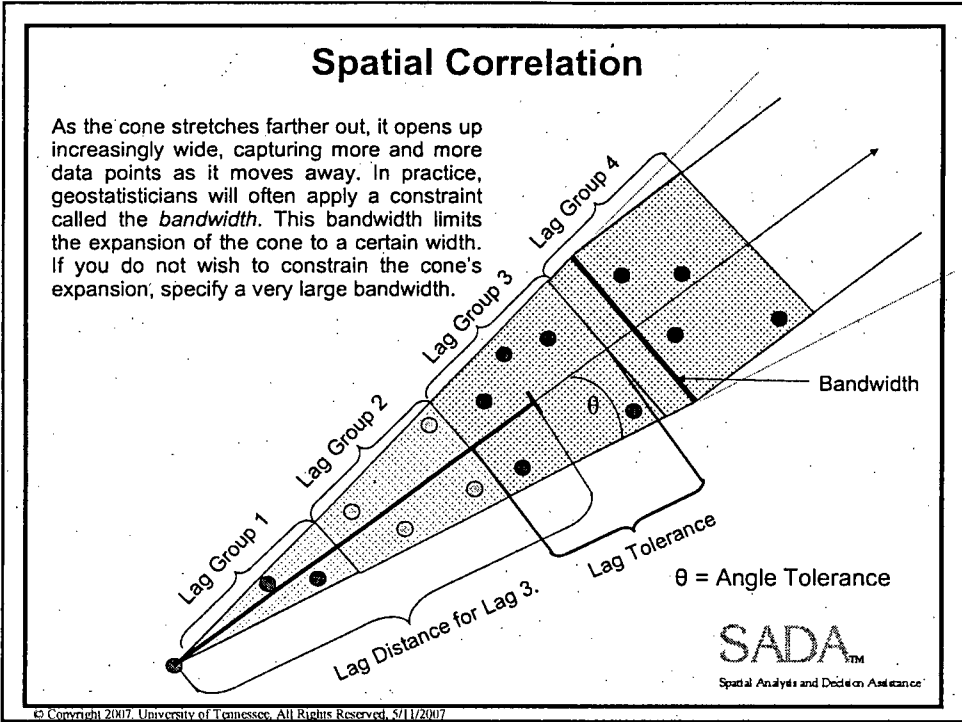
Spatial Correlation

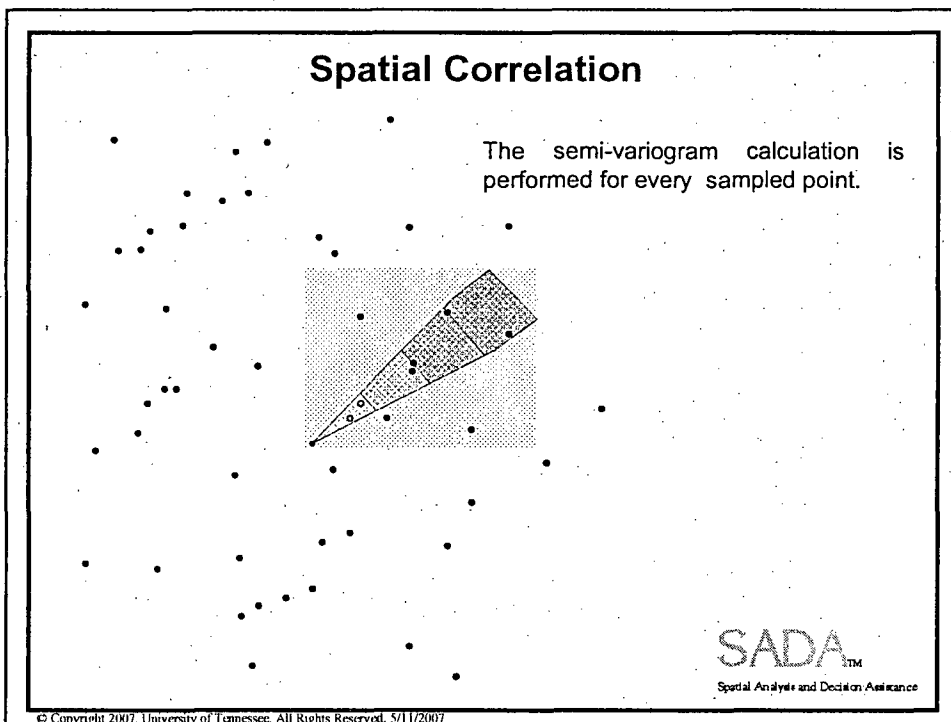
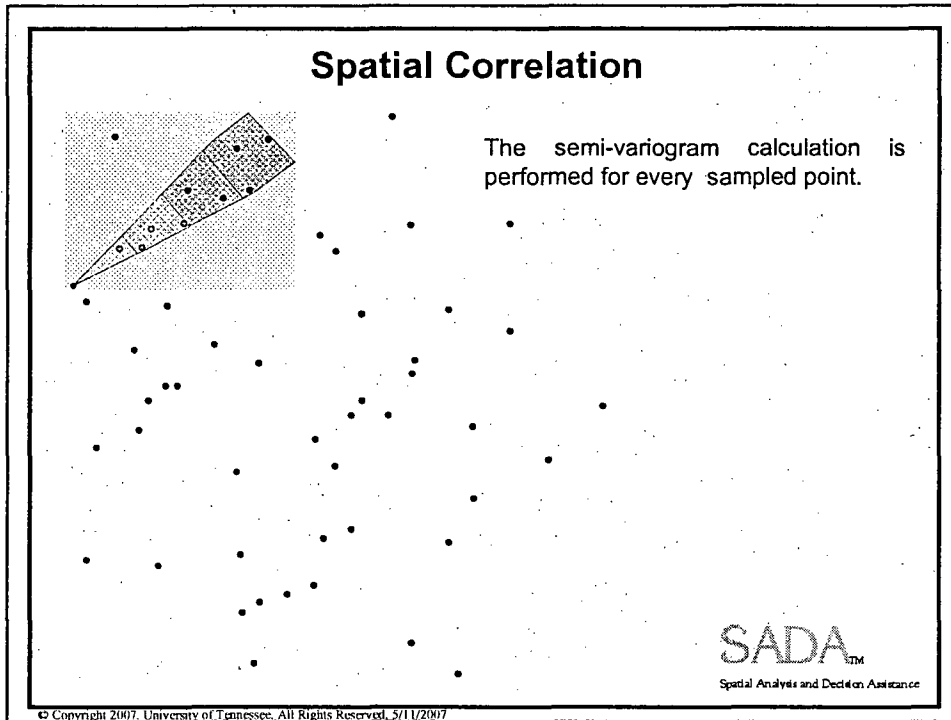
If we repeat this operation for a number of lag distances, we would generate a cone shaped object expanding outward from the point of interest. This cone would be partitioned by lag groups centered about our lag distances.

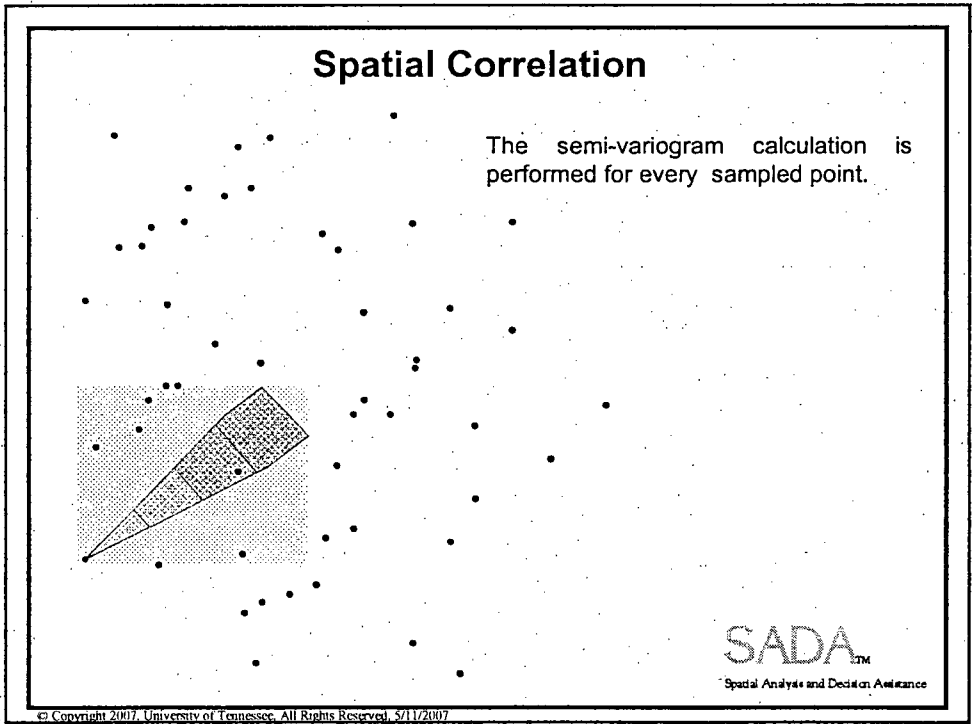
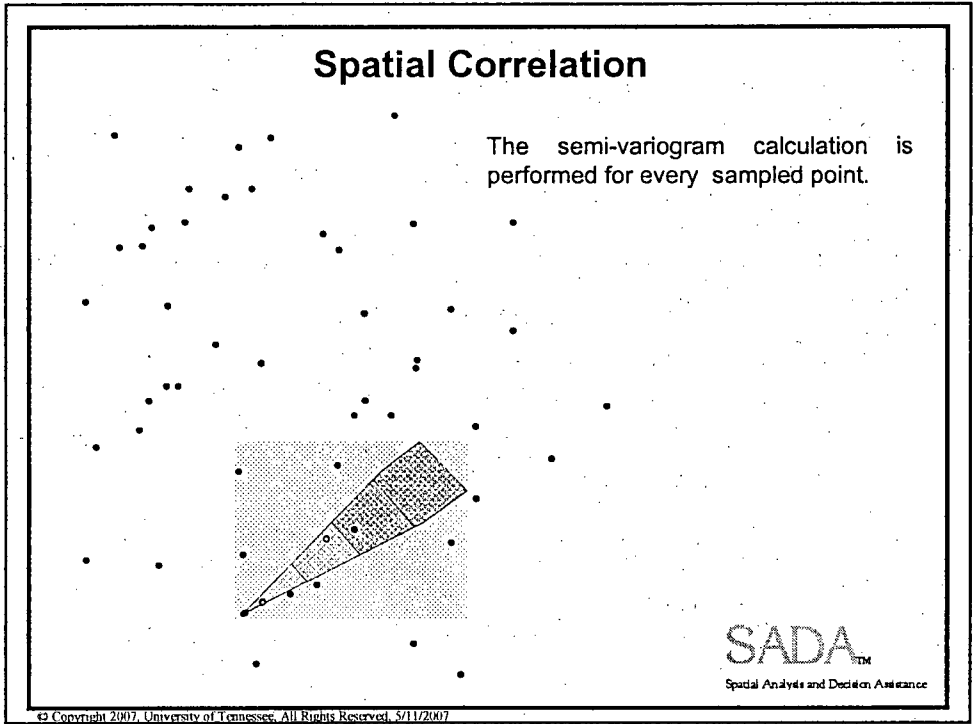


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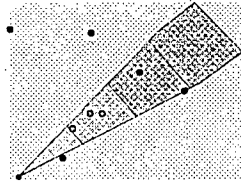




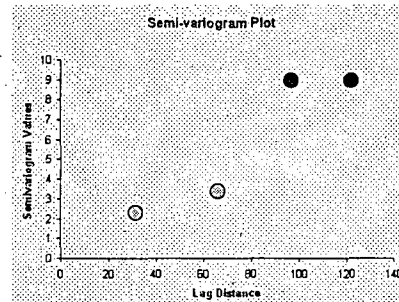


Spatial Correlation

The semi-variogram values are then plotted.



Lag	Distance	Value
1	32	2.3
2	67	3.4
3	98	8.9
4	123	8.9

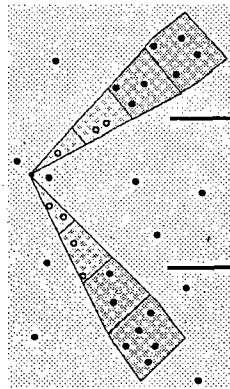


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Spatial Correlation

Note though, by specifying an angle α , we are excluding all those data points located outside of the cone from $\alpha - \theta$ degrees to $\alpha + \theta$ degrees. In other words, we are exploring how data are correlated in a particular direction. If we find that data are more correlated in one direction than another, the data are said to be *anisotropic*. This means that data in the direction α are more alike than in other directions.



Lag	Distance	Value
1	32	2.3
2	67	3.4
3	98	8.9
4	123	8.9

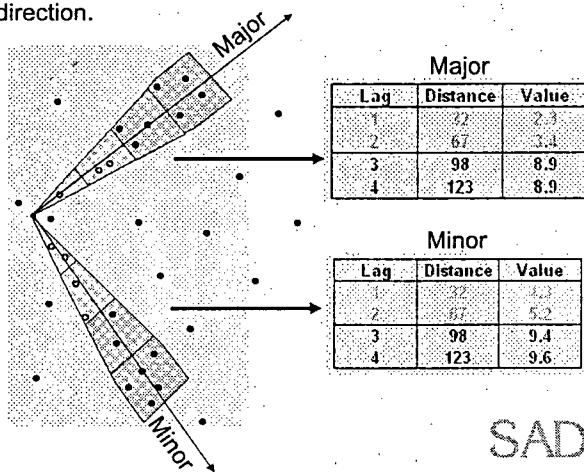
Lag	Distance	Value
1	32	1.3
2	67	5.2
3	98	9.4
4	123	9.6

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Spatial Correlation

In fact, if anisotropic conditions exist, the direction of highest correlation is considered the *major direction* of anisotropy. The perpendicular direction is referred to as the *minor direction* of anisotropy. The *major direction* of correlation will exhibit semi-variogram values that increase at a slower rate than any other direction.



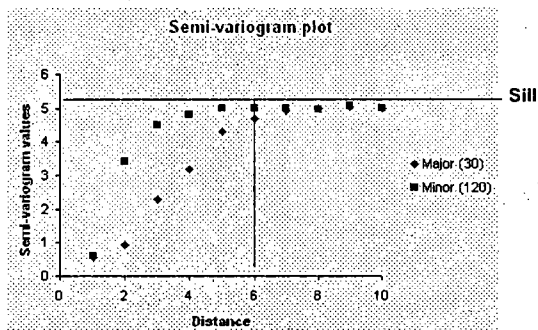
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Spatial Correlation

Theoretically, the semi-variogram values will continue to rise until they reach the *sill* value. The sill is the point at which the data are now far enough apart to be independent. The sill value should be roughly equivalent to the variance of the data set. A *semi-variogram plot* is useful in detecting the sill value and location.

Lag	Major (30)	Minor (120)
1	0.56	0.6
2	0.95	3.4
3	2.3	4.5
4	3.2	4.8
5	4.3	5
6	4.7	5
7	4.9	5
8	5	4.95
9	5.01	5.05
10	4.99	5



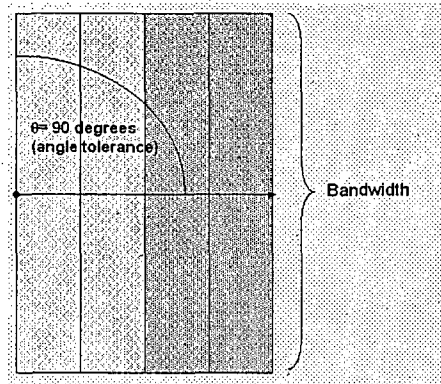
In the above example, we see a major direction at 30 degrees and the corresponding minor direction at 120 degrees. A sill value of approximately 5 is detected around 6 feet of separation.

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Isotropic Variograms

In order to calculate an isotropic or *omni-directional* variogram, simply set the angle tolerance to 90 degrees and make the bandwidth significantly larger than the site. This will force the cone to consider the entire spectrum of data points.



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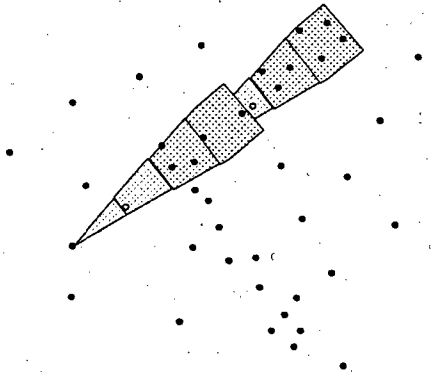
Spatial Correlation

What about in the opposite direction?

It is assumed that correlation is symmetrical. If data are varying a certain amount at 30 degrees, then they are varying the same amount at 120 degrees.

Why don't we include those sample points in the 120 degrees direction to improve our semi-variogram calculation?

We do. Our current point of interest will be captured by the cone of those points behind it.



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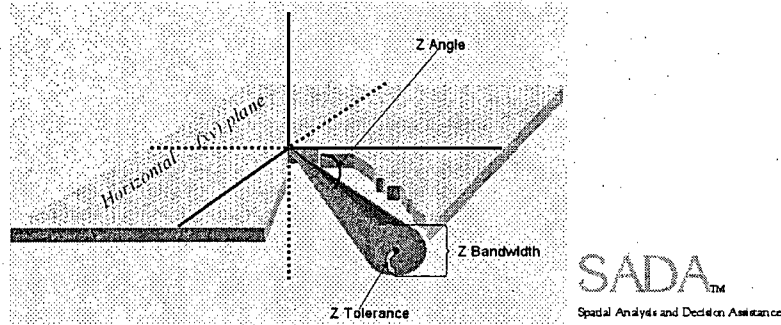
Three-Dimensional Variography

Three-dimensional semi-variogram calculation is the same approach as in the two-dimensional case. In addition to the previously defined parameters, a z angle (dip), z tolerance, and z bandwidth must be specified.

Z Angle (Dip) – The angle below the horizontal plane that the cone should dip.

Z Tolerance – The tolerance on this dip angle.

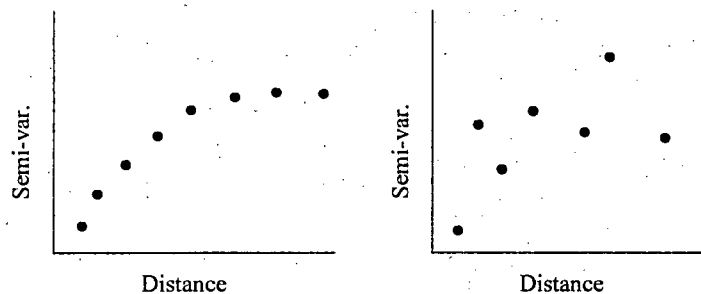
Z Bandwidth – The maximum distance the vertical component of the cone is permitted to go.



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Semi-variogram Behaviors

- Semi-variograms often do not conform to the well behaved monotonic increasing variogram structures seen in text book examples.

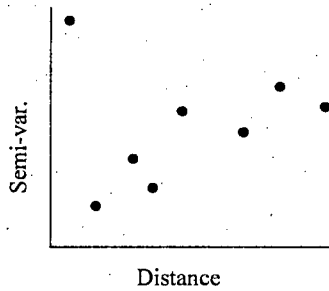


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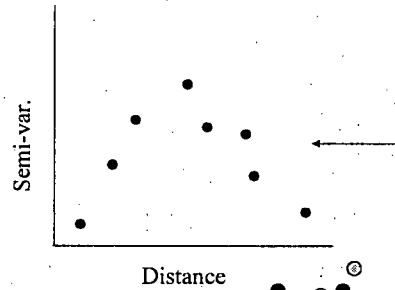
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Semi-variogram Behaviors

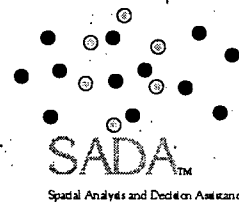
- Semi-variograms often do not conform to the well behaved monotonic increasing variogram structures seen in text book examples.



A high sample occurs close to a small value.



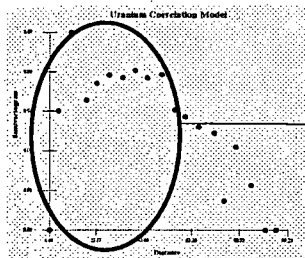
Samples have spatial oscillating distribution.



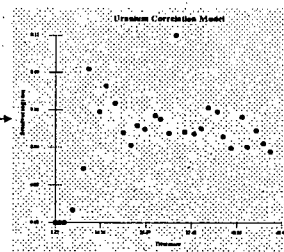
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Semi-variogram Behaviors

- Sometimes the variability is really short range and you have your lags set too large. This blurs the true spatial structure and can result in bizarre cases especially as the cone distance increases. In the case of indicator kriging below we can see this effect.



Lag Dist = 5



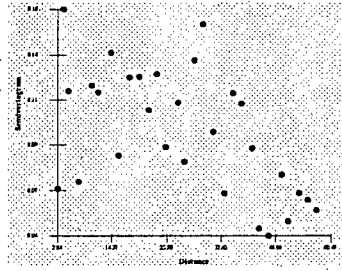
Lag Dist = 2

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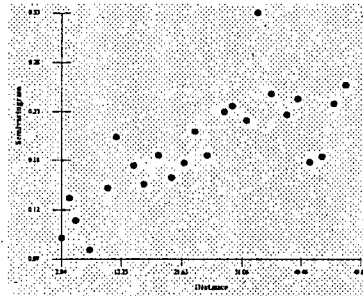
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Semi-variogram Behaviors

- In 3d dimensional applications DIP can be very important.



