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Defensible Statistical Sampling Design and Geophysical Data Analysis for Site Characterization

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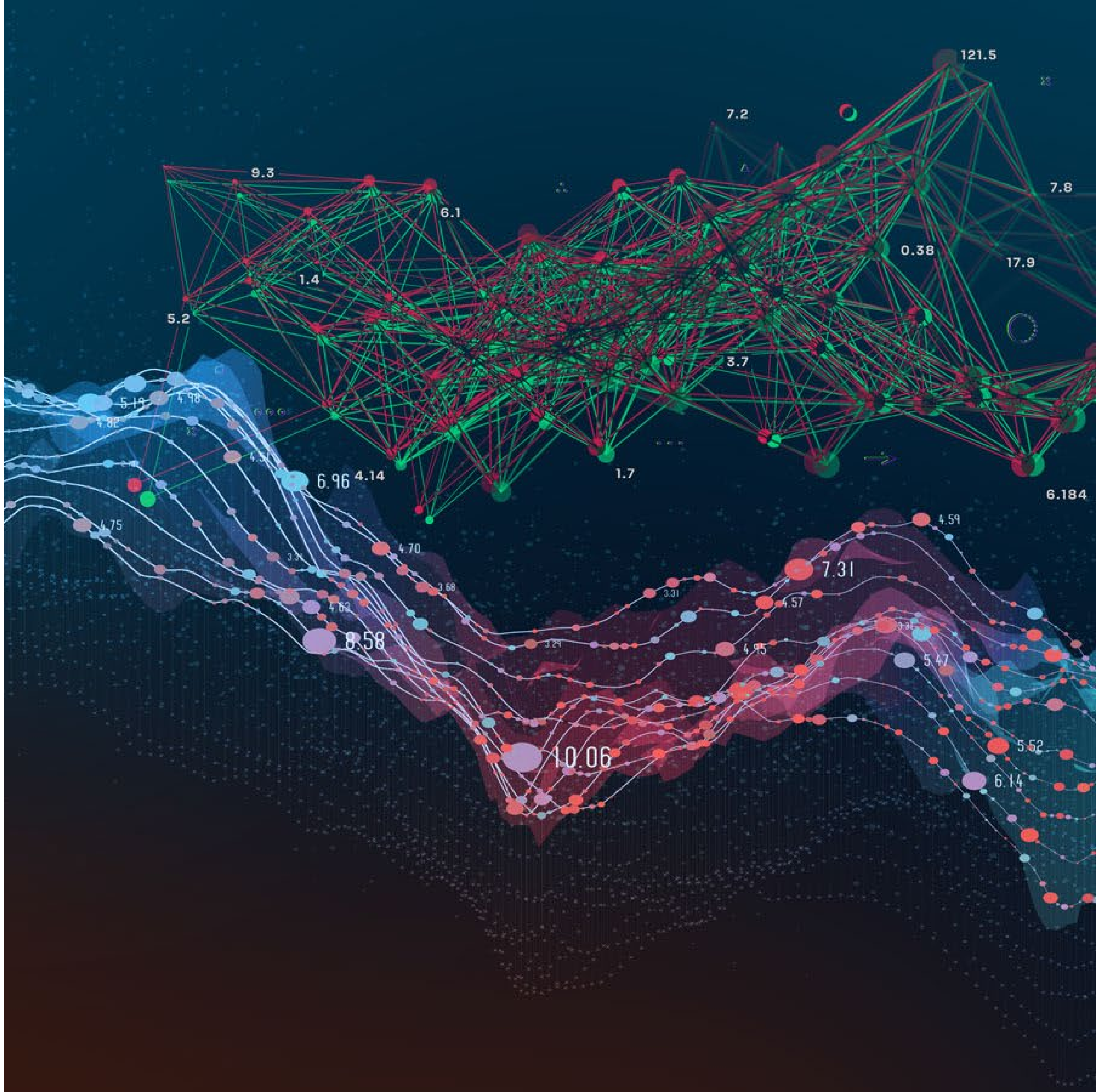
Pacific Northwest National Laboratory