Dip = 0



Lag Dist = 2

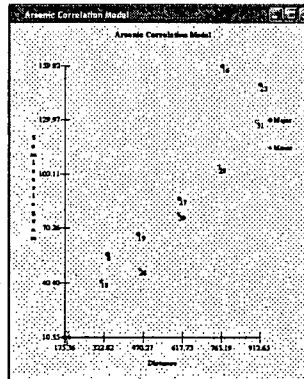
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Setting Variography Model

To calculate semivariogram values, select **Correlation Modeling** from the **Steps Window** and enter the appropriate information on the **Parameters Window**. The results of two separate cones are viewed at once to provide visual comparison and check for anisotropic correlation. Press **Show Me**.

Parameter	Value	Unit
Scale	Major	Minor
Cartoon	Major	Minor
Lag Number	4	8
Lag Distance	1.00	1.00
Lag Tol	1.00	85
Length	90	42
Tol	45	70
Dist	1000	1800
Dip	0	0
CTM	70	90
CTol	1000	1000

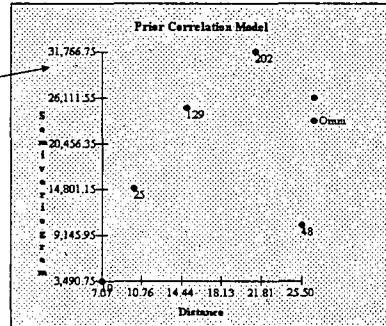
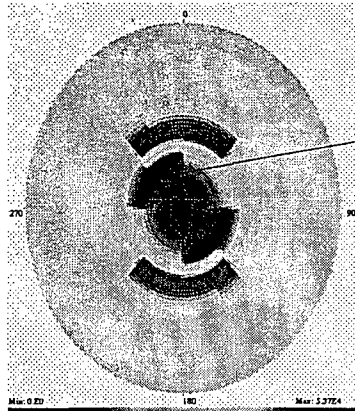


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Rose Diagrams

Rather than viewing only on angle at a time, users can view semivariogram values in all directions at once. They can then choose an angle of interest by clicking on the rose diagram map. SADA will show the semivariogram values for that direction.



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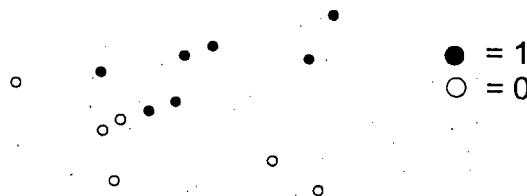
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Indicator Variograms

To this point, all variograms we have calculated have been on the actual data points. This type of variography is necessary for ordinary kriging. Indicator kriging requires variography be calculated on the *indicator transformed* values. When performing an indicator transform, you need a threshold value t . All sample values greater than t become equal to 1, and all values less than t are 0. We can write the indicator transform of the data as follows

$$I(u_i) = \begin{cases} 0 & \text{if } u_i > t \\ 1 & \text{if } u_i \leq t \end{cases} \text{ for all } i$$

If we plot the transformed data values, they would look something like this.



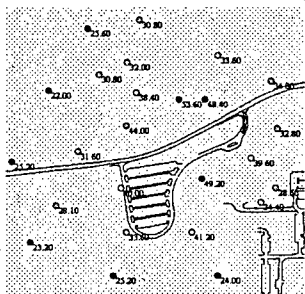
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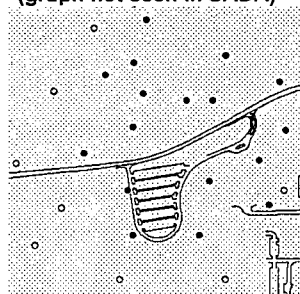
Indicator Variograms

The following example shows Arsenic data that has been indicator transformed at a threshold of 30 mg/kg.

Raw Data



Indicator Transformed
(graph not seen in SADA)



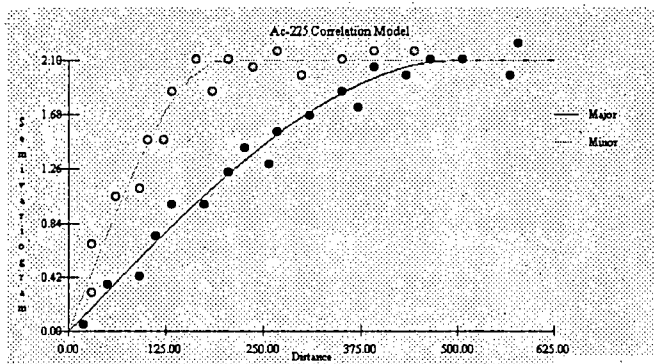
Calculations of the variogram of the indicator transformed data then proceed exactly as in the case of the untransformed data.

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Spatial Covariance

When the kriging models are used, they will require that the semi-variogram values are known for any distance h . At this point, we only have these values for a few discrete distances. Therefore, we need to fit a model to the data so that a semi-variogram value is available for every distance.

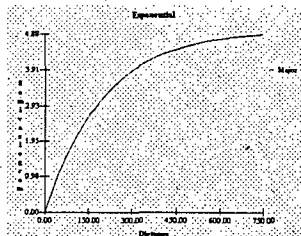
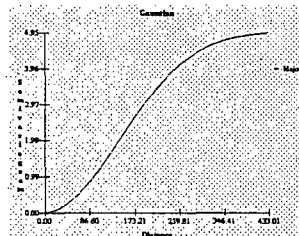
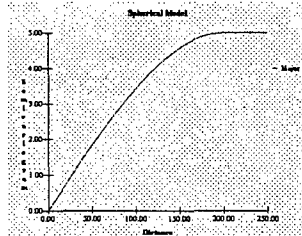


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Spatial Covariance

SADA provides 3 standard correlation models that provide a great deal of flexibility in semi-variogram data: Spherical, Exponential, and Gaussian.



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Spatial Covariance

All three models require the same set of parameters. Most of these parameters were encountered while specifying a search neighborhood.

2D and 3D

- Major Range – distance to sill or *correlation length* along the major anisotropic axis.
- Minor Range – distance to sill or *correlation length* along the minor anisotropic axis.
- Angle – the angle of anisotropy

3D

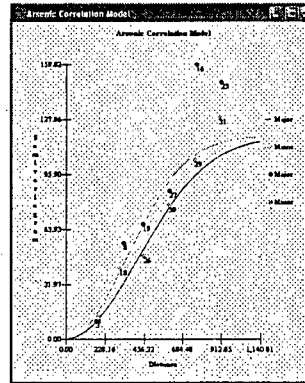
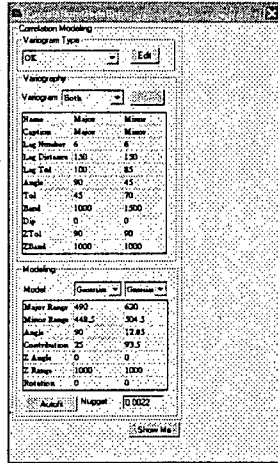
- Z Angle – the angle of anisotropy in the Z plane (equal to the Dip parameter in experimental variography).
- Z Range – a value describing how anisotropy behaves in the z minor direction, relative to major axis.
- Rotation – how the anisotropic ellipsoid is rotated about its major axis.
- Contribution – The model's contribution to the sill (maximal model value)
- Nugget – where the model should cross the y axis (white noise)

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Setting Correlation Model

To fit a correlation model to the semivariogram results, enter appropriate values in the second table on the **Parameters Window**. SADA provides three standard models: Spherical, Exponential, and Gaussian. In addition to these three models, a nugget effect is also available. Press **Show Me**.

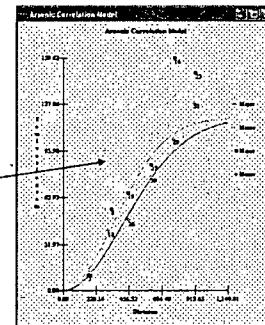
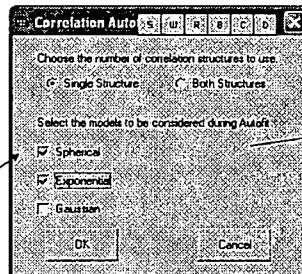
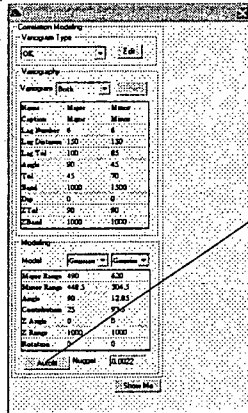


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Estimating the Correlation Model

SADA can estimate the model and associated parameters to use for a given set of semi-variogram values. Press the **Autofit** button and select the models and whether a nested model is needed. Typically, users will only choose a single structure and choose from spherical or exponential. Estimation quality can vary from variogram set to variogram set and results should only be used as a basis for adjusting the correlation model parameters.



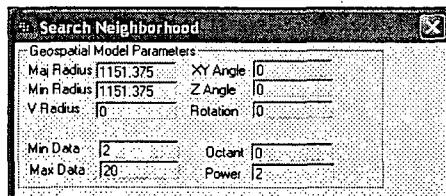
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Search Neighborhoods

Inverse distance requires a neighborhood definition for estimating concentration values at a point. A neighborhood is defined as an area around the point in which data values will be used to estimate the concentration value. Data values outside the neighborhood will be excluded.

The neighborhood is always defined by a search ellipse that can be manipulated in shape and size to include or exclude various data. The parameters which control the shape and size of the search ellipse are entered on the **Parameters Window** when **Search Neighborhood** is selected from the **Steps Window**.



Geospatial Model Parameters			
Maj Radius	1151.375	XY Angle	0
Min Radius	1151.375	Z Angle	0
V Radius	0	Rotation	0
Min Data	2	Octant	0
Max Data	20	Power	2

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Search Neighborhoods

The Major Radius, Minor Radius, and XY Angle parameters control the size and shape of the search ellipse.

Major Radius

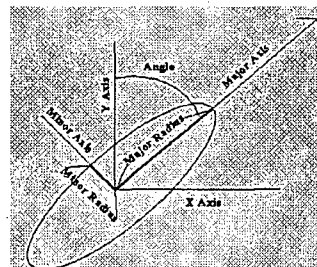
The long radius of the ellipse.

Minor Radius

The short radius of the ellipse.

XY Angle

The angle or direction the long radius points. This angle is measured clockwise from the positive Y axis (0 deg is North). The minor elliptical axis is perpendicular to the major axis.



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Search Neighborhoods

For three-dimensional data, the ellipse becomes an ellipsoid. The following parameters, in addition to those listed before, describe the search ellipsoid in 3D space.

Z Angle

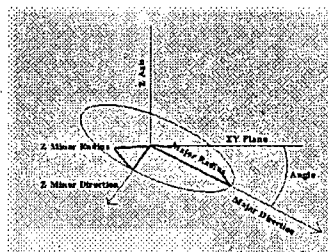
The angle or dip below the XY plane at the point of estimation. This angle is measured as negative degrees below the plane.

V Radius

Also referred to as Z minor radius, it is the radius of the ellipse in the vertical direction.

Rotation

The parameters described to this point fully form the body of the ellipsoid in 3D space. The rotation parameter then rotates this ellipsoid about the major axis the specified number of degrees.



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Search Neighborhoods

The following view shows the effect of the rotation parameter on the ellipsoid body along the major elliptical axis. The rotation angle rotates two orthogonal directions clockwise relative to the major elliptical axis when looking toward the origin. The following parameters define the search criteria within the search ellipse.

Min Data

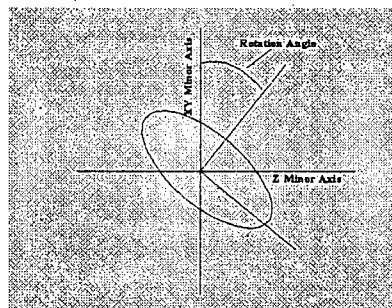
The minimum number of data required for estimating the concentration. If the minimum is not met, SADA returns un-estimated values that become empty spaces in the plot.

Max Data

The maximum number of data to use in estimating a point.

Octant

The ellipsoid is divided into quadrants, four if two-dimensional, eight if three-dimensional. If the Octant value is greater than zero and there are fewer data points than the octant value in each quadrant, the point will not be estimated.

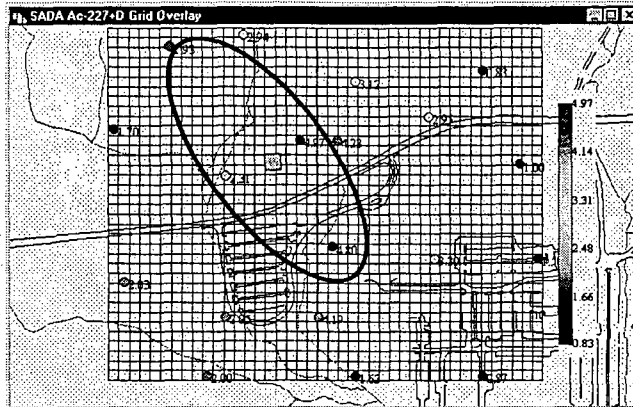


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Search Neighborhoods

Neighborhoods allow the user to search for a single unsampled point.

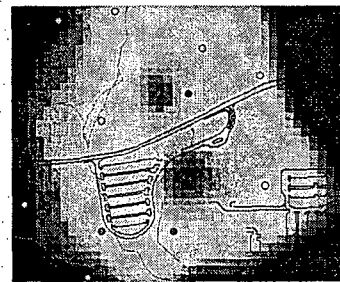
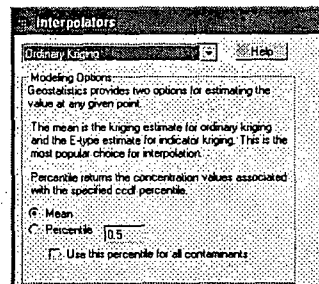


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Ordinary Kriging in SADA

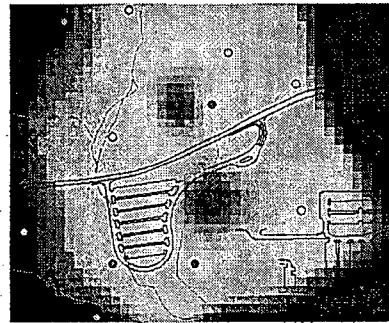
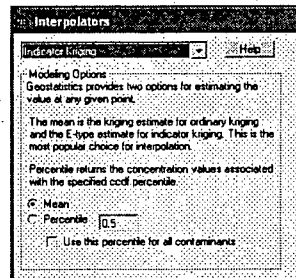
- Select the analysis, data type and data name of interest
- Select **Interpolate My Data** from the **Interview** list (or any other spatial model map)
- Define a grid by selecting **Set Grid Specs.**
- Press **Interpolation methods**, and then select Ordinary Kriging from the list of available interpolants.
- Select **Correlation Modeling** and set variography and correlation models.
- Setup an appropriate search neighborhood and specify the power parameters after selecting **Search Neighborhood.**
- Press **Show The Results** to see the map.



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Indicator Kriging in SADA

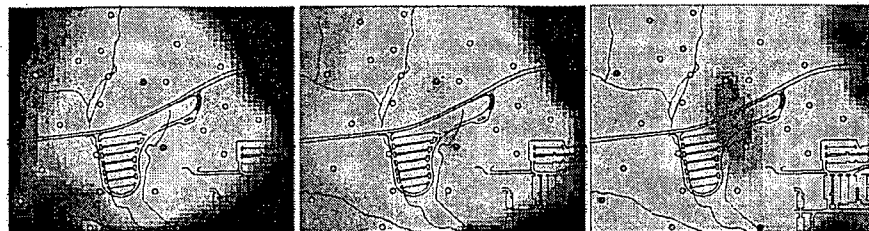
- Select the analysis, data type and data name of interest
- Select **Interpolate My Data** from the **Interview** list (or any other spatial model map)
- Define a grid by selecting **Set Grid Specs.**
- Press **Interpolation methods** and then select Indicator Kriging from the list of available interpolants.
- Select **Correlation Modeling** and set variography and correlation models for a range of threshold values.
- Setup an appropriate search neighborhood and specify the power parameters after selecting **Search Neighborhood.**
- Press **Show The Results** to see the map.



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Plotting Percentile Maps

- Allows one to be conservative (e.g. percentiles > .5)
- Allows one to spatially ascertain the difference between an “optimistic, realistic, and pessimistic” (e.g. 25th, 50th, and 75th) maps.
- Helps identify regions that could benefit from further sampling.



“optimistic”

P=.25

“realistic”

P=.5

“pessimistic”

P=.75

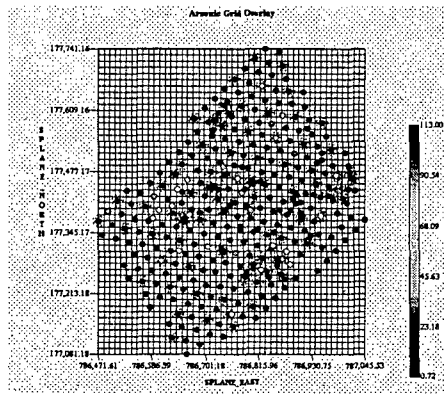
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Overview of LISA Maps

- Local Index of Spatial Association (LISA) displays show maps of moving window statistics, these statistics are calculated at each grid node and the results displayed
- Ripley's K- sampling intensity with each window
- Moran's I- measure of correlation between all points in each window
- Geary's C- semivariance calculation (average dissimilarity) between points within each window



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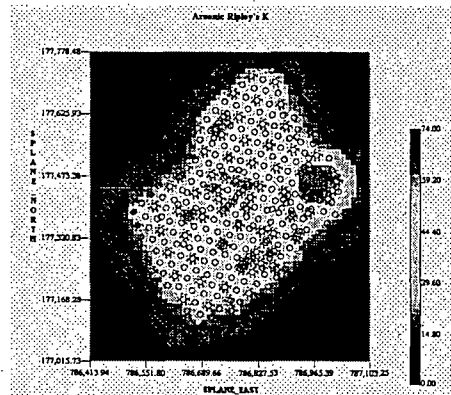
Ripley's K

- Ripley's K- sampling intensity with each window
- Users must first specify a LISA Search Radius
- Quantifies the spatial pattern intensity of points for various sizes of a circular search window
- Computes the overall mean number of points located within a search window of radius t :

$$\bar{K}(t) = \frac{\lambda^{-1} \sum_{i=1}^n \sum_{j=1}^n I_i(e_i, e_j)}{n}$$

for $i \neq j$ and $t > 0$

- γ is point intensity (n/A), I_i is an indicator of whether inside search window
- There is an edge correction effect for grid areas on the fringe

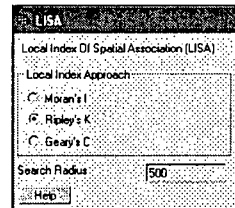
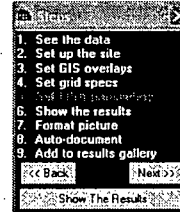
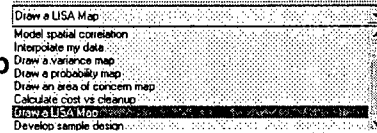


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Producing LISA Maps

- Select **Draw a LISA Map** from interview menu
- Click **Set LISA Parameters Step**
- Select a **Local Index Approach**
- Enter a **Circular Search Radius** for the moving window
- Click **Show the Results**



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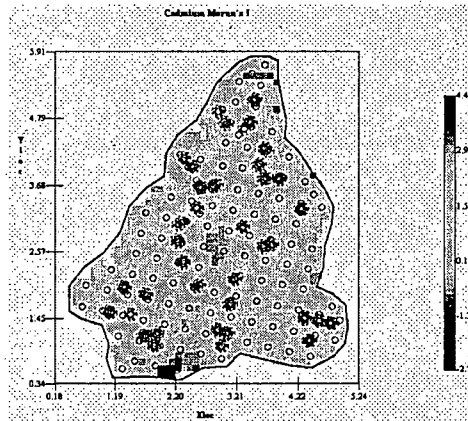
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Moran's I

- Moran's I- measure of correlation between all points in each window
- Users must first specify a LISA search radius
- Computes the degree of correlation between the values of a variable as a function of spatial lags
- Similar to Pearson's correlation coefficient, ranges from -1 (-correlation) to 1 (+ correlation), expected value close to 0

$$I(d) = \frac{\sum \sum w_{ij}(d)(x_i - \bar{x})(x_j - \bar{x})}{W(d) \sum (x_i - \bar{x})^2}$$

- $w_{ij}(d)$ indicates whether pairs are in the same distance class, $w(d)$ is the sum of $w_{ij}(d)$



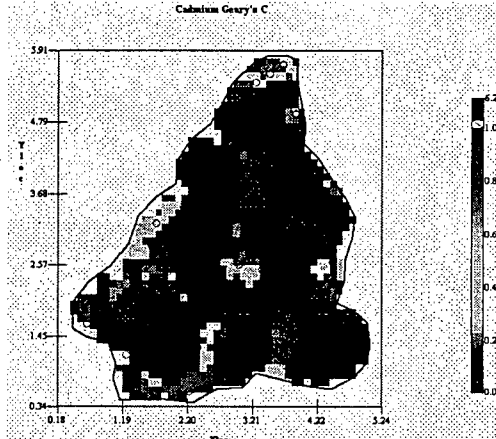
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Geary's C

- Geary's C- semivariance calculation (average dissimilarity) between points within each window
- Needs pretty high sampling densities to be informative
- Users must first specify a LISA Search Radius
- Measures the semivariance (average dissimilarity) among values of a variable at nearby locations

$$c(d) = \frac{\sum \sum w_{ij}(d)(x_i - x_j)^2}{2W(d)} \cdot \frac{\sum (x_i - \bar{x})^2}{(n-1)}$$



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Geospatial References

- Applied Geostatistics, Isaaks and Srivastava
- Geostatistical Software Library (GSLIB), Deutsch and Journel
- Geostatistics for Natural Resources Evaluation, Pierre Goovaerts
- Geostatistics in Five Easy Lessons; Journel
- Spatial Data, Cressie

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Questions?

Comments?

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Practice Session Advanced Spatial Analysis Tools

The objective of this lesson is to practice setup and use of the Ordinary Kriging method. Cross validation techniques are also used.

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Practice Session: Advanced Spatial Analysis Tools

1. Open up "Lesson4.sda". Choose the "Interpolate My Data" interview and turn on the polygon "Boundary".
2. Choose set grid specs and draw. Notice the part outside the polygon turns grey.
3. Click on *Correlation Modeling*. Try the following omni-directional parameters. Type these in for both Major and Minor.
 - a. Caption = Major or Minor
 - b. Lag Number = 8
 - c. Lag Distance = 25
 - d. Lag Tol = 25
 - e. Angle = 0
 - f. Tol = 90 *Note this makes the lag calculations omni directional in the horizontal plane.*
 - g. Band = 1000
 - h. Dip = 0
 - i. ZTol = 90 *Note this makes the lag calculations omni directional in vertical plane.*
 - j. Zband = 1000

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Practice Session: Advanced Spatial Analysis Tools

4. Choose to plot the major direction only for now and press the *Show Me* button in the lower right hand corner (*note: do not press the Show The Results button in the blue area on the left*). This is an omni directional variogram out to 200 feet.
5. Now, we want to see correlation behavior in all directions at once. Press the *Rose* button. Note that the semivariogram values are now represented by color from lowest (purple) to highest (red). Also note that they are the same in all directions. This is how an omni directional variogram should appear – the same in all directions.

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Practice Session: Advanced Spatial Analysis Tools

6. Now, we'll try an anisotropic view of the semivariogram values. Under the major and minor direction, choose 45 for the Tol value. This restricts our tolerances to half the field of view for any direction we may be looking at. Note how the rose diagram changes dramatically. Note also that the rose diagram only looks at the values in the major direction. We changed both to 45 for consistency.
7. Now we see a fairly clear line of anisotropic behavior at an angle from about 32 to 42 degrees (measured from due north) and different behavior perpendicular to this direction. Click on the map to obtain the raw variogram values. This direction becomes our major direction of anisotropy. Our minor direction of anisotropy should be exactly perpendicular to this major direction. Let's choose 35 degrees for our major direction and 125 degrees ($35+90=125$) for our minor. Type these values into the Angle parameter boxes respectively. Press *Show Me*.

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Practice Session: Advanced Spatial Analysis Tools

8. Now we want to fit a model to these values. Try a major range and minor range of about 250, angle of 35, contribution of 3800, zangle = 0, zband = 1000, rotation = 0, nugget = 0.
9. Now plot only the minor direction. Press *Show Me*. Change the Minor range to be 50. Press *Show Me*. The green line is the minor direction model. Does this seem like a reasonable fit? One can use cross validation to check sensitivity and accuracy later.
10. Now turn on both major and minor directions. The blue line follows the major direction while the green follows the minor. It can look messy with all the points involved.

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Practice Session: Advanced Spatial Analysis Tools

11. Press the save button.
11. Choose ordinary kriging to be the interpolant. For the search neighborhood, we want the major and minor directions to mirror our correlation model findings. Use 200 and 75 for major and minor, respectively. Use an angle of 35 for our XY angle.
12. Press the *Show the Results* button. Save the results to the result gallery as "Ordinary Kriging".

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Practice Session: Advanced Spatial Analysis Tools

14. Perform Cross validation. Enter the results here.

Mean Error _____

Absolute Mean Error _____

Mean Squared Error _____

15. Compare these results to the more basic interpolants, such as inverse distance and natural neighbor. Now try inverse distance again with the new major, minor, and xy angle values derived during correlation modeling. How does the cross validation compare with the previous result in Lesson 3?

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Spatial Analysis and Decision Assistance (SADA) Version 4 3-D Visualization

Environmental Assessment Methods in SADA
University of Tennessee, Knoxville

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3d Modeling and Visualization

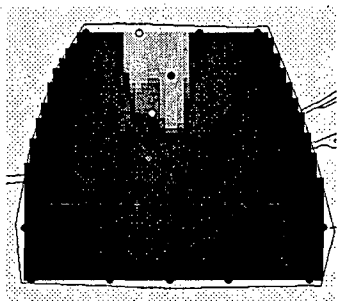
- Spatial modeling in SADA is the same in 2d and 3d, with the exception of 3 additional terms that appear both in the correlation modeling and in the search neighborhood. In both, we must specify a z angle, a z width (or vertical radius), and a rotation value. These concepts have been previously covered.
- Viewing in 3d can be done in two ways in SADA: *single layer* or *volume view*.
 - The single layer view is the default. It is the usual view-one-layer-at-a-time approach.
 - The volume view requires the use of SADA's three dimensional visualization module.

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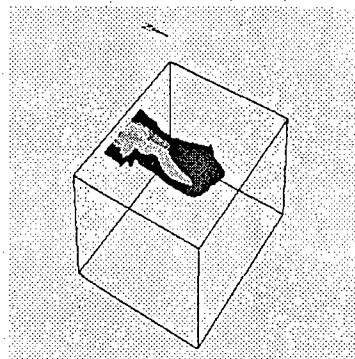
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3d Modeling and Visualization

Layer View (1st layer)



3d View

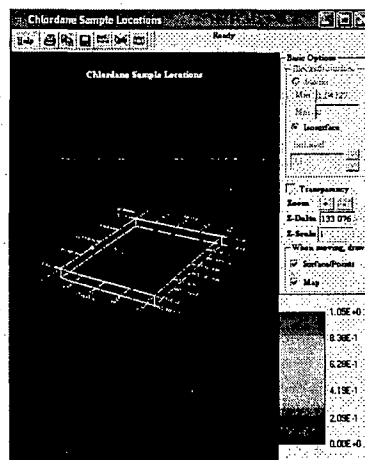


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3d Viewer

- Open Threedimensional.sda. This file contains 3d chlordane data. Switch to the **Interpolate my data** interview.
- You can view both data and modeled results in the 3d viewer.
- To use the 3d viewer choose **Graphics** → **View 3d**. The 3d viewer appears in the place of the 2d view. Depending on the speed of your computer, it may take some time to render the 3d view.
- This training will focus on only the most frequently used features of the 3d viewer. Refer to the help file for more detailed information.



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3d Viewer Commonly Used Features

The screenshot shows the SADA 3D Viewer window titled "Chlordane Sample Locations". The main area displays a 3D view of the data points. On the right side, there is a "Basic Options" panel with several settings:

- View options:** A toolbar with icons for different view modes.
- Apply button:** A button with a checkmark icon to apply changes.
- Status bar:** A bar at the top right showing the current status.
- Type of view:** A dropdown menu to select the view type.
- Isosurface value:** A numerical input field for setting the isosurface value.
- Z Scale:** A numerical input field for setting the Z-axis scale.
- Legend:** A vertical legend showing color-coded values from 1.00E+0 to 0.00E+0.

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3d Viewer: Z Scale

- The initial view shows the data values as they appear normally.
- Usually, the view is quite flat, because the horizontal extents are usually larger than the vertical.
- In the Z-Scale box, enter a value of 10 and press the **Apply** button.

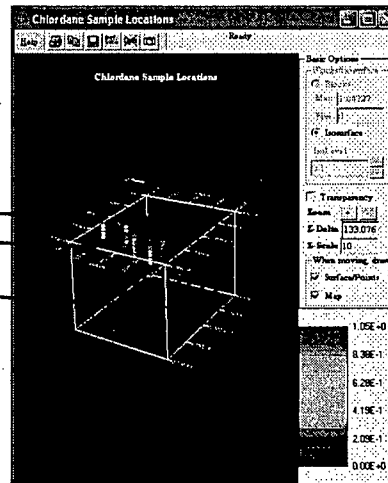
The screenshot shows the same SADA 3D Viewer window. The "Z Scale" input field in the "Basic Options" panel is circled in red, indicating where the user should enter a value of 10. The 3D view shows a flat rectangular area representing the sample locations.

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3d Viewer: Remove Axis Marks

- The default view shows all the axis tick marks. This can make the view somewhat cluttered.
- The easiest way to turn off the axis tick marks is to right mouse click on each axis to toggle the tick marks on and off.
- You can also turn them off using the options button (discussed later)

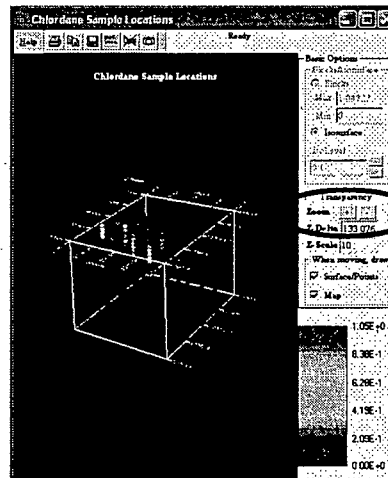


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3d Viewer: Zooming

- You can control how close or far the 3d view appears to you.
- Simply press the Zoom buttons (+ and -) until the view is where you want it.
- Remember that each press of the zoom button generates a new view. You might have to wait a second for each press to update the view.

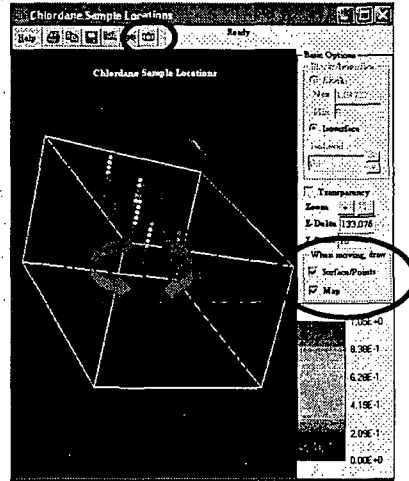


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3d Viewer: Rotating the view

- To rotate the view around, left mouse click on the picture. While holding the mouse button down, move the mouse around.
- The picture rotates accordingly.
- The view will actually rotate faster if you turn off the Surface/Points and Map options under **When moving, draw** option.
- Remember if you turn these off to press the **Apply** button again to render your picture after each rotation.

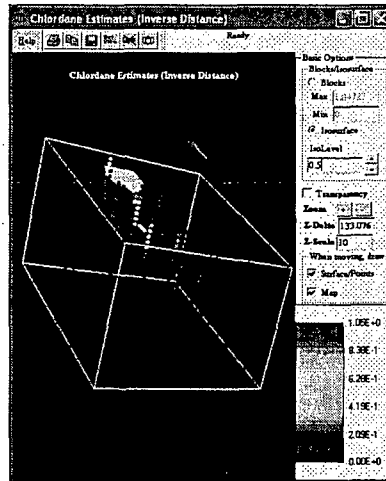


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3d Viewer: Viewing the model

- With **Interpolate my data** interview selected, press the **Show me the results** button.
- The file Threedimensional.sda has been set up for you to run ordinary kriging in 3d.
- Any time the view appears not to be fully rendered after the status bar reports it complete, simply press the **Apply** button again.
- SADA should respond by showing you an isosurface map of your inverse distance results.

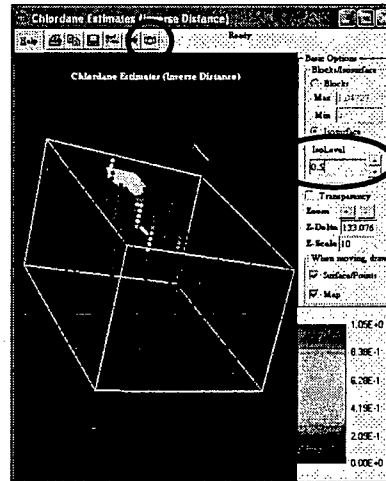


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3d Viewer: Setting the isosurface

- The isosurface level is the value above which all volume is plotted.
- For example, if the isosurface is .1 mg/kg, SADA will plot all regions of the volume that are greater than .1 mg/kg.
- Change the IsoLevel parameter to .1 and press Enter.

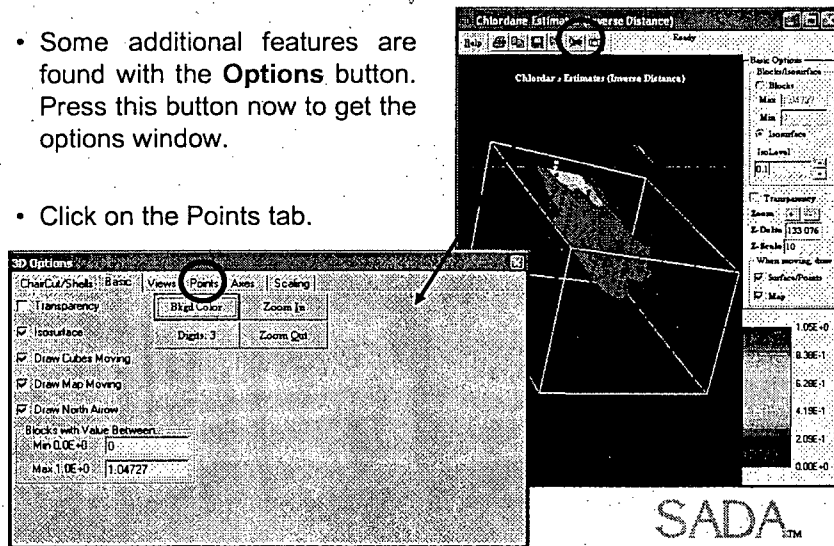


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3d Viewer: Using the options button

- Some additional features are found with the **Options** button. Press this button now to get the options window.
- Click on the Points tab.

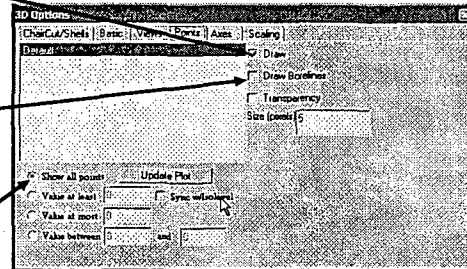


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3d Viewer: Manipulating Data Points

- The most commonly used feature of the points tab is to turn the drawing of sample points on and off.
- Drawing borelines (vertical well holes through each data point) can help visualize which data points belong to the same well log.
- You can also show only data points within certain ranges and even synchronize these ranges with the Isolevel.
- Turn off the **Draw** option and click **Update Plot**.
- Click on **ChairCut/Shells**.

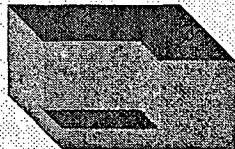
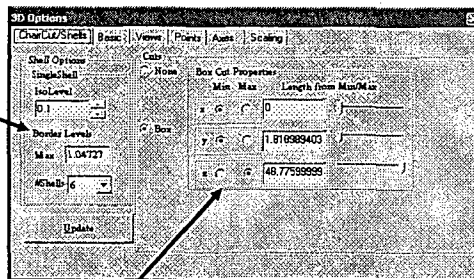


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3d Viewer: Chair Cuts

- Some of the shell options we've seen before are repeated here.
- The most common reason for visiting this tab is to perform *chair cuts* or *box cuts*.
- A box cut slices through regions of the volume and gets its name from the box-like removal produced.



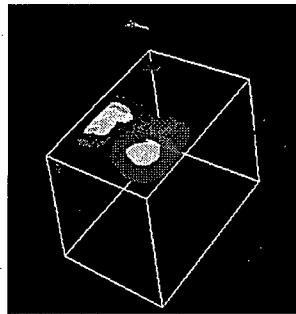
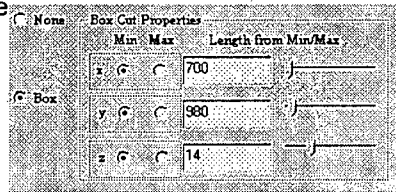
- Specify the start of your chair cut along each axis and how far down the axis the chair (box) will extend.
- It takes some practice becoming familiar with this tool. Orientation in space is the hardest aspect of this tool for new users.

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3d Viewer: Chair Cuts

- Under Box Cut Properties, Choose X Min with value 700.
- Choose Y Min with value 980
- Choose Z Min with value 14.
- Press the **Update** Button



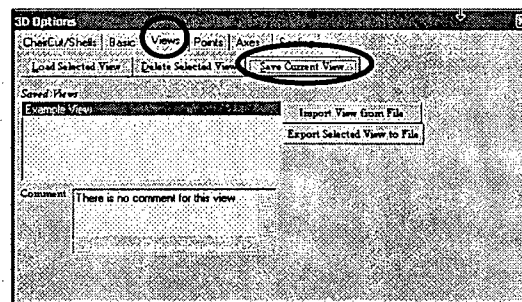
Box Cut

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3d Viewer: Saving Views



- Click on the **Views** Tab. Here, you can save and recall specific view setups, such as the one we just created. Later, you can recall this view without having to repeat all these steps.
- Press **Save Current View** and enter name My View. Press **Save View**.

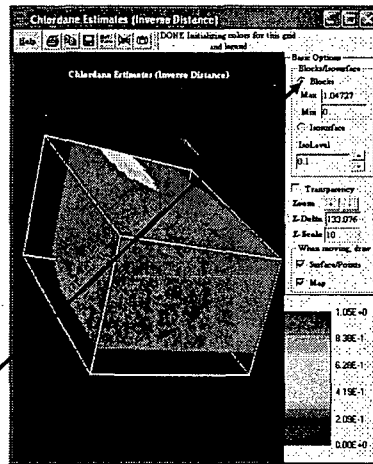


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3d Viewer: Block Views

- Anytime the 3d options window disappears, simply repress the options button. 
- To remove the options window, press this button again. 
- Save your ThreeDimensional.sda file.
- You can also see a block view of your model results. This view is typically slower and is not often used. To see the raw block values, click on the Block view option.

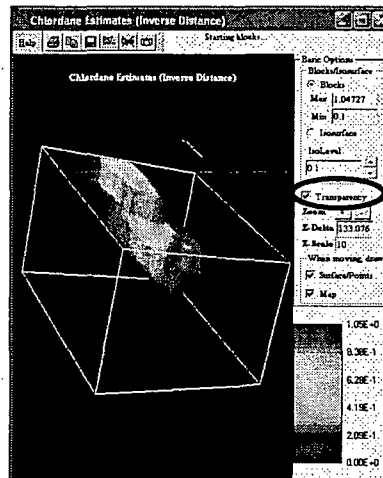


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3d Viewer: Block Views

- As with the isosurface view, you can specify a range of values for which to plot the blocks.
- Use Max = 1.04727 and Min = .1
- One feature of the block view is the *transparency option*.
- The transparency option will makes the opaque quality of the block proportional to the concentration value of the block.
- For example, high values appear solid and low values appear vapor like.
- This allows you to “see through” the low areas of contamination to the higher values.
- Click this value on.



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Questions?

Comments?

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Spatial Analysis and Decision Assistance (SADA) Version 4 Human Health Risk

Environmental Assessment Methods Using SADA
University of Tennessee, Knoxville

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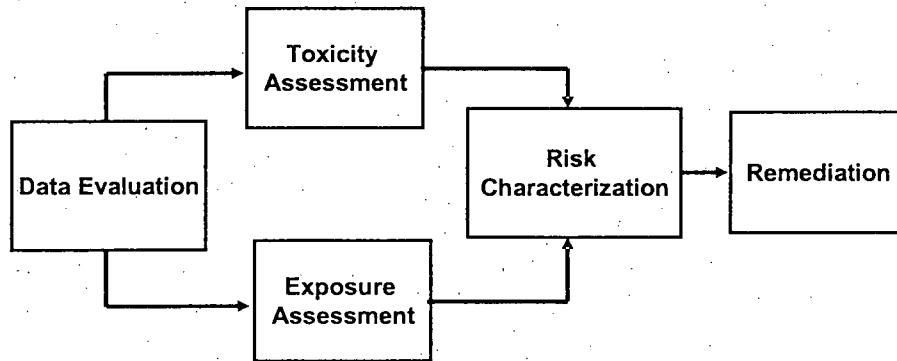
Human Health Risk

- SADA implements EPA methods for conducting human health risk assessments
- Calculation of site-specific preliminary remediation goals
- Exposure modeling for humans for five different land use scenarios
- Contains IRIS/HEAST toxicity databases for calculating risk from exposure
- Contains EPA default exposure parameters for the risk models
- Tabular screening and risk results
- Point screens
- Risk and dose mapping

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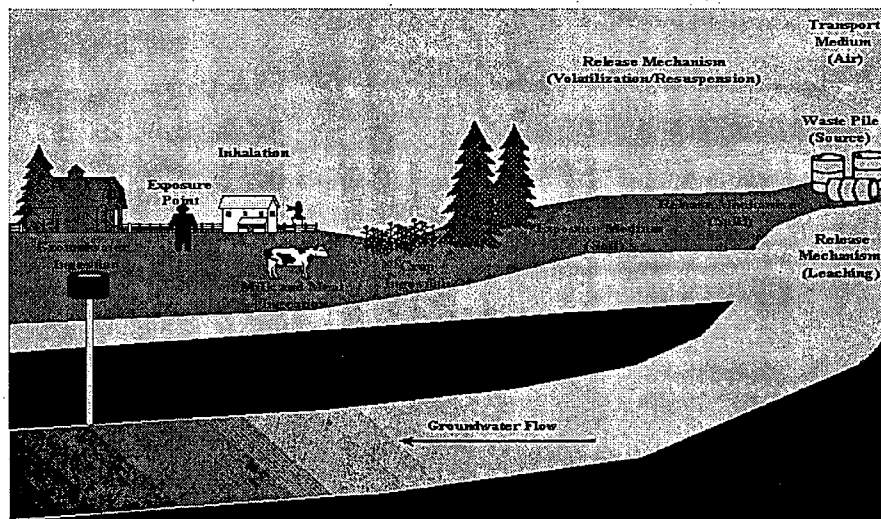
Standard Steps of a Risk Assessment



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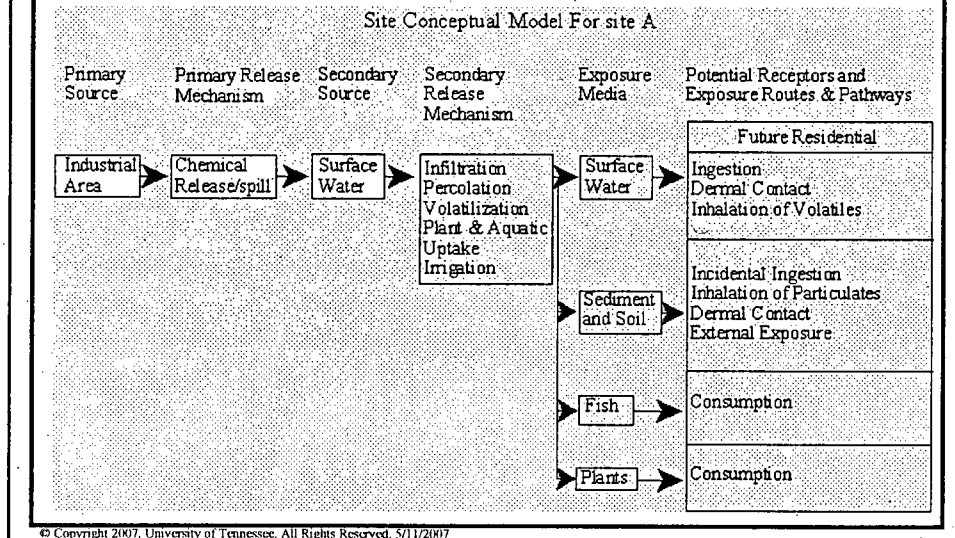
Risk Assessment- Exposure Assessment



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Risk Assessment- Exposure Assessment

Conceptual Site Model



Residential Land Use

- Residents are expected to be in frequent, repeated contact with contaminated media
- Provides a conservative assessment of risk, a residential land use scenario is assumed as one of the potential receptors for all EPA baseline risk assessments
- Exposure is calculated for a lifetime, which includes exposures for the receptor as both child and adult
- Exposure routes considered:
 - ingestion of ground or surface water,
 - inhalation of vapors from ground or surface water during water use in the home,
 - dermal contact with ground or surface water while showering,
 - incidental ingestion of soil or sediment,
 - inhalation of particulates and/or vapors emitted from soil or sediment,
 - dermal contact with contaminated soil or sediment, and
 - external exposure to ionizing radiation emitted from contaminants in soil or sediment.

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Recreational Land Use



- Recreational scenario addresses exposure to children and adults who spend a limited amount of time at or near the site while engaging in outdoor activities such as playing, fishing, hunting, or hiking.
- Recreational land use scenario can also be parameterized to serve as a "trespasser" or "site visitor" scenario
- Exposure routes considered:
 - incidental ingestion of surface water,
 - dermal contact with surface water,
 - incidental ingestion of soil or sediment,
 - inhalation of particulates and/or vapors emitted from soil or sediment,
 - dermal contact with contaminated soil or sediment,
 - external exposure to ionizing radiation emitted from contaminants in soil or sediment, and
 - consumption of fish.

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Industrial Land Use



- Under the industrial land use, adult workers are assumed to be routinely exposed to contaminated media within a commercial area or industrial site.
- Exposures are based on the potential for the use of heavy equipment and related traffic in and around contaminated soil and sediment in an unrestricted industrial scenario
- Exposure routes considered:
 - incidental ingestion of ground or surface water,
 - incidental ingestion of soil or sediment,
 - inhalation of particulates and/or vapors emitted by soil or sediment,
 - dermal contact with contaminated soil or sediment, and
 - external exposure to ionizing radiation emitted from contaminants in soil or sediment.

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Agricultural Land Use



- Under agricultural land use, residents are assumed to be exposed to farm products in addition to the primary exposure pathways of the residential scenario.
- Farming practices vary regionally, parameters such as irrigation rates should be customized to reflect regional practices.
- Exposure routes considered:
 - consumption of vegetables,
 - consumption of whole milk, and
 - consumption of beef.

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Excavation Scenario



- Under excavation land use, individuals are assumed to be exposed to contaminated soil or sediment infrequently and for only a short period of time
- frequency is assumed to be one month of the worker year, or approximately 20 days per year. In addition, excavation is assumed to be a rare occurrence, so the exposure duration for any one worker is assumed to be one year.
- Due to the short duration, risk calculations use subchronic (where available) reference doses (RfDs) for all pathways
- Exposure routes considered:
 - incidental ingestion of soil or sediment,
 - inhalation of particulates and/or vapors emitted by soil or sediment,
 - dermal contact with contaminated soil or sediment, and
 - external exposure to ionizing radiation emitted from contaminants in soil or sediment.

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*Sub chronic
exposure -
Subchronic
values first*

Risk Assessment- Toxicity Assessment

- Gather toxicological information
 - Typically no development of new data
 - Relies on EPA approved information
- Identify appropriate toxicity values
- Evaluate chemicals without toxicity values
- Evaluate uncertainties of toxicity information

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Toxicity Assessment

- Toxicity Value Classifications
 - Radionuclide - chemical that undergoes nuclear decay and emits radiation (e.g., Uranium-238)
 - Nonradionuclide - chemical that does not undergo nuclear decay or emit radiation (e.g., Iron)
 - Organic - chemical or compound that contains a carbon skeleton (e.g., Acetone)
 - Inorganic - chemical or compound that does not contain a carbon skeleton (e.g., Mercury)
 - Carcinogen - agent that may produce or incite cancer (e.g., Polychlorinated Biphenyls (PCBs), Vinyl Chloride)
 - Noncarcinogen - agent that typically does not produce or incite cancer (e.g., Antimony, Beryllium)

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Toxicity Assessment

- Exposure Durations
 - Chronic - exposure lasting more than 7 years ("lifetime" exposures, typically low levels)
 - Subchronic - exposures lasting from 2 weeks to 7 years ("limited occupational" or "event" exposures, e.g. remediation worker)

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Risk Characterization

- Risk Characterization
 - Risk Characterization incorporates the outcomes of the previous activities (Data Evaluation, Exposure Assessment, and Toxicity Assessment) and calculates the risk or hazard resulting from potential exposure to chemicals via the pathways and routes of exposure determined appropriate for a site.
- Calculate risks by media and land-use
 - Quantify risk for each chemical
 - Quantify risks from multiple chemicals
 - Combine risks across exposure pathways
 - Assess uncertainty
- Identify chemicals, media, and land-uses of concern
 - Support development of cleanup goals

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Risk Characterization

- Basic Risk and Hazard Equations

$$\text{Risk} = \text{CDI} \times \text{SF} \qquad \text{HQ} = \frac{\text{CDI}}{\text{RfD}}$$

where:

Risk = unitless probability of individual developing cancer over lifetime

HQ = hazard quotient

CDI = chronic daily intake or dose [mg/kg-day; and risk/pCi]

SF = slope factor, expressed in [(mg/kg-day)⁻¹; pCi/risk]

RfD = chronic reference dose

If HQ > 1 remediation is needed

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Data!

- Risk Assessments are data driven:
 - as quality and confidence increases in data, then
 - so does the quality and confidence increase in the risk estimates.
- SADA offers reliable and effective data storage, visual analysis, and synthesis that can enhance risk assessments. But ultimately, the quality of the risk assessment is dependent upon the quality and quantity of the data.

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SADA Human Health Functionality

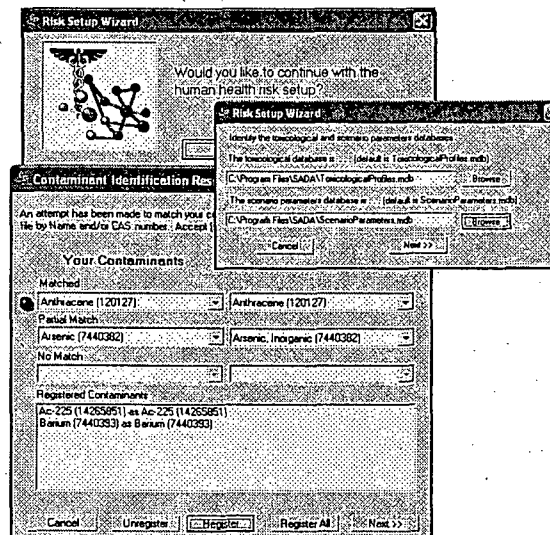
- Setting Up Human Health
- Viewing Scenario Parameters
- Viewing Toxicological Parameters
- Changing Target Risk/Hazard Index
- Setting Screening and Exposure Statistics
- PRG Tables
- PRG Screen Tables
- Risk Tables
- Spatial PRG Screens
- Point Risk Maps
- Rematching a Single Contaminant

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Setup Human Health

- After a SADA file is created
- Imports toxicity and exposure data to the SADA file
- Link contaminants in toxicity file to those in SADA file

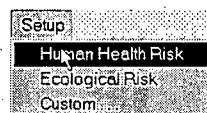


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Setup Human Health

- Select **Setup** -> **Human Health Risk**
- Click **Yes** on Risk Setup Wizard
- Browse for ToxicologicalProfiles.mdb
- Select **Open**, Then **Next** (or **Reset**)
- Browse for ScenarioParameters.mdb
- Select **Open**, Then **Next** (or **Reset**)
- **Register** Contaminants
- Select **Next**

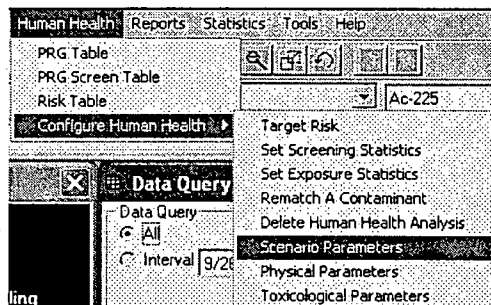


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Viewing Scenario Parameters

- Select Human Health on Analysis Drop Down List
- Select **Human Health** -> **Configure Human Health** -> **Scenario Parameters**

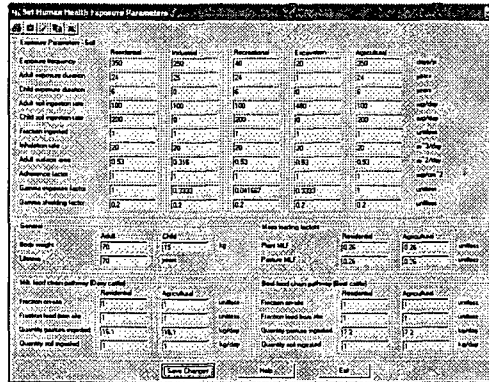


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Viewing Scenario Parameters

- For each media
 - Soil, Sediment, Surface Water, Groundwater
- Exposure Scenarios
 - Residential, Industrial, Recreational, Agricultural, Excavation
- Exposure Pathways
 - Ingestion, Inhalation, Dermal Contact, Food Chain (Beef, Milk, and Vegetable Ingestion)
- Customizable

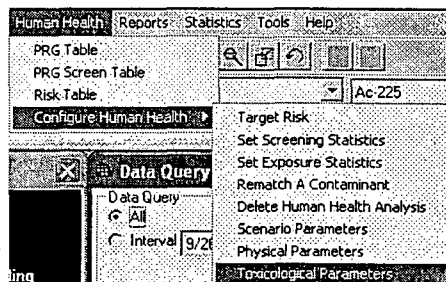


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Viewing Toxicological Parameters

- Select Human Health on Analysis Drop Down List
- Select **Human Health** -> **Configure Human Health** -> **Toxicological Parameters**



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Viewing Toxicological Parameters

- IRIS and HEAST Toxicity Databases

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Viewing Physical Parameters

- Select Human Health on Analysis Drop Down List
- Select Human Health -> Configure Human Health -> Physical Parameters

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Viewing Physical Parameters

- Physical Parameters
 - Bioaccumulation Factors
 - Volatilization, Particulate Emission Factors
 - Permeability Constants, Absorption Factors
 - Saturation Coefficients, Radionuclide Half-Lives

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Setting Target Risk/Hazard Index

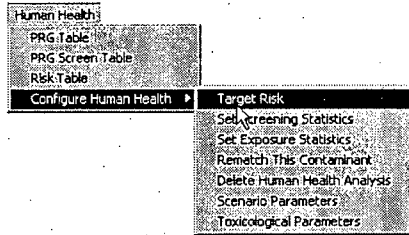
- Default values of 1E-6 for carcinogenic risk and 1 for Hazard Index
- User can change
- Select Human Health on Analysis Drop Down List. Then, select **Human Health -> Configure Human Health -> Target Risk**

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Setting Target Risk/Hazard Index

- Select Human Health on Analysis Drop Down List
- Select **Human Health -> Configure Human Health -> Target Risk**



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Human Health Statistics

- Default values are maximum detected value for screening calculations and lesser of the maximum detected value and the UCL95 for exposure calculations.
- User can change the approach:
 - Maximum Value: the maximum concentration, detected or nondetected, for normal or lognormal distribution
 - Maximum Detected Value: the maximum detected concentration for normal or lognormal distribution
 - UCL95: the 95% upper confidence limit on the mean for normal or lognormal distribution
 - Mean: the average concentration over all values for normal or lognormal distribution

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Setting Statistics

- Select Human Health on Analysis Drop Down List. Then, select Human Health -> Configure Human Health -> Set Screening Statistics or Set Exposure Statistics.

The screenshot shows the 'Setting Statistics' process in a software application. At the top, a navigation menu is visible with 'Human Health' selected. Below the menu, two dialog boxes are shown side-by-side. The left dialog is titled 'Screening Calculation Options' and the right is 'Exposure Calculation Options'. Both dialog boxes contain a list of statistical approaches with radio buttons. In the 'Screening Calculation Options' dialog, 'Maximum Detected Value' is selected. In the 'Exposure Calculation Options' dialog, 'Maximum Detected Value' and 'Minimum of Max Detect and UCL95' are selected. Both dialog boxes also have a note: 'If a detection ID field has been specified during setup, then these values will be zero when current calculation contains no detected data.' At the bottom of each dialog are 'OK' and 'Cancel' buttons.

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Preliminary Remediation Goals (PRGs)

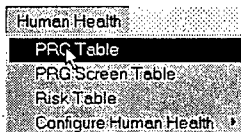
- Definition of PRG
Chemical-specific preliminary remediation goals (PRGs) are concentration goals for individual chemicals in specific medium and land use combinations which are used by risk managers as targets during the analysis and selection of remedial alternatives
- Application
 - develop during the project scoping phase to facilitate development of appropriate detection limits and remedial alternatives or to identify data needs or limitations
 - can be used as screening tools to focus concern on a specific medium or COPC, support no further action recommendations, or support the need for additional study
 - can be used as toxicity screens
 - Can be used as a risk-based concentration goal and considered a final remediation level
 - identify data needs and limitations (e.g., detection limits are greater than risk-based PRGs)
 - focus future sampling and analysis on chemicals and exposure pathways of potential concern
 - establish appropriate detection limits for subsequent environmental sample analysis
 - support a No Further Investigation Determination
 - quantitatively support the need for additional study

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PRG Tables

- View site-specific Preliminary Remediation Goals for media and pathway(s) combinations
- Carcinogenic risk or noncarcinogenic hazard basis
- Select Human Health on Analysis Drop Down List. Then, select Human Health -> PRG Table



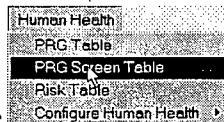
Name	CAS	Ingestion			Inhalation			Dermal			Vegetables		
		HQ (Adult)	HQ (Child)	R	HQ	R	HQ	R	HQ	R	HQ	R	
Barium	7440393	5.1E+4	5.5E+3		6.9E+5		6.7E+4					2.4E+2	
Arsenic, Inorg	7440392	2.2E+2	2.3E+1	4.3E-1		7.5E+2		1.7E+3		8.9E+0		1.1E+0	
Anthracene	120127	2.2E+5	2.3E+4				3.1E+5					9.7E+2	

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PRG Screen Tables

- For a given set of points, SADA finds the maximum value
- Calculates a PRG for the contaminant, exposure scenario, and target risk level. Returns "Yes" if maximum is equal to or higher, Blank if lower or no PRG is available
- Select Human Health on Analysis Drop Down List. Then, select Human Health -> PRG Screen Table



Screening Results: Target risk = 0.000001 / Target Health Index = 1

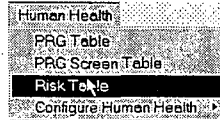
Name	CAS	Conc	Ingestion			Inhalation			Dermal			Vegetables		
			HQ (Adult)	HQ (Child)	R	HQ	R	HQ	R	HQ	R	HQ	R	
Barium	7440393	104.8												
Arsenic, Inorg	7440392	53.6			Yes	Yes						Yes	Yes	
Anthracene	120127	9.5												

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Risk Tables

- For a given set of values, SADA finds the minimum of the UCL95 and the maximum value
- Using this exposure concentration, calculates risk based on the contaminant and exposure scenario
- Select Human Health on Analysis Drop Down List. Then, select **Human Health -> Risk Table**



A screenshot of the 'Human Health Risk Results' window. It displays a table with columns for Name, CAS, Conc, Ingestion, Inhalation, and Dermal. The table lists Benzene, Arsenic, and Anthracene with their respective risk values.

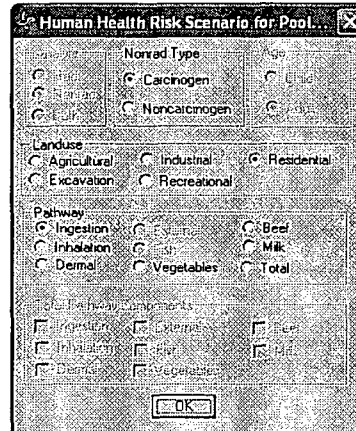
Name	CAS	Conc	Ingestion		Inhalation		Dermal		Veg
			HQ (Ad.)	HQ (Ch.)	R	HQ	R	HQ	
Benzene	7440399	382463842	1.8E-3	1.7E-2	1.3E-4	1.4E-3			
Arsenic	7440382	315399452	1.9E-1	1.8E+0	9.7E-5	5.9E-8	2.4E-2	4.7E-5	
Anthracene	120127	909065391	1.7E-5	1.6E-4			1.2E-5		
Total	55831	609599954	1.9E-1	1.8E+0	9.7E-5	1.3E-4	5.9E-8	2.4E-2	4.7E-5

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Spatial PRG Screens

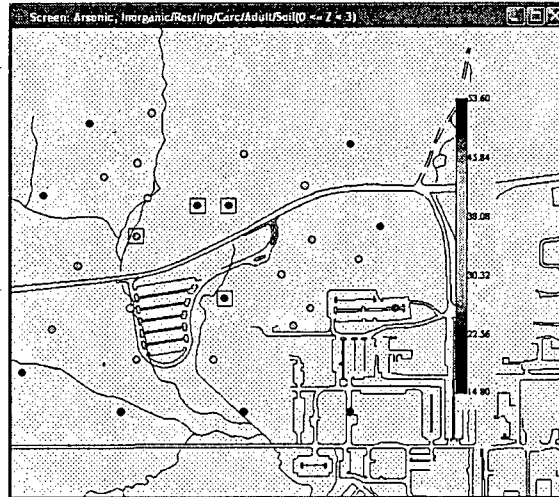
- SADA calculates a PRG for the contaminant, exposure scenario, and target risk level
- Compares the concentration at each location to the PRG
- Location is boxed if it exceeds PRG
- Select Human Health on Analysis Drop Down List. Then, select **Draw a Data Screen Map** from the Interview list
- Press **Show the Results** and select the exposure scenario and pathways when prompted



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Spatial PRG Screen Results



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Point Risk Maps

- SADA calculates risk for each sampling point based on contaminant and exposure scenario.
- Legend scale changes to risk.
- Select Human Health on Analysis Drop Down List. Then, select Draw a Point Risk Map from the Interview list.
- Press Show the Results and select the exposure scenario and pathways when prompted.

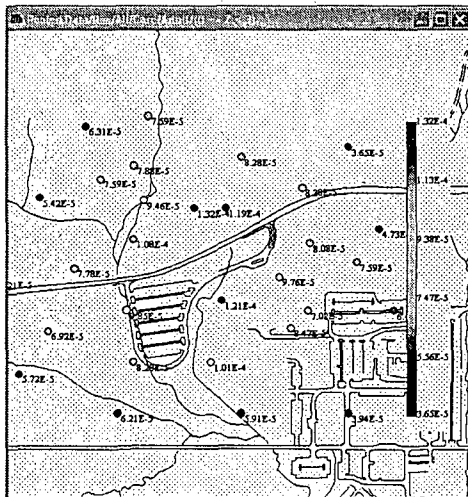
<input type="radio"/> Total <input type="radio"/> Nonrad <input type="radio"/> Carcinogen <input type="radio"/> Noncarcinogen	Nonrad Type <input checked="" type="radio"/> Carcinogen <input type="radio"/> Noncarcinogen
<input type="radio"/> Agricultural <input type="radio"/> Excavation	<input type="radio"/> Industrial <input type="radio"/> Recreational
<input checked="" type="radio"/> Ingestion <input type="radio"/> Inhalation <input type="radio"/> Dermal	<input type="radio"/> Meat <input type="radio"/> Beef <input type="radio"/> Milk <input type="radio"/> Vegetables <input type="radio"/> Total
<input type="checkbox"/> Ingestion <input type="checkbox"/> Inhalation <input type="checkbox"/> Dermal	<input type="checkbox"/> Meat <input type="checkbox"/> Beef <input type="checkbox"/> Milk <input type="checkbox"/> Vegetables

OK

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Point Risk Map Results



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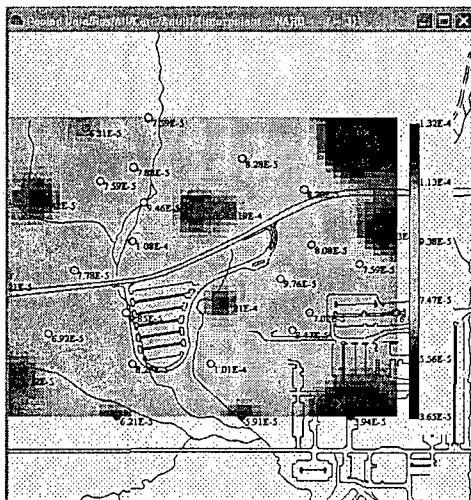
Contoured Risk Maps

- SADA displays a modeled map of concentration to risk based on contaminant and exposure scenario
- Legend scale changes to risk
- Select Human Health on Analysis Drop Down List. Then, select Draw a Contoured Risk Map from the Interview list
- Press **Show the Results** and select the exposure scenario and pathways when prompted

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Contoured Risk Map Results

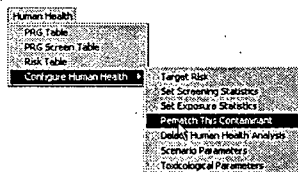
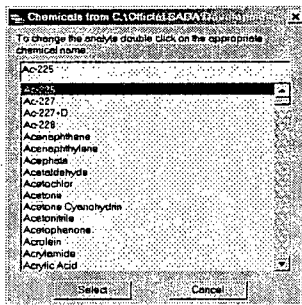


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Rematching a Single Contaminant

- Allows user to change the toxicity information that a contaminant is linked to
- Preferable to resetting up the entire file
- Select Human Health on Analysis Drop Down List
- Select **Human Health** -> **Configure Human Health** -> **Rematch This Contaminant**



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Human Health Help File

- Extensive documentation of human health methods and parameters in SADA help file

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Future Capabilities for Human Health Risk

- ProUCL95 (confidence limits, automatic distribution testing)
- Additional tox info, target organs
- RAGS Part D reporting format
- Screening PRGs as benchmarks
- Air, dermal modifications
- Uncertainty analysis

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Questions?

Comments?

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Spatial Analysis and Decision Assistance (SADA) Version 4 Ecological Risk

Environmental Assessment Methods Using SADA
University of Tennessee, Knoxville

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Ecological Capabilities in SADA

- SADA implements EPA methods for conducting ecological risk assessments
- Benchmark database for contaminant effects on ecological receptors
- Exposure modeling for over 20 other terrestrial species
- Contains EPA default exposure parameters for the risk models where available
- Tabular screening and risk results.
- Point screens
- Risk and dose mapping

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Hazard v. Risk Assessment

- Ecological Hazard Assessment- a comparison of an environmental concentration to an estimated toxic threshold for a particular contaminant
 - Most common method for examining effects of chemicals in environment
 - Comparison of environmental exposure concentration to a toxic threshold (benchmark)
 - Iterative (or tiered) implementation
 - Number of toxicity data sets for soil, sediment, and surface water available for screening
- Ecological Risk Assessment- explicitly attempts to estimate the probability and magnitude of the effects of exposure to contamination

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Limitations of Hazard Assessment

- Lack of consensus
- Conservative benchmarks
- Inappropriate receptors
- Combined exposures
- No probability
- No magnitude

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Ecological Functionality

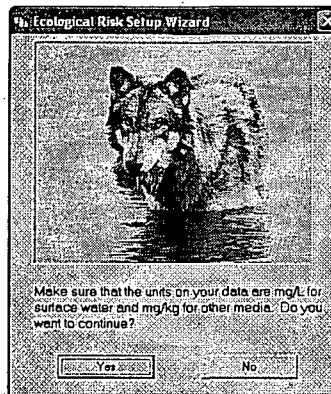
- Setting Up Ecological Risk
- Ecological Risk Assessment Procedure
- Setting Physical Parameters
- Description of Ecological Benchmark Database
- Histograms of Benchmark Values
- Tables of Benchmark Values
- Setting Screening and Exposure Statistics
- Area Result Tables (Screens, Ratios)
- Map Result Values (Screens, Ratios)
- Rematching a Single Contaminant
- Checking Ecological Version
- Terrestrial Dose Modeling

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Setup Ecological Risk

- Identify source benchmarks database
- Match contaminants in data to benchmark contaminants
- Adds ecological information to SADA file

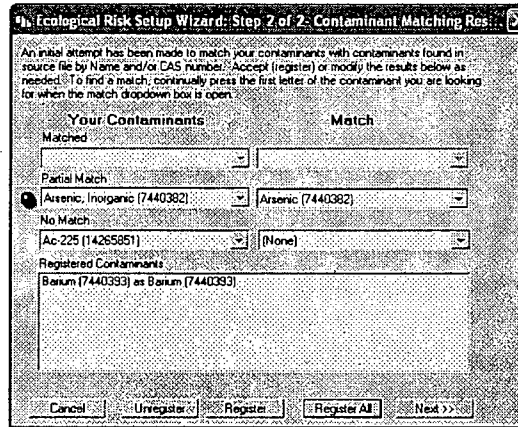
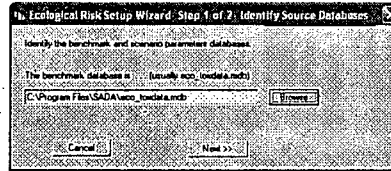


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Setup Ecological Risk Steps

- Select **Setup Ecological Risk** ->
- Click **Yes** on Risk Setup Wizard
- Browse **eco_toxdata.mdb** for
- Select **Next>>** (or **Cancel**)
- Register Contaminants



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Step 1 – Eco Hazard Identification

- First step, done primarily by comparing environmental measurements to benchmarks
- Benchmarks are environmental effects concentrations derived from toxicity testing
- Comparison process is called “screening”
- Benchmarks can be tailored to the site a bit- function of environmental variables where appropriate

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Benchmark Screening

- SW/SD/SO concentration benchmarks
- Choice of statistics (max, percentile, UCL95, etc.)
- Hierarchy of media-specific benchmarks for screening
- Spatial and tabular display of ratios
- Derivation of Benchmarks:
 - Toxicity testing (acute or chronic)
 - regression of concentration-response data
 - hypothesis testing
 - Extrapolation from another benchmark
 - Simulation of an assessment endpoint

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Ecological Benchmarks Databases

- Surface Water (15 Benchmarks)
- Sediment (17 Benchmarks)
- Soil (11 Benchmarks)
- Biota (8 Benchmarks)
- Suitable for performing benchmark screening
- Benchmarks are function of environmental variables, where appropriate (pH, Hardness, Organic Carbon, etc.)

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Surface Water Screening Benchmarks

- Canadian Water Quality Guidelines
- Test EC20s and estimated test EC20s
- Population Ec20s
- EPA Region 4 (Acute and Chronic)
- EPA Region 5 EDQLs
- Lowest CVs in the literature
- Great Lakes Tier II Values

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Sediment Screening Benchmarks

- EPA Great Lakes Assessment and Remediation of Contaminated Sediment (ARCS-NEC, TEC, PEC)
- Canadian ISQL
- Canadian PEL
- Consensus TEC PEC
- EPA Region 4
- EPA Region 5 EDQL
- Florida Department of Environmental Protection (TEL, PEL)
- National Oceanic and Atmospheric Administration (ER-L, ER-M)
- Ontario Ministry of the Environment (LEL, SEL)
- OSWER Ecotox Thresholds
- Washington State Apparent Effects Threshold (NEL, MAEL)

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Soil Screening Benchmarks

- Dutch (Target, Intervention)
- Eco-SSL (Avian, Inverts, Mammalian, Plants)
- EPA Region 4
- EPA Region 5 EDQL
- ORNL (Invertebrates, Microbes, Plants)

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Tissue Residue Benchmarks

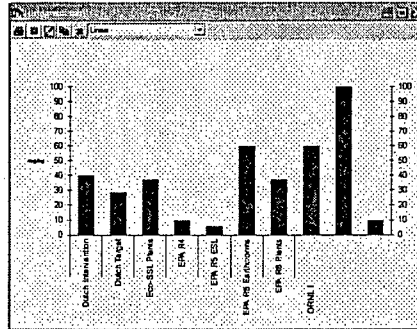
- ECW (Avian, Mammalian)
- British Columbia MELP (Piscivorous wildlife)
- Commission of European Communities (Fish)
- Canadian Council of Ministers of the Environment (Fish, Aquatic organisms)
- Environment Ontario (Piscivorous wildlife)
- Niagara River Biota Contamination Project (Piscivorous wildlife)

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Browse Benchmark Histogram

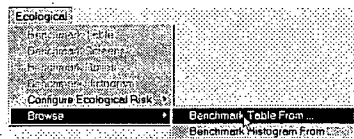
- Can be used to browse benchmarks in master benchmark file or any SADA file
- Shows all available benchmarks in histogram view
- Based on physical properties saved in file when appropriate (hardness, pH, etc.)



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Browse Benchmark Tables



Analyte	EPA-R4-Acids	EPA-R4-Chronic	EPA-RS-ESL	Tier 1 SAV	Tier 1 SOV
1,1,1-Trichloroethane	5.28	0.528	0.088	0.2	0.011
1,1-Dichloroethane			0.047	0.03	0.047
1,1-Dichloroethene	1.03	0.303	0.078	0.45	0.025

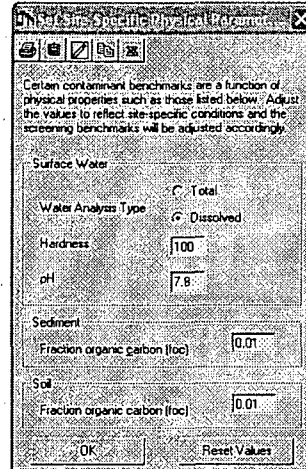
- Can be used to browse benchmarks in master benchmark file or in any SADA file
- Shows available benchmarks in table view, select which benchmarks to see
- Will update based on changed physical properties (hardness, pH, etc.)

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Setting Physical Parameters

- Allows users to set site-specific parameters for organic carbon, hardness, pH, and water analysis type
- Benchmarks that are a function of these parameters will be updated
- Parameters primarily affect bioavailability



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Setting Statistics

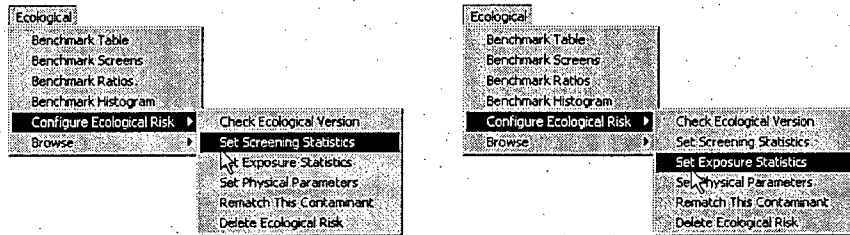
- Default values are maximum detected value for screening calculations and lesser of the maximum detected value and the UCL95 for exposure calculations.
- User can change the approach:
 - Maximum Value: the maximum concentration, detected or nondetected, for normal or lognormal distribution
 - Maximum Detected Value: the maximum detected concentration for normal or lognormal distribution
 - UCL95: the 95% upper confidence limit on the mean for normal or lognormal distribution
 - Mean: the average concentration over all values for normal or lognormal distribution

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Setting Statistics

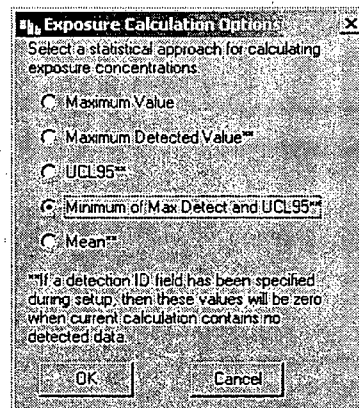
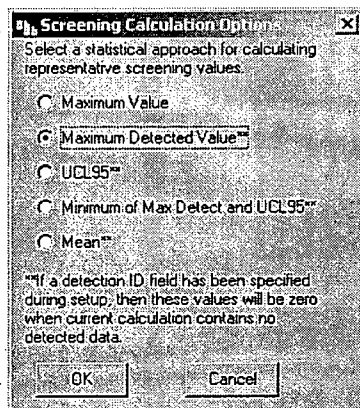
- Select Ecological on Analysis Drop Down List
- Select Ecological -> Configure Ecological Risk -> Set Screening Statistics or Set Exposure Statistics.



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Setting Statistics



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Exposure Area Result Ratios

- Provides a concentration to benchmark ratio based on the min (UCL95, max) for the selected area
- User selects the benchmarks to be screened
- Select Ecological on Analysis Drop Down List. Then, select Ecological -> Benchmark Ratio

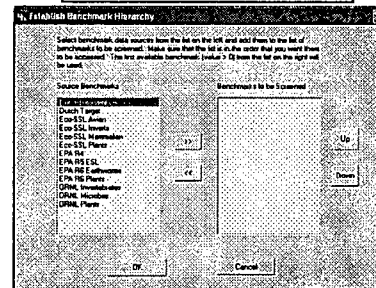
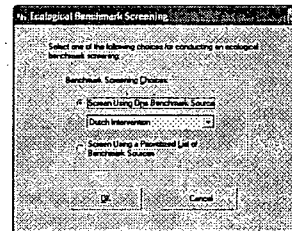
Analyte	Concentration	Units	UCL95	Dutch Target	Dutch Intervention	EPA R4	EPA R5 ESL
Anthracene	3.0337	mg/kg	3.0337			30.3369	0.002
Arsenic	34.822	mg/kg	34.822	1.2006	0.8706	3.4822	6.1091
Barium	74.4157	mg/kg	74.4157	0.4651	0.1191	0.451	71.5536

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Map Result Screens

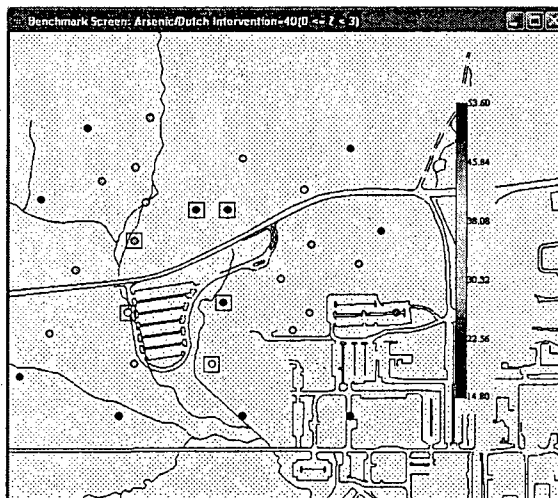
- Screens concentration against benchmarks at each sample location
- Places a box around locations that exceed benchmark
- Can use one benchmark source or establish a site-specific hierarchy
- Select Ecological on Analysis Drop Down List. Then, select Draw a Data Screen Map from the Interview list
- Press Show the Results and select the ecological benchmarks for screening



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Map Result Screens

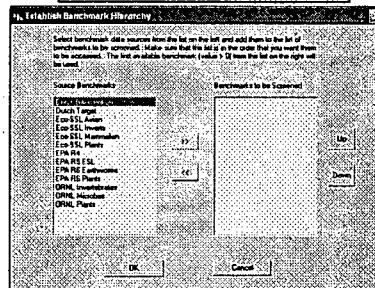
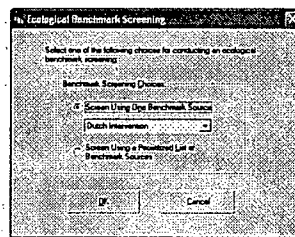


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Map Result Ratios

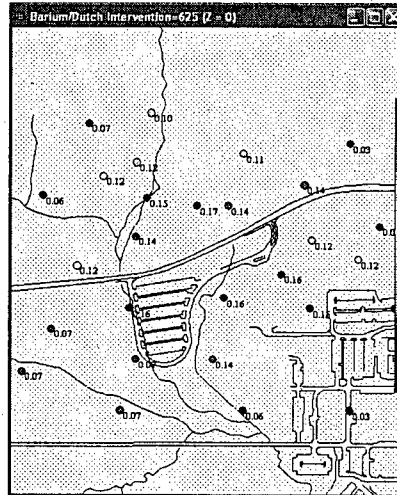
- Provides a concentration to benchmark ratio at each sample location
- Legend changes accordingly
- Can use one benchmark source or establish a site-specific hierarchy
- Select Ecological on Analysis Drop Down List. Then, select Draw a Point Risk Map from the Interview list
- Press Show the Results and select the ecological benchmarks for screening



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Map Results Ratios

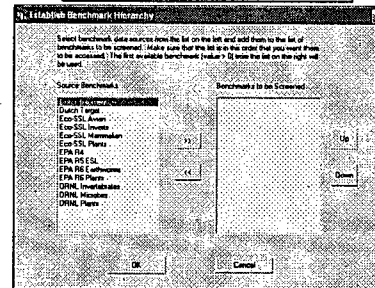
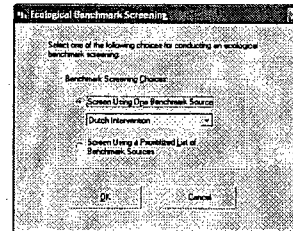


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Contoured Risk

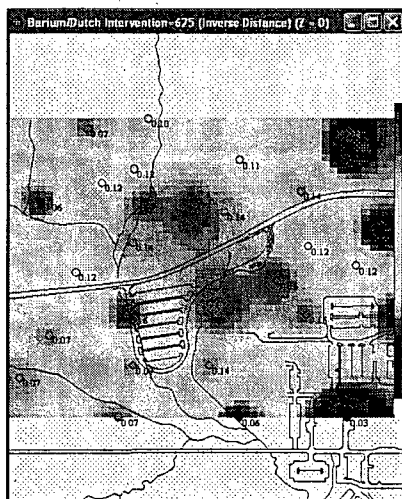
- Displays a modeled map of concentration to benchmark
- Legend changes accordingly
- Can use one benchmark source or establish a site-specific hierarchy
- Select Ecological on Analysis Drop Down List. Then, select Draw a Contoured Risk Map from the Interview list
- Press Show the Results and select the ecological benchmarks for screening



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Contoured Risk Results

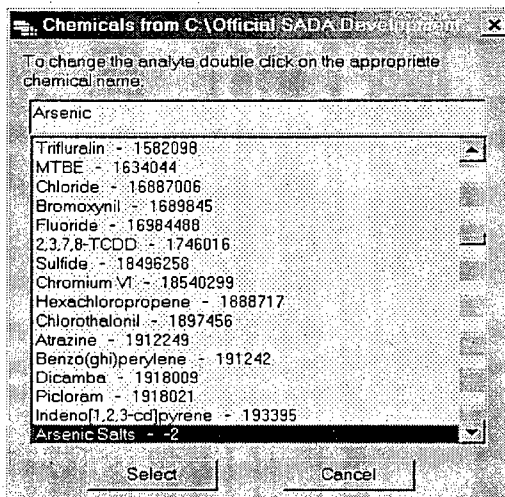
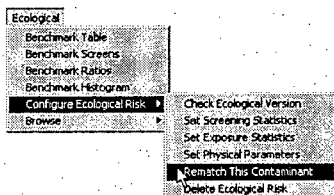


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Rematch a Contaminant

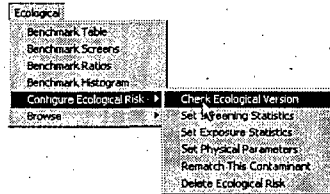
- Allows user to change the benchmark information that a contaminant is linked to
- Preferable to resetting up the entire file



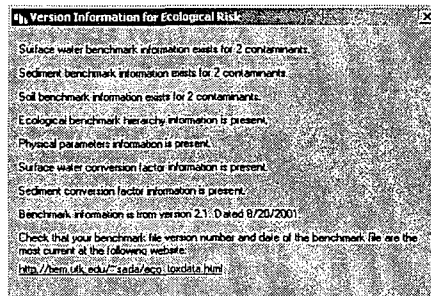
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Check Ecological Version



- Allows user to see if ecological benchmark information has been updated since the file was initially created



- Version and date stamp
- Web address to get latest version

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Step 2 – Dose-Response Evaluation

- Human health- EPA has a constantly maintained database of reference doses and carcinogenic slope factors for determining dose responses
- Ecological- do it yourself, can be pulled out of same data used to generate screening benchmarks, no central vetted database approved for use

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Step 3 – Exposure Assessment

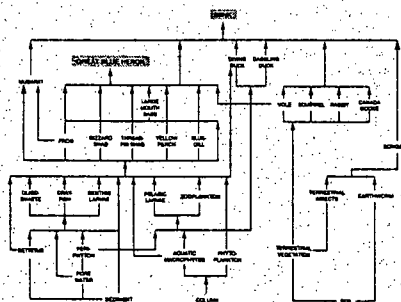
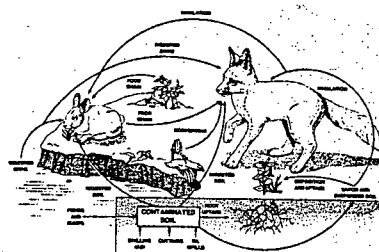
- Decide ecological receptors and pathways to model
- Estimates of daily intake
- Can take into account bioavailability, behavior, growth, spatial distribution
- Easier for a theoretical individual than to build a distribution for a population
- Can also be directly measured via measurements of body burdens or tissue residues



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Conceptual Site Model

- Describe environment
- Obtain source term information
- Suitable habitat determination
- Endpoint definition
 - Socially relevant
 - Biologically relevant
 - Clear operational definition
 - Accessibility to prediction and measurement
 - Susceptibility to the hazardous agent
- Representative Endpoint Species selection
- Exposure Pathway delineation
- Representative diagram



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Ecological Risk Characterization

- Exposure Assessment
 - Species parameter database
 - Exposure Pathways
 - Uptake models
 - Exposure Concentration Determination

- Effects Assessment
 - Predicted effects scale (dose levels)
 - No observed effect
 - No observed adverse effect
 - Low observed adverse effect
 - Probable effects level
 - Severe effects level
 - Correlation/Confirmation with toxicity testing
 - Population surveys

- Risk Characterization
 - Integration of exposure and effects assessment
 - Exposure concentrations
 - Exposure duration
 - Proportion of organisms, populations, or communities responding
 - Severity of the effect

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SADA Terrestrial Dose Modeling

- SADA calculates dose (mg/kg BW d) from food ingestion, soil ingestion, dermal contact, and inhalation for terrestrial exposures as well as total dose summed over all pathways selected.
- SSL, Female, Male, or Juvenile
- Number of different species



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Ingestion Pathway

Model for dose to wildlife receptor from ingestion of contaminated food:

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

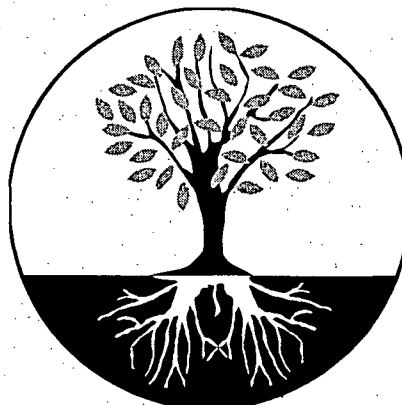
where	<p>FIR_{BW} = Dry food ingestion rate as a function of body weight (kg dry food/kg BW/d)</p> <p>C_{plant} = Chemical concentration in plant (mg/kg dry weight). Estimated from regression equation, or estimated as C_{plant} = C_{soil} x BAF_{plant}</p> <p>BAF_{plant} = soil to plant bioaccumulation factor (mg/kg dry plant per mg/kg dry soil)</p> <p>P_{plant} = Plant ingestion as a percentage of diet (unitless)</p> <p>C_{invert} = Chemical concentration in invertebrate (mg/kg dry weight). Estimated from regression equation, or estimated as C_{invert} = C_{soil} x BAF_{invert}</p> <p>BAF_{invert} = soil to invertebrate bioaccumulation factor (mg/kg dry invertebrate per mg/kg dry soil)</p> <p>P_{invert} = Soil invertebrate ingestion as a percentage of diet (unitless)</p> <p>C_{mamm prey} = Chemical concentration in vertebrate, primarily small mammalian, prey (mg/kg dry weight). Estimated from regression equation, estimated as C_{mamm prey} = C_{soil} x BAF_{soil-to-mamm}, or, if transfer factor is diet-to-tissue, as C_{mamm prey} = C_{diet} x BAF_{diet-to-mamm}</p> <p>BAF_{soil-to-mamm} = soil to mammal bioaccumulation factor (mg/kg dry plant per mg/kg dry soil)</p> <p>C_{diet} = Chemical concentration in diet of mammalian prey (mg/kg dry weight), measured or estimated as C_{diet} = (C_{plant} x P_{plant}) + (C_{invert} x P_{invert}) + (C_{soil} x P_{soil}) with C_{plant}, C_{invert}, P_{plant}, P_{invert}, and P_{soil} referring to mammalian prey parameters rather than the focal receptor.</p> <p>BAF_{diet-to-mamm} = food to mammal bioaccumulation factor (mg/kg dry mammal per mg/kg dry food)</p> <p>P_{mamm} = Proportion of vertebrate prey in the diet (unitless)</p> <p>AF = Absorbed fraction of chemical from ingested food. Assumed = 1. (unitless)</p> <p>AUF = Area use factor = ratio of animal's home range to area of site. Maximum is 1, which assumes animal is on-site 100% of the time. Default is 1. (unitless)</p>
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Terrestrial Plants

root absorption, leaf
deposition



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Soil -> Plant

Kow-based soil-to-plant BAFs were generated using the following equation from EPA (2000):

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

where BAF_{plant} = soil to plant foliage bioaccumulation factor ($\frac{mg / kg \text{ dry plant}}{mg / kg \text{ dry soil}}$)
 K_{ow} = octanol-water partitioning coefficient.

Soil-to-plant tissue regression relationships are of the form:

$$C_{tissue} = e^{\text{slope} \times \ln(C_{soil}) + \text{intercept}}$$

where C_{tissue} = Chemical concentration in plant tissue (mg/kg, dry weight)
 C_{soil} = Chemical concentration in dry soil (mg/kg)
 Slope = coefficient for slope of the regression model
 Intercept = value for the y-intercept of the regression model.

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Soil -> Invertebrates

Kow-based soil-to-invertebrate BAFs were generated using the following equation from EPA (2000):

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

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

Soil-to-invertebrate tissue regression relationships are of the form:

$$C_{tissue} = e^{\text{slope} \times \ln(C_{soil}) + \text{intercept}}$$

where C_{tissue} = Chemical concentration in invertebrate tissue (mg/kg, dry weight)
 C_{soil} = Chemical concentration in dry soil (mg/kg)
 Slope = coefficient for slope of the regression model
 Intercept = value for the y-intercept of the regression model.

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Soil/Diet -> Vertebrates

Soil-to-vertebrate tissue regression relationships are of the form:

$$C_{tissue} = e^{\text{slope} \times \ln(C_{soil}) + \text{intercept}}$$

where C_{tissue} = Chemical concentration in vertebrate tissue (mg/kg, dry weight)
 C_{soil} = Chemical concentration in dry soil (mg/kg)
 Slope = coefficient for slope of the regression model
 Intercept = value for the y-intercept of the regression model.

No Diet-to-Tissue regression relationships have been included in SADA, but users who have developed their own relationships may enter the slope and intercept values under Diet-to-Small Mammal Concentration, Tissue Regression if the Diet-to-vertebrate tissue regression relationship is of the form:

$$C_{tissue} = e^{\text{slope} \times \ln(C_{diet}) + \text{intercept}}$$

where C_{tissue} = Chemical concentration in vertebrate tissue (mg/kg, dry weight)
 C_{diet} = Chemical concentration in diet (mg/kg, dry weight)
 Slope = coefficient for slope of the regression model
 Intercept = value for the y-intercept of the regression model.

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Ingestion of Contaminated Soil

Model for dose to wildlife receptor from ingestion of contaminated soil:

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

where 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. Maximum is 1, which assumes animal is on-site 100% of the time. Default is 1. (unitless).

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Dermal Contact with Soil

Model for estimation of dose to terrestrial receptors from dermal contact:

$$D_{dermal} = \frac{C_{soil} \times SA \times AdF \times AbF}{BW}$$

where C_{soil} = Chemical concentration in dry soil (mg/kg)
 SA = Receptor's surface area (cm²/d)
 AdF = Adherence Factor, a measure of tendency of soil to adhere to skin.
 AbF = Absorption Fraction, a measure of the fraction of chemical in contact with skin that is actually absorbed into the body. (unitless)
 BW = Receptor's body weight (kg)

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Inhalation Dose

Model for estimation of dose to terrestrial receptors from inhalation:

$$D_{inhalation} = \frac{IR_{air} \times C_{air}}{BW}$$

where IR_{air} = Receptor's inhalation rate (m³/d)
 C_{air} = Concentration of chemical in air, calculated as C_{soil} x PEF for nonvolatile chemicals or as C_{soil} x 1/VF for volatile chemicals (mg/m³)
 C_{soil} = Chemical concentration in dry soil (mg/kg)
 PEF = Particulate Emissions Factor, estimate of concentration of dust particles in the air (kg/m³)
 VF = Volatilization Factor, a chemical-specific soil-to-air volatilization factor (m³/kg)
 BW = Receptor's body weight (kg)

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SADA Terrestrial Dose Modeling

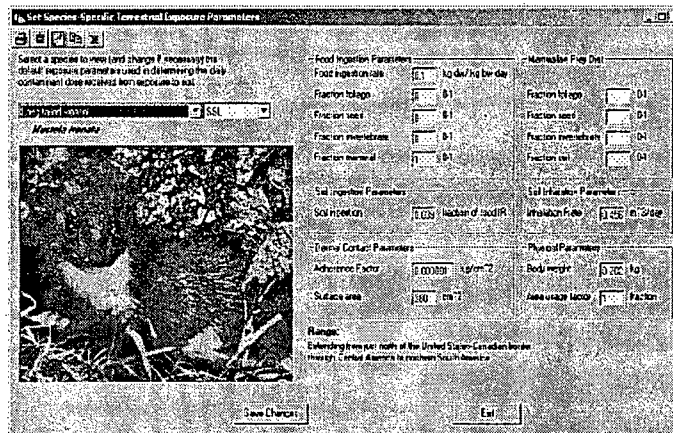
- SADA calculates dose (mg/kg BW d) from food ingestion, soil ingestion, dermal contact, and inhalation for terrestrial exposures as well as total dose summed over all pathways selected.
- SSL, Female, Male, or Juvenile
- Number of different species

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Set Species Exposure Parameters

- Customize model parameters
- 21 species available for version 4



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Set Contaminant Uptake Parameters

- Set chemical constants for contaminants
- Choose bio-accumulation model type and values

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Calculate Exposure for Home Range

- Use a polygon to identify home range
- Select species/sex
- Click exposure pathways
- Returns dose in mg/kg/day for each exposure pathway

Analyte	Concentration	Food Ingestion	Soil Ingestion	Dermal Contact	Inhalation	Total
Arsenic	34.822033566	0.75737923007	0.6059033844	1.17818910564	NA	1.36

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Point Dose Maps

- Provides dose calculation at each point based on species and exposure assumptions
- Legend changes accordingly
- Select Ecological on Analysis Drop Down List. Then, select **Draw an Eco Point Dose Map** from the Interview list
- Press **Show the Results** and select the species and exposure assumptions

Terrestrial Dose Calculation

Select a species and a set of exposure assumptions for terrestrial dose calculation.

Receptor

Species: Meadow vole

Exposure Type: SSL

Check the exposure pathways that are to be summed for terrestrial exposure.

Exposure Pathways

Food Ingestion

Soil Ingestion

Dermal Contact

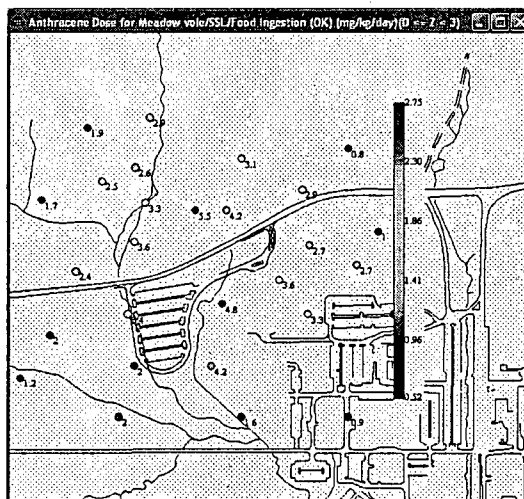
Inhalation

OK Cancel

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Point Dose Maps



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Contoured Eco Dose Maps

- Provides a modeled map of dose based on species and exposure assumptions
- Legend changes accordingly
- Select Ecological on Analysis Drop Down List. Then, select **Draw a Contoured Eco Dose Map** from the Interview list
- Press **Show the Results** and select the species and exposure assumptions

Terrestrial Dose Calculation

Select a species and a set of exposure assumptions for terrestrial dose calculation.

Receptor

Species: Meadow vole

Exposure Type: SSL

Check the exposure pathways that are to be summed for terrestrial exposure.

Exposure Pathways

Food Ingestion

Soil Ingestion

Dermal Contact

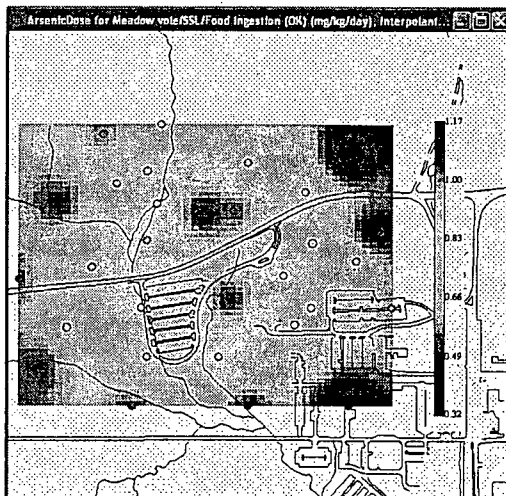
Inhalation

OK Cancel

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Contoured Eco Dose Maps



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Ecological Risk

- Additional benchmarks
- Radionuclide benchmarks and dose assessment methods
- Terrestrial movement and habitat models
- Eco PRG tables/calculations
- Aquatic dose models
- Uncertainty for dose assessment

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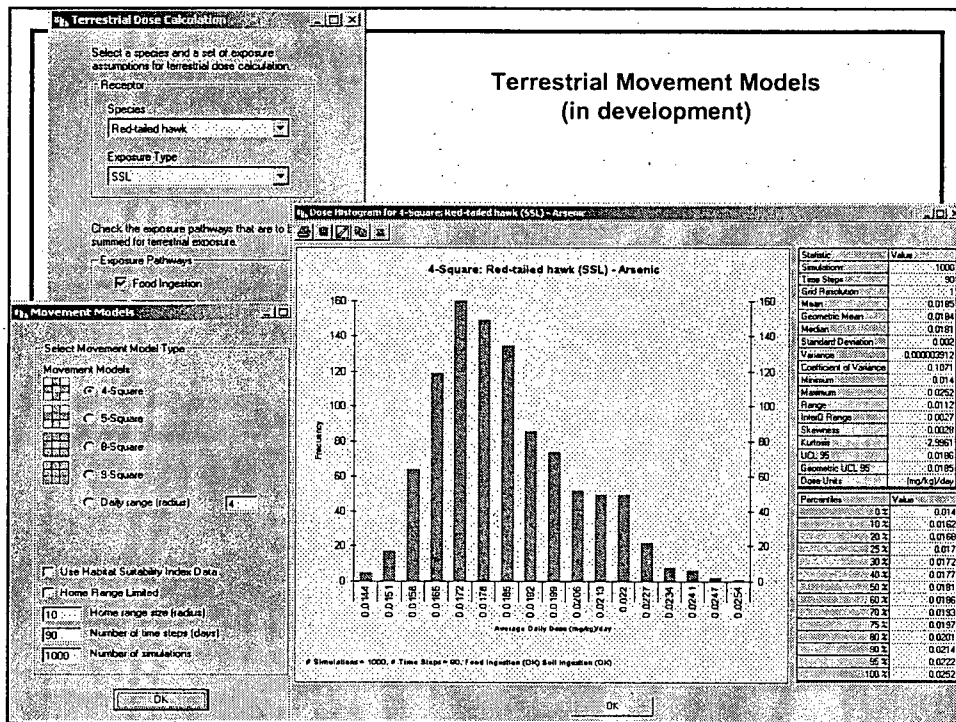
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Spatially Explicit Ecological RA

- Use spatial distribution of contamination with dynamic movement models that also incorporate:
 - Habitat quality
 - Foraging behavior
 - Ecological interactions
- Number of movement models available in the literature

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Questions? Comments?

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Practice Session Human Health and Ecological Risk Assessment

The objective of this lesson is to be able to add human health and ecological risk functionality to a SADA file, then generate risk assessment results both in a tabular form and using the spatial interpolation capabilities of SADA.

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Practice Session: Human Health and Ecological Risk Assessment



I-40/I-640 Site

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Practice Session: Human Health and Ecological Risk Assessment

1. Open the file you created earlier called lesson2.sda.
2. Setup human health risk assessment capabilities using the setup wizard. Accept all partial matches, find matching names for contaminants with no match. Save the file.
3. Configure Target risk to carcinogenic risk of 0.00001 and noncarcinogenic hazard of 0.1.
4. Select Pooled Data and View PRG table. Select Arsenic and the ingestion, dermal contact, and inhalation pathways. For the residential scenario, what are the:
Noncarcinogenic PRG _____
Carcinogenic PRG _____

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Practice Session: Human Health and Ecological Risk Assessment

4. Draw a polygon around the sinkhole, then perform a tabular PRG screen, which set of contaminants are a problem for the recreational scenario (with ingestion, dermal contact, and inhalation selected)?

5. Generate tabular risk results for pooled data, what is the total agricultural risk and noncarcinogenic hazard?
Risk _____
Hazard _____
6. Draw a point risk map for pooled data and the recreational scenario (select ingestion, dermal contact, and inhalation).
7. Select Arsenic and choose an interpolation method (inverse distance, search radii = 50, min data = 1, max data = 20, power =2), then draw a contoured risk map for carcinogenic residential ingestion.
8. Change the adult residential soil ingestion rate from 100 mg/day to 40 mg/day and regenerate the arsenic map.

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Practice Session: Human Health and Ecological Risk Assessment

9. Setup ecological risk with this same database. Be sure to match up Aroclor-12xx to PCB-12xx and DDE to 4,4-DDE, etc. Save the file.
10. Select pooled data and view benchmark tables and screen tables.
11. For the sinkhole area polygon, select view benchmark ratio tables, what is the ratio for lead versus the EPA Region 4 benchmark?

12. With lead selected, select view benchmark histogram, what is the most conservative benchmark value for lead (you may have to show the benchmarks on the log scale)?

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Practice Session: Human Health and Ecological Risk Assessment

13. View the terrestrial exposure parameters for the long-tailed weasel. Change the food ingestion rate for the male long-tailed weasel to 0.12. Calculate the total dose from food and soil ingestion for the male long-tailed weasel for lead and enter it here. _____
14. Select Lead and choose an interpolation method (inverse distance, search radii = 50, min data = 1, max data = 20, power =2), draw a contoured eco dose map for the male long-tailed weasel's exposure to lead from food and soil ingestion.
15. Select Mercury and choose an interpolation method (inverse distance, search radii = 50, min data = 1, max data = 20, power =2), Draw a contoured risk map for the ratio of mercury concentration to the benchmark, use a benchmark hierarchy of
 1. Eco-SSL Mammalian
 2. Eco-SSL Avian
 3. Dutch Target
 4. EPA R4What source and value was used as the benchmark?

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Spatial Analysis and Decision Assistance (SADA) Version 4.1 Custom Analysis

Environmental Assessment Methods in SADA
University of Tennessee, Knoxville

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Custom Analysis

- What is intended for Custom Analysis
- Setting Up A Custom Analysis
- Viewing Custom Values Table
- Setting Screening Statistics
- Custom Value Screen Table
- Spatial Custom Value Screen
- Rematching a Single Contaminant

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Role Of Custom Analysis

- Custom analysis refers to any outside values that can be imported into SADA.
- Once imported into SADA, these values can be used to screen data, determine area of concern, and support sample design.
- Custom analyses are imported into SADA the same fashion as ecological and human health.
- One can have an unlimited number of custom analyses.

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Setting Up a Custom Analysis

- From the main menu, select **Setup** and then **Custom**.
- Choose **Next**.
- Select the file with the custom values you need. In this example, choose **browse**, select Microsoft Access Database as the file type and choose CustomCriteria.mdb.
- When you select a database, you are presented with the available recordset from that database. In this example, select Custom Analysis.
- Next, choose the column from the recordset associated with contaminant names and CAS numbers.
- Accept or modify the contaminant matches and you're finished.

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Viewing Custom Values

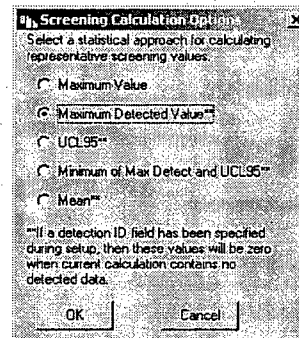
- In the analysis list box, choose custom analysis.
- You will now see the name of your custom analysis appear as a menu table.
- Under this menu, choose **Custom Analysis Table**.
- The custom decision values for the currently selected contaminant are presented in a table.

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Setting Screening Statistics


- Select Custom Analysis on Analysis Drop Down List.
- Select **Custom Analysis -> Configure Custom Analysis -> Set Screening Statistics**.
- Default value is maximum detected value.
- User can change value.
 - Maximum Value: the maximum concentration, detected or nondetected, for normal or lognormal distribution
 - Maximum Detected Value: the maximum detected concentration for normal or lognormal distribution
 - UCL95: the 95% upper confidence limit on the mean for normal or lognormal distribution
 - Mean: the average concentration over all values for normal or lognormal distribution



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Screening Custom Values (Tabular)

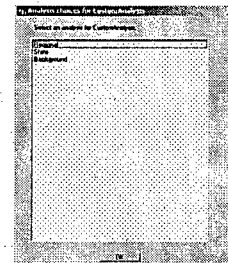
- In the analysis list box, choose custom analysis.
- You will now see the name of your custom analysis appear as a menu table.
- Under this menu, choose Custom Screen Table or press the Screen Button. 
- If a data value exceeds the custom criteria value, a Yes will appear in the corresponding box.

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Screening Custom Values (Spatial)

- In the analysis list box, choose custom analysis.
- Under Decision Basis on the Decision tab of the control panel, make sure that the current custom analysis option is selected.
- Press the Data Screen Button. 
- You will be presented with all the possible screening criteria in your custom analysis. Choose one.
- SADA responds with the result. If your choice has no value or has a non-numeric value, SADA will prompt you to use zero or just quit.



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Spatial Analysis and Decision Assistance (SADA) Version 4 Decision Analysis

Environmental Assessment Methods in SADA
University of Tennessee, Knoxville



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Part 8: Decision Analysis

- Probability Maps
- Area of Concern Maps
 - Block Framework
 - Site Framework
- Cost Benefit Analysis
 - Cost Lines
 - Cost Line Query

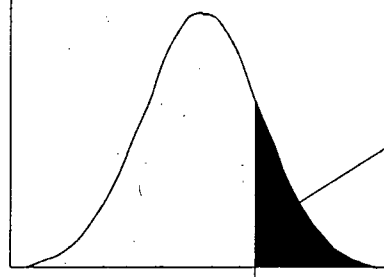


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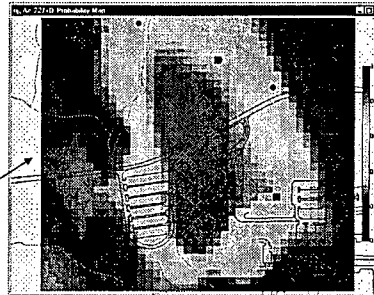
Probability Maps

- A probability map spatially delineates the probability of exceeding a specified threshold.
- The probability of the center of each block exceeding the threshold value is calculated.
- Probability maps can only be created with ordinary or indicator kriging.

Probability > 3.0 pCi/G



Probability > 3.0 pCi/G



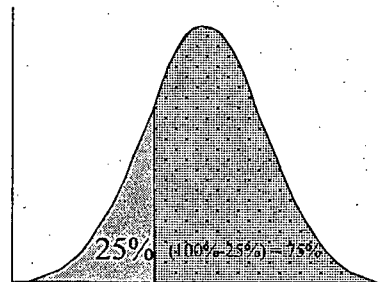
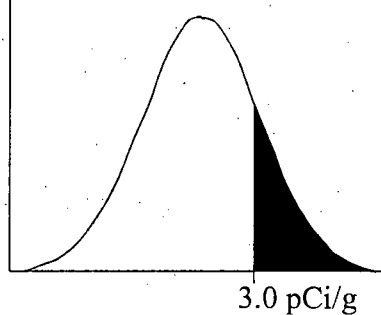
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Percentile Maps vs Probability Maps

- In a percentile, we fix the probability and determine what concentration is associated with that probability in each block. So you get a map of concentrations.
- In a probability map, we fix the concentration and calculate the probability associated with that concentration.

Probability > 3.0 pCi/G

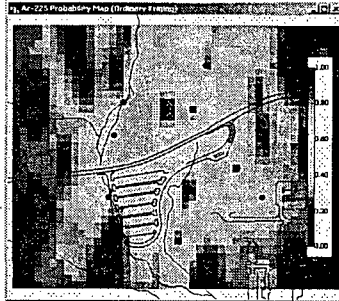


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Creating Probability Maps

- Select the analysis, data type and data name of interest
- Select **Draw a Probability Map** from the Interview list.
- Define a grid by selecting **Set Grid Specs**.
- Press **Interpolation methods** and then select Ordinary or Indicator Kriging.
- Select **Correlation Modeling** and then set variography and correlation models.
- Select **Search Neighborhood** and define the search neighborhood parameters.
- Press **Show The Results**.
- SADA will ask for the applicable decision criteria, depending on the analysis type, and then present the results in the **Results Window**.



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Area of Concern Maps

- Draws the area of concern based on the modeled values, a threshold value, and a decision framework.
- Can be drawn with any of the five available interpolants.
- Threshold values can come from user-defined concentrations, human health risk, ecological risk, or custom analysis.
- Three decision frameworks are available
 - *Block Scale* (Nearest Neighbor, Natural Neighbor, Inverse Distance)
The decision criteria is applied to individual blocks.
 - *Confidence Based Block Scale* (Ordinary and Indicator Kriging)
The decision criteria, which now includes a remedial confidence parameter, is applied to individual blocks.
 - *Site Scale* (All Five Interpolants)
The decision criteria is applied to the site. Individual blocks are "remediated" until the site-wide model average satisfies the specified threshold.
- Density and Post Remediation Parameters

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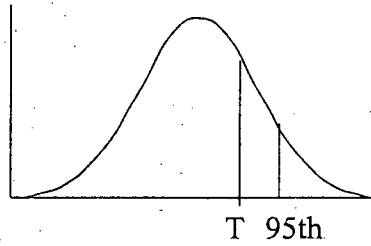
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Decision Scales

- **Block Scale**
 - If the estimated block value is above the threshold value, it must be remediated. For ordinary and indicator kriging, set the confidence parameter equal to .5.

- **Block Scale (Confidence)**
 - Given a threshold value, if the 95th percentile is greater than the threshold value, then remediation is required. Otherwise, there is at least a 95% chance the true value falls below the threshold.

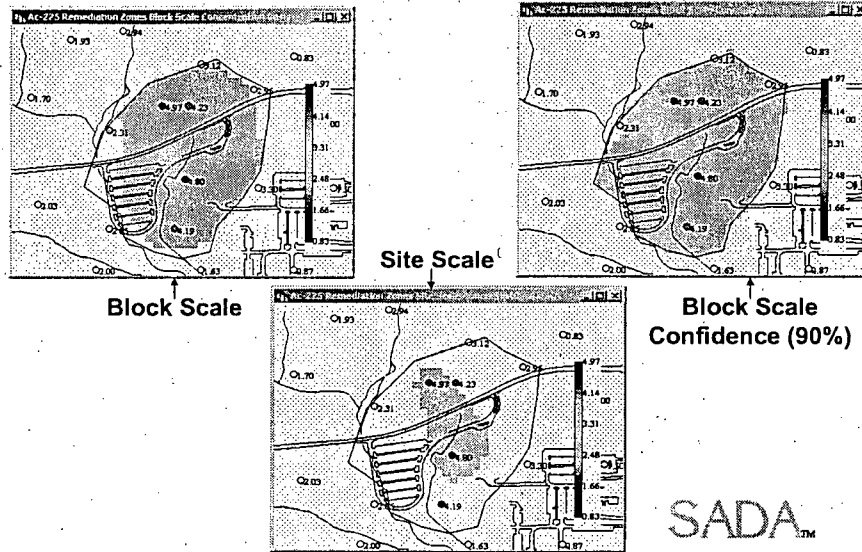
- **Site Scale**
 - If the site-wide model average is above the threshold value, "remediate" the individual blocks from worst to least contaminated until the average, including post remedial concentrations, drops below the threshold value.



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Decision Framework Results



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Creating Area Of Concern Maps

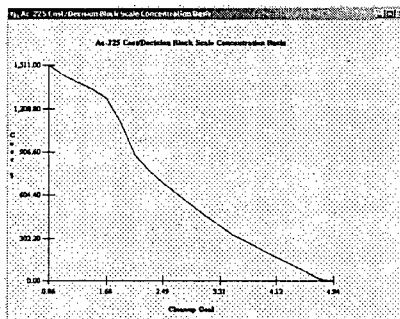
- Select the analysis, data type and data name of interest
- Select **Draw an Area of Concern Map** from the **Interview** list.
- Define a grid by selecting **Set Grid Specs**.
- Press **Interpolation methods** and then select the method from the list of available interpolants.
- Select **Correlation Modeling** (for Ordinary and Indicator Kriging) and then set variography and correlation models.
- Select **Search Neighborhood** and define the search neighborhood parameters.
- Select **Specify Decision Criteria**. Choose a **Site** or **Block** scale.
- Press **Show The Results**.
- SADA will ask for the applicable decision criteria, depending on the analysis type, and then present the results in the **Results Window**.

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Cost Benefit Analysis

- The decision framework (block, block confidence, site) determines the associated cost for a range of cleanup goals.
- Cost is calculated by determining the area of concern (or volume for 3d) for a threshold value, then multiplying the number of blocks in this area by the remedial cost per block.
- After the threshold value range is calculated, cost is calculated for each incremental value in this range.



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Performing A Cost Benefit Analysis

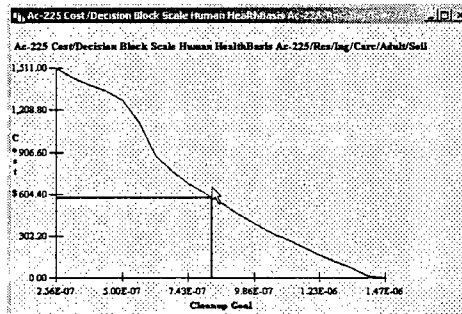
- Select the analysis, data type and data name of interest
- Select **Calculate Cost versus Cleanup** from the **Interview** list.
- Define a grid by selecting **Set Grid Specs**.
- Press **Interpolation methods** and then select the method from the list of available interpolants.
- Select **Correlation Modeling** (for Ordinary and Indicator Kriging) and then set variography and correlation models.
- Select **Search Neighborhood** and define the search neighborhood parameters.
- Select **Specify Decision Criteria**. Choose a **Site** or **Block** scale.
- Set the cost information by selecting **Set Cost Information**.
- Press **Show The Results**.
- SADA will ask for the applicable decision criteria, depending on the analysis type, and then present the results in the **Results Window**.

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Cost Lines

Click the **Line Pointer** button and you will now see two blue lines which will help guide you as you interpret the graph. On the bottom Status bar, the actual XY's are displayed.



Line Pointer

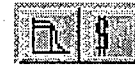
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Cost Line Query

Click the **Line Query** button and the following window appears. Type a specific cleanup concentration into one of the top boxes and leave the corresponding cost box empty. Press the **Calculate** button. SADA reads the cost value from the graph. Conversely, by leaving the concentration box empty and entering a cost value, SADA will report the cleanup concentration.

	Scenario 1	Scenario 2	Scenario 3
Cleanup Concentration	1E-6		
Cleanup Cost	2,471.00		



↑
Line Query

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Questions?

Comments?

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Practice Session Decision Analysis

The objective of this lesson is to combine the skills learned for risk assessment and spatial analysis in a number of decision making frameworks, including area of concern and cost benefit analysis.

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Practice Session: Decision Analysis

1. Open up "Lesson6.sda". Choose the "Draw a Data Screen map" interview and turn on the polygon "Boundary".
2. Produce a data screen map for Arsenic, Inorganic using a screening value of 100 mg/kg. Notice where the data points are exceeding this value.
3. We want to screen the Arsenic data for values that are too high for a child living on the site who might incidentally ingest the soil. We are interested in noncarcinogenic effects at a target health index of 1. In other words, we want to produce a data screen map for this human health scenario: nonrad, noncarcinogenic, residential, ingestion, child. What is the PRG? Notice where the data points are exceeding this value.

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Practice Session: Decision Analysis

1. Now, we want to evaluate, in a spatial context, the probability of exceeding certain important values where we have not yet sampled. Switch to the "Draw a probability map" interview. Choose Ordinary kriging for your interpolant. Switch the analysis to Human Health. The ordinary kriging model has been parameterized from the previous lesson. Note the areas that are green in the large unsampled areas in the north. Does this make sense?

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Practice Session: Decision Analysis

6. Given the samples we now have and the ordinary kriging model we've parameterized, where should we clean up? We want to clean up any portion of the site that is too high for our human health scenario.
7. Switch to the "draw an area of concern map" interview. Under the decision criteria, we need to choose block scale to clean up any portion that is too high for our scenario. Set the confidence level to .5. Set the density parameter to 1. What area do we clean up at a confidence of .5? What is the number of blocks? The total volume?
8. What about .7? .9?

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Practice Session: Decision Analysis

9. Now, suppose the regulator only states that the average site concentration be acceptable for the human health scenario. We would want to just clean the worst areas so that the site-wide model average is below the threshold value for the residential child scenario. So, we're going to clean up those areas and backfill them with "clean" soil. However, the "clean" soil contains some naturally occurring arsenic. The background value in the soil is 2 mg/kg. Using site scale, determine what areas require remediation.
10. We want to quantify the impact of slightly lowering or raising the health index on the overall cost of the project. If we raised it only slightly, could we still make the site safe while lowering costs? Switch to the "cost vs cleanup" interview. Let's calculate for a block scale framework at a confidence of .5. For the cost of cleanup, enter \$1 per block. This will allow us to see how many blocks we'll need to clean. (In a real scenario, you would enter the actual cost of cleaning up a block of this size.)

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Practice Session: Decision Analysis

11. Press the *Show the results* button and choose the usual human health scenario. How much does it cost to clean up for a health index result equal to one?
Hint: Use the cost line query tool, found by right mouse clicking over the picture. It should be around \$393.
12. What if we raised the index to 1.1 (slightly more dangerous)? What if we lowered it to .9 (slightly safer)?

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Spatial Analysis and Decision Assistance (SADA) Version 4 Secondary Sample Design

Environmental Assessment Methods in SADA
University of Tennessee, Knoxville

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Part 12: Secondary Sample Designs

- Threshold Radial
- Adaptive Fill
- High Value
- Extreme Value
- Area of Concern Boundary
- Minimize/Maximize Area of Concern
- Ripley's K
- Moran's I
- Geary's C

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Simulated vs Unsimulated Sample Designs

Simulated Sampling

Simulated sampling finds each successive new sample. That sample is placed and the estimated value is added to the conditioning data as if they were real values. Since real values are not used, error rates are incurred in the process, which increase with each new additional sample location.

Unsimulated Sampling

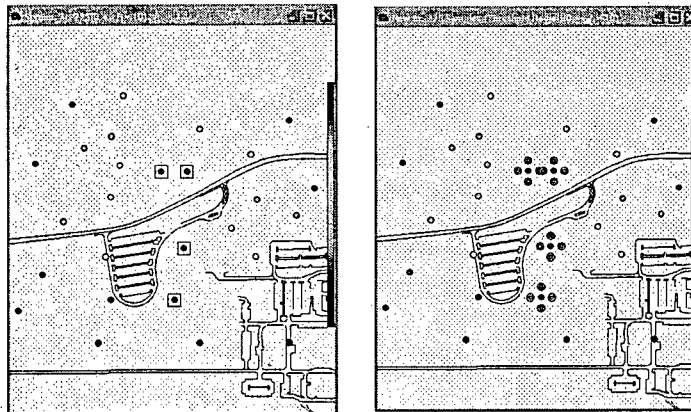
Unsimulated sampling simply locates all new samples off the same geospatial map without attempting to update the map after each point is found. The method is quick but does not always reflect the type of behavior the model will exhibit after each new sample is found, particularly for those methods that depend on measures of geospatial uncertainty.

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Threshold Radial

Threshold Radial is a straightforward secondary sample design places samples in a radial pattern around existing data points that exceed a decision threshold. The user has control over the pattern of the surrounding new sample points. They can be circular or rectangular.

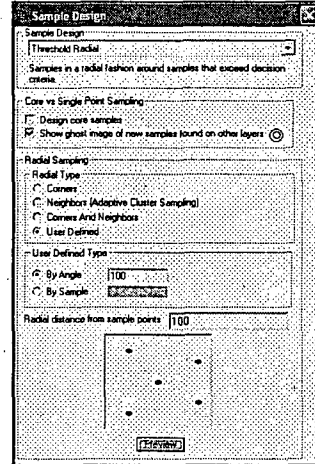
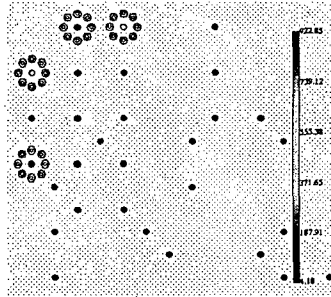


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Threshold Radial

Select **Threshold Radial** from the drop down list under **Sample Design**. Then select the radial type and enter the radial distance.



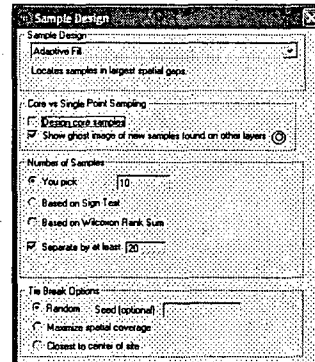
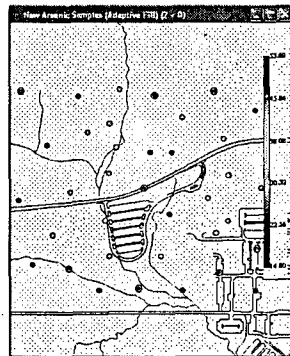
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Adaptive Fill

Adaptive Fill is a secondary sample design that spatially fills data gaps, independent of geospatial interpolation.

Select **Adaptive Fill** from the drop down list under **Sample Design**. Then select the number of samples. Enter a value for **Separate By At Least** in order to use the secondary minimum distance constraint.



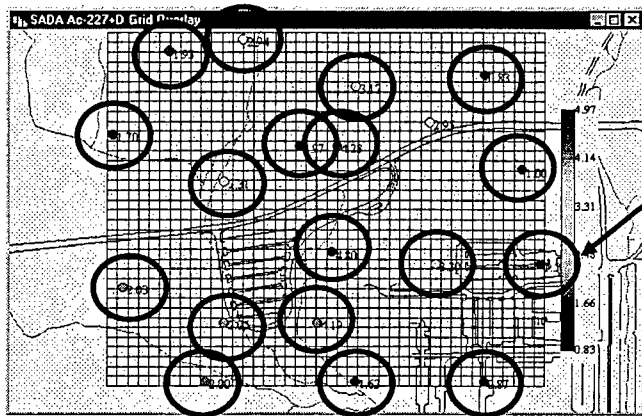
Press **Show the Results** and SADA will randomly select your new sample locations.

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Secondary Minimum Distance Constraint

This constraint prevents clustering by setting the minimum distance a new sample point can exist from an existing new or actual sample point through a limiting sphere. All nodes within the sphere are eliminated from consideration as a new sample candidate.



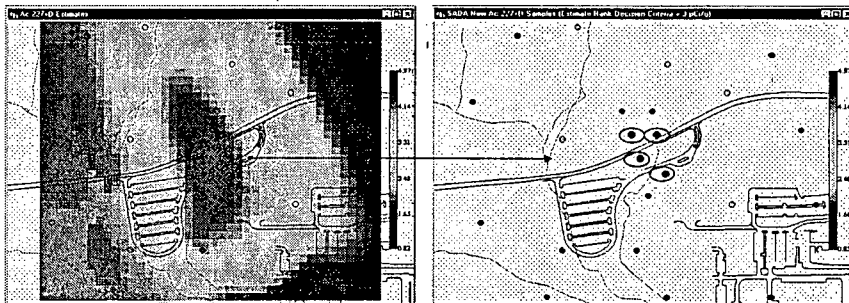
Limiting Spheres

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High Value

- Places new samples where modeled values are highest
- Good for confirming hot spots



Contour Map

High Value Design

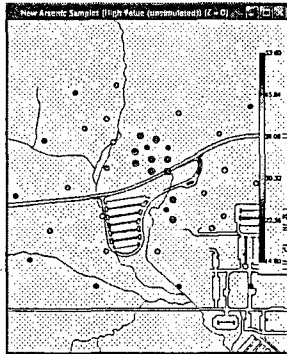
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High Value

High Value is a secondary sample design that generates new samples in locations with high interpolation estimates. This design may be useful for verifying the extent of hot spot regions.

Select **High Value** from the drop down list under **Sample Design**. Then select the number of samples. Enter a value for **Separate By At Least** in order to use the secondary minimum distance constraint.

A screenshot of the "Sample Design" dialog box in the SADA software. The "High Value" option is selected in the "Sample Design" dropdown menu. The "Core vs Single Point Sampling" section has "Design core samples" checked and "Show ghost image of new samples found on other layers" selected. The "Number of Samples" section has "You pick" selected with a value of 10. The "Separate by at least" field is set to 20. The "Simulated Sampling" section has "Simulated Sampling" checked. The "Break Options" section has "Random" selected for "Seed (optional)".

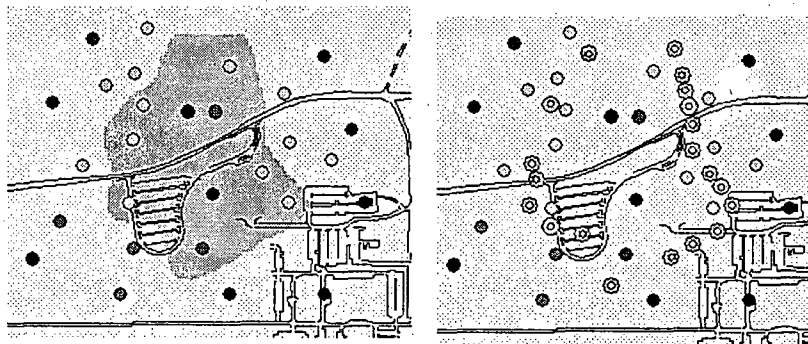
Press **Show the Results** and SADA will select your new sample locations.

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Area of Concern Boundary Design

Area of Concern Boundary is a secondary sample design that places new samples in locations along the decision boundary.

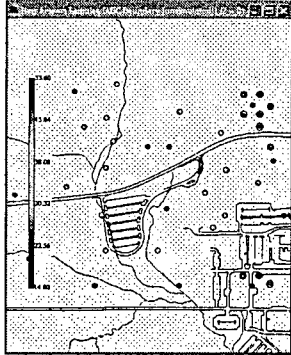


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Area of Concern Boundary

Select **Area of Concern Boundary** from the drop down list under **Sample Design**. Then select the number of samples. Enter a value for **Separate By At Least** in order to use the secondary minimum distance constraint.



Sample Design

Area of Concern Boundary

Locates samples where interpolator's estimates are closest to decision criteria.

Core vs Single Point Sampling

Design core sampler

Show ghost image of new samples found on other layers

Number of Samples

You pick: 10

Based on Sign Test

Based on Wilcoxon Rank Sum

Separate by at least: 100

Simulated Sampling

Tie Break Options

Random: Seed (optional):

Minimize spatial coverage

Closest to center of site

Press **Show the Results**. SADA will ask for a decision goal and remedial confidence and then display your new sample locations.

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Questions?

Comments?

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Practice Session Secondary Sample Design

The objective of this lesson is to use two secondary sample design strategies to better delineate the extent of contamination across the site.

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Practice Session: Secondary Sample Design

1. Open "Lesson7.sda". Choose the "Develop a sample design" interview and turn on the polygon "Boundary".
2. Suppose we have cause to believe that the extreme value points found in the southeast portion of the site are probably disjoint. We want to find out the extent of the local hot spots. Use the *Threshold Radial* sample design to encircle the hot sample locations and "chase" the extent of the local hot spot. Since the hot values were discovered at the edge of the boundary, we need to extend ours its boundary so that the sample design can extend beyond the current site boundary. We'll also need to remove the boundary polygon.

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Practice Session: Secondary Sample Design

3. We want the samples to be 25 feet apart and in a circle (use corners and neighbors). Using the human health scenario we have been working with in previous lessons (nonrad, noncarcinogenic, residential, ingestion, child scenario) for arsenic, apply the *threshold radial* design.

Hint: Click on the zoom out button.

4. Suppose we do not know if there are disjoint discoveries. We want to find out if they are part of a larger contamination zone. Use the *High value* sample design to place new samples where the model believes a highly contaminated zone exists. This should confirm or disprove the presence of a larger zone of contamination. You can only afford 10 new samples. We want to space them apart for better coverage, so separate them by at least 25 feet. Keep the

polygon turned off and press *Show the Results*.
What do you get as a secondary sample design?



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Practice Session: Secondary Sample Design

5. Suppose we know that the extreme value points found in the southeast portion of the site are in fact part of a larger contaminated zone. At this point, we want to better refine the boundary area between the contaminated and uncontaminated zones. To do this, we'll use the *Area Of Concern boundary* sample design. Again, we can only afford ten new samples, and we want them to be spaced apart by about 25 feet. Since the Area of Concern boundary design is based on the same principles as area of concern, specify a scenario (use the same human health scenario). Turn the *Boundary* polygon on and press *Show The Results*. Notice how the new sample design differs from the previous two.



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Practice Session: Secondary Sample Design

6. Auto-document the result. In practice, you may want to submit part or all of this report to the sampling team.
7. Now import the results of this second round of sampling into SADA. The file is called "AOCBoundaryLesson7.csv" (match SADADepth1 to Depth when the SADA asks)
8. Check your correlation structure. Is the sill now lower than in the first round? Adjust accordingly (sill ~ 2400) and generate the probability map. Notice the reduction in previous areas of uncertainty.

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Spatial Analysis and Decision Assistance (SADA) Version 4 MARSSIM

Environmental Assessment Methods Using SADA
University of Tennessee, Knoxville

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Part 10: MARSSIM Functionality in SADA 4

- Calculate sample size based on Sign Test and WRS Test; incorporating DCGLs, decision variables, area factors, instrument sensitivity
- Develop initial sample design (MARSSIM grid or simple random)
- Post sampling analysis (A site passes or fails)
- Detecting and Defining Elevated Areas

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I want to create a MARSSIM sample design

- (1) Identify the survey area
- (2) Set Class I, II, or III based on extent of contamination suspected/known
- (3) Set WRS or Sign (background or not)
- (4) View/edit DCGL and associated values (DCGL_w, LBGR, alpha, beta, sigma)
- (5) Show power curve, return N, alpha, beta
- (6) Get grid area (survey area/N)
- (7) Get grid area-area factor curve
- (8) Update AF for new grid area, calculate DCGL_{emc}, get MDC
- (9) Instrument sensitivity check
 - (1) If pass
 - (1) Show 2D Elipgrid results for circular hot spot of size grid area
 - (2) If fail
 - (1) Query for area factor based on updated grid area of (needed scan factor/DCGL)
 - (2) Recalculate N based on updated grid area and survey area
 - (3) Show elipgrid probabilities for both Ns and update grid area
 - (4) Accept original N and higher risk of missing circular hotspot or new N and lower risk of missing same hotspot size
- (10) Show MARSSIM grid or simple random sample design based on Class type

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Determining Number of Samples Sign Test

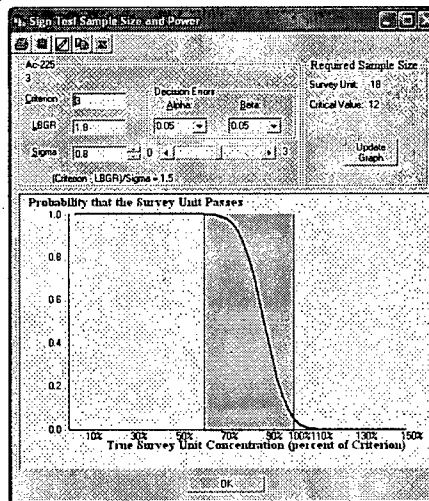
Use if contamination is not present in background and measurements are radionuclide-specific or use if background levels are a small fraction of the DCGL

Evaluates whether the median of the data is above or below the DCGL_w

Survey reference area is not necessary

Compare contaminant levels with DCGL values

Each measurement below the DCGL contributes evidence that the survey unit is clean and the null hypothesis should be rejected



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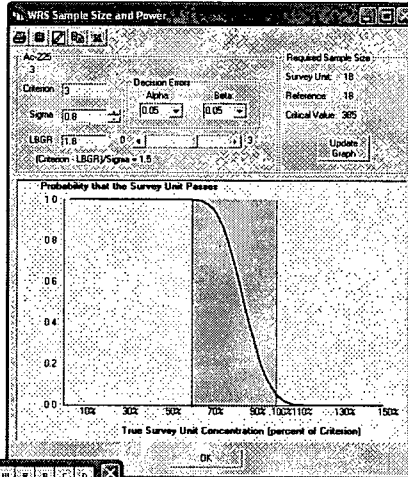
Determining Number of Samples Wilcoxon Rank Sum

Use if contamination is present in background

Evaluates whether the difference between the median of the data in the survey unit and the median in the reference area is above or below the DCGL_w

Compare survey unit concentration data with reference area data *adjusted by adding the DCGL*

Each survey unit measurement below an adjusted reference area measurement contributes evidence that the survey unit is clean and the null hypothesis should be rejected



SADA

You need a total of 36 samples. You need 18 in your area of interest and 18 in your reference area. SADA will now plot the 18 samples in your area of interest.

OK

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Import Area Factor-Grid Area Curves

- User can import grid area-area factor curves from the Resrad-MARSSIM Excel output for a survey site

Area Factor	Grid Area	Area Factor
1	1.0000	10.74074
2	1.064944	10.46195
3	1.089172	10.36622
4	1.104	10.10724
5	1.13921	9.860506
6	1.18442	9.564482
7	1.22555	9.216308
8	1.24494	9.200803
9	1.28326	8.990451
10	1.34718	8.663347
11	1.3724	8.53807
12	1.43341	8.270597
13	1.45217	8.151361
14	1.51906	7.925718
15	1.56681	7.7
16	1.61545	7.5
17	1.66153	7.3
18	1.7036	7.1
19	1.75389	6.9
20	1.8227	6.7
21	1.89462	6.5
22	1.97004	6.3
23	1.97739	6.5
24	2.0411	6.4
25	2.11397	6.2
26	2.18186	6.1
27	2.25669	6.0
28	2.31586	5.8
29	2.3576	5.7
30	2.47836	5.5
31	2.56424	5.101363
32	2.62314	5.428366
33	2.74992	5.262913
34	2.8398	5.166743
35	2.86203	5.120443
36	2.97952	4.996686
37	3.09568	4.869752
38	3.14304	4.826115

Retrieve Grid Area-Area Factor Relations

Grid Area-Area Factor for Ca-137

Select Grid Area: 143341

Corresponding Area Factor: 8.270597

OK Cancel

Instrumentation Check

MARSSIM Parameters for Default

Grid Area (Survey area/ Sample N): 150.8287 (8676.75/54)

Area Factor (AF) Corresponding to Grid Area: 1.2

DCGL_w: 5

DCGL_{enc}: 6

Minimum Detectable Concentration for Instrument: 12

Current check of instrumentation has failed.

When the instrumentation check has failed, one can also find the sample size that is necessary to meet the MDC for the instrument. Enter or retrieve an area unit corresponds to the needed Area Factor below to find the five sample size that meets the MDC. In the next step, you will be to choose between the original sample size and this new sample size.

Corresponding Grid Area: 146

Corresponding Area Factor: 6.9

Check Instrumentation OK Cancel Next

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MARSSIM- Instrument Check (Scan MDC)

- Check of $DCGL_{EMC}$ versus Minimum Detectable Concentration

MARSSIM Parameters for Default

Grid Area (Survey area/
Sample N) 158.8267 (1576.75/54)

Area Factor (AF)
Corresponding to Grid Area 1.2 Retrieve AF from
RESRAD-MARSSIM

DCGL_w 5

DCGL_{EMC} 6

Minimum Detectable
Concentration for
Instrument 1

Current check of instrumentation has passed.

Instrument Check Cancel Next

MARSSIM Parameters for Default

Grid Area (Survey area/
Sample N) 185.3754 (10006.49/54)

Area Factor (AF)
Corresponding to Grid Area 1.2 Retrieve AF from
RESRAD-MARSSIM

DCGL_w 5

DCGL_{EMC} 6

Minimum Detectable
Concentration for
Instrument 1

Current check of instrumentation has failed.
When the instrumentation check has failed, one can also find the sample
size that is necessary to meet the MDC for the instrument. Enter or retrieve
the grid area that corresponds to the needed Area Factor below to find the
alternative sample size that meets the MDC. In the next step, you will be
asked to choose between the original sample size and this new sample
size.

Grid Area Corresponding
to needed AF 146 Retrieve Grid Area from
RESRAD-MARSSIM

Sample N Corresponding to
Grid Area equal to MDC 63

Instrument Check Cancel Next

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MARSSIM- Instrument Check Fail

Sample Size Needed to Detect Elevated Areas

If $\text{scan MDC} > DCGL_{EMC}$,

- (1) Find the area factor that satisfies

$$\text{Area Factor} = \text{scan MDC} / DCGL_w$$

- (2) Find the Grid Area corresponding to that Area Factor

- (3) Calculate the number of sample points needed to produce that Grid Area,

$$n_{EA} = (\text{Survey Unit Area}) / (\text{Grid Area})$$

- (4) Compare elipgrid hit probabilities for two different Ns and select one

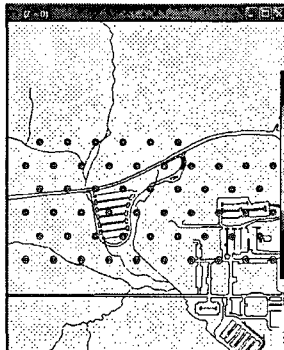
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Calculate Probability of Missing Hotspot for Grid

With Hot Spot: Calculate Probability, the user defines the grid and the hot spot size, shape and orientation.

Select **Hot Spot: Calculate Probability** from the drop down list under **Sample Design**. Select a square, triangle, or rectangle grid style and enter the applicable parameters.



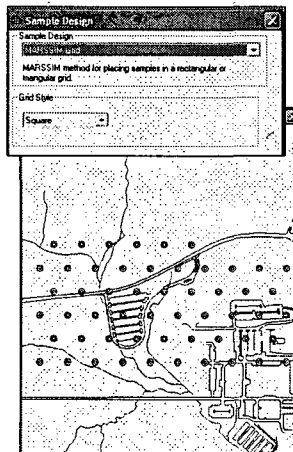
Press **Show the Results** and SADA will calculate the probability of missing a hotspot of the specified size with N samples in the MARSSIM grid.

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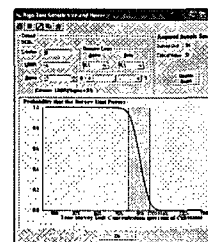
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Class I or II- MARSSIM Grid

MARSSIM grid is a 2d initial sample design for empty sada files that relies on a grid style to generate locations for new samples. Can be based on square or triangular grids.



- Class 1: areas that have, or had, a potential for contamination or known contamination above the $DCGL_w$
- Class 2: areas that have, or had, a potential for contamination or known contamination but that contamination is not expected to exceed the $DCGL_w$



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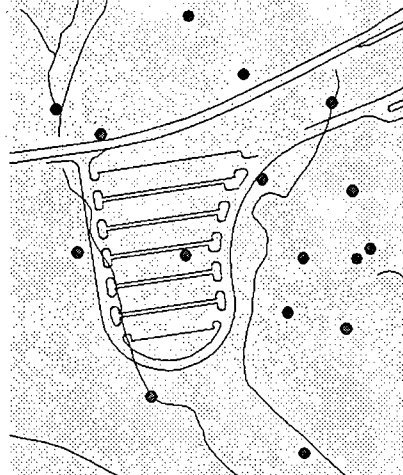
Class III- Simple Random

Description

- Samples are distributed across the site based on the generation of coordinate values to create the new samples.

Class III

- Areas not expected to contain residual contamination or expected to contain levels that are a small fraction of the $DCGL_w$



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I want to perform a MARSSIM data analysis (no background)

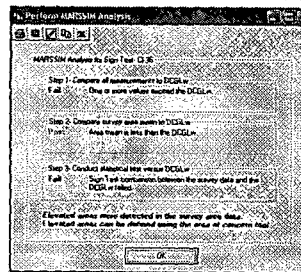
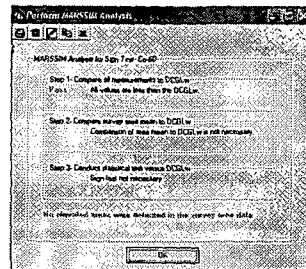
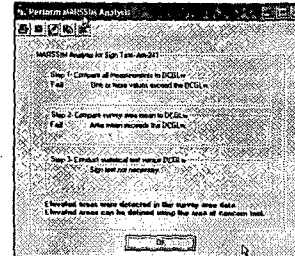
- (1) Identify the survey area
- (2) Set Class I, II, or III based on extent of contamination suspected/known
- (3) Set Sign (no background)
- (4) View/edit DCGL and associated values (DCGL_w, LBGR, alpha, beta, sigma)
- (5) Compare all measurements versus DCGL_w
- (6) Compare survey average versus DCGL_w
- (7) Conduct Sign test versus DCGL_w

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Detect Elevated Areas- Sign Test (Class changes)

- Compares all measurements to DCGLw
- Compares area mean to DCGLw
- Performs Sign Test if necessary



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I want to perform a MARSSIM data analysis (with background)

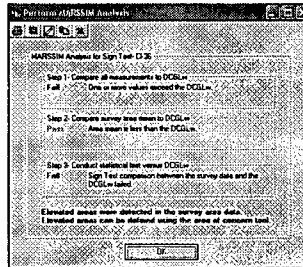
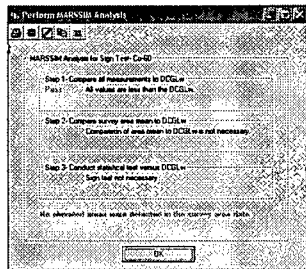
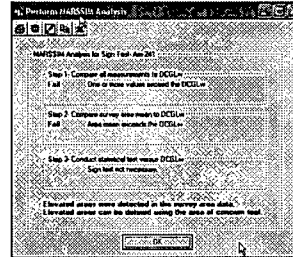
- (1) Identify the survey area
- (2) Set Class I, II, or III based on extent of contamination suspected/known
- (3) Set WRS (background)
- (4) Import/identify background data source
- (5) View/edit DCGL and associated values (DCGLw, LBGR, alpha, beta, sigma)
- (6) Compare site measurements (Max Survey – Min reference) versus DCGLw
- (7) Compare average difference of survey area and reference data versus DCGLw
- (8) Conduct WRS test for data (Reference Area + DCGLw versus Survey Area)

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Detect Elevated Areas- WRS Test (Class changes)

- Compares all measurements to DCGLW
- Compares area mean to DCGLW
- Performs WRS Test if necessary

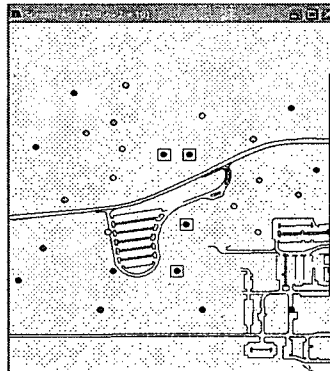


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MARSSIM- If check for elevated areas fails

- If fail, then SADA can be used to define elevated areas with the Area of Concern tool.
- Also, extent of the elevated area can be sampled with the threshold radial sample design



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I want to define a MARSSIM elevated area

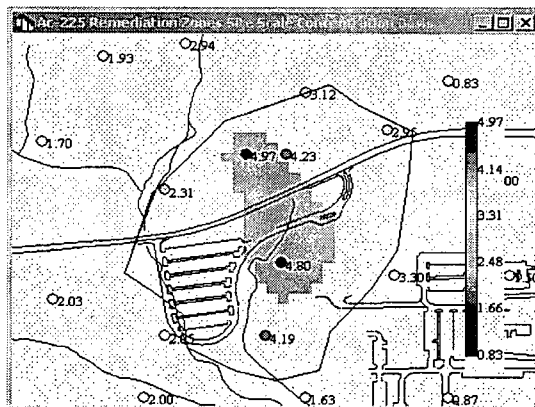
- (1) Identify the survey area
- (2) Set Class I, II, or III based on extent of contamination suspected/known
- (3) Import/identify background data source
- (4) View/edit DCGL and associated values (DCGLw, LBGR, alpha, beta, sigma)
- (5) All measurements versus DCGLw or DCGLEmc depending on Class
- (6) If fail:
 - (1) Define elevated area using a DCGL, interpolant, and AOC tool
 - (2) Perform radial or judgmental sampling
 - (3) Import additional data
 - (4) Elevated area averages versus DCGLEa (user inputs F_{actual})
- (7) Conduct Quantile test (version 5)

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MARSSIM- Define Elevated Area with AOC Tool

- Use the area of concern tool with an interpolant to estimate the size of the elevated area(s)

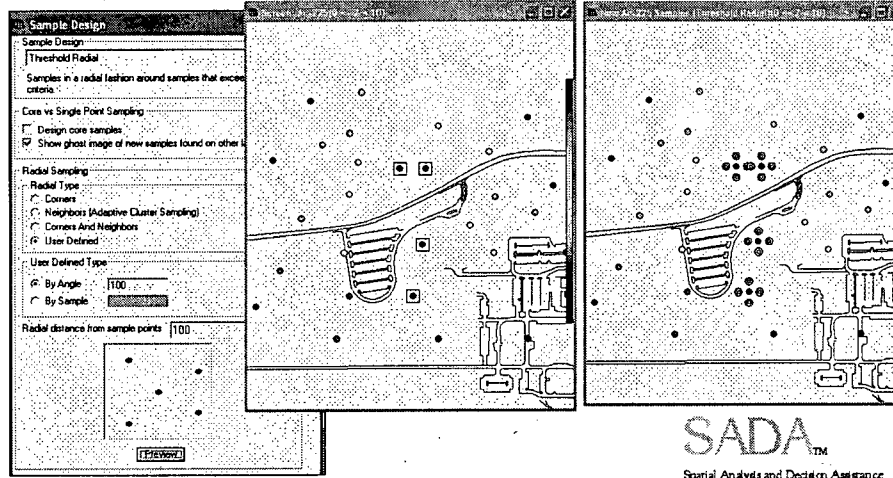


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Threshold Radial for Elevated Areas

Threshold Radial can be used to place samples in a radial pattern around existing data points that exceed the DCGLmc.



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MARSSIM Functionality in SADA 4

- Calculate sample size based on Sign Test and WRS Test; incorporating DCGLs, decision variables, area factors, instrument sensitivity
- Develop initial sample design (MARSSIM grid or simple random)
- Post sampling analysis (A site passes or fails)
- Detecting and Defining Elevated Areas

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