PNNL-SA-185087

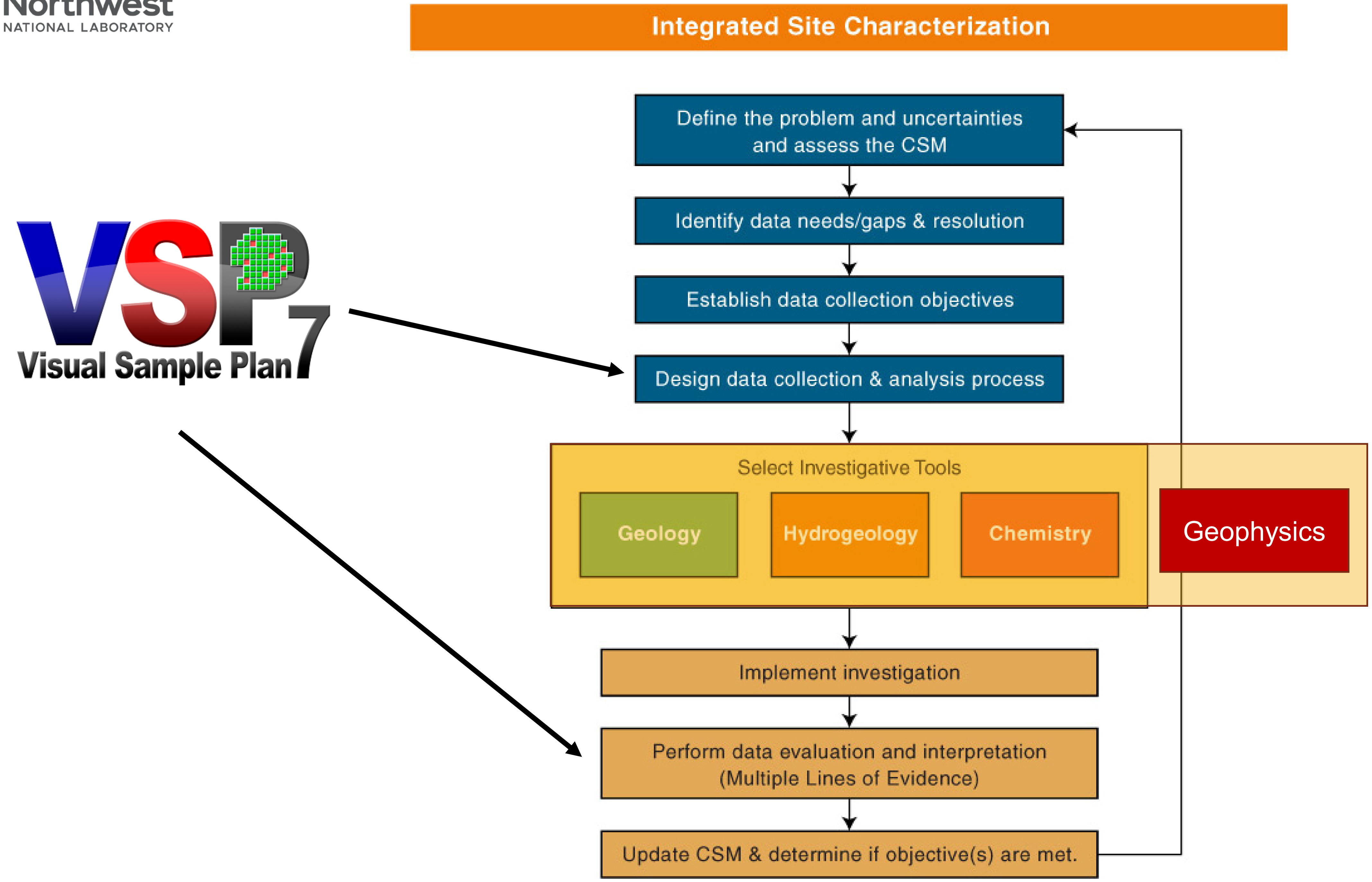


U.S. DEPARTMENT OF ENERGY BATTELLE

Data Analysis and Statistical Sampling for Site Characterization

- Statistical sampling and analysis methods for later phases of site remediation are well established
  - Often required by regulations and guidance
  - Data collection driven by statistical requirements
- Challenges of characterization phase
  - Various vintages, sources and types of data
  - Conceptual site model (CSM) is continually evolving
  - Analysis is often subjective / qualitative and not reliant on external criteria
- Systematic planning, data quality assurance (DQA), geophysical data analysis, and statistical sampling design can assist in site characterization

Site Characterization and CSM Refinement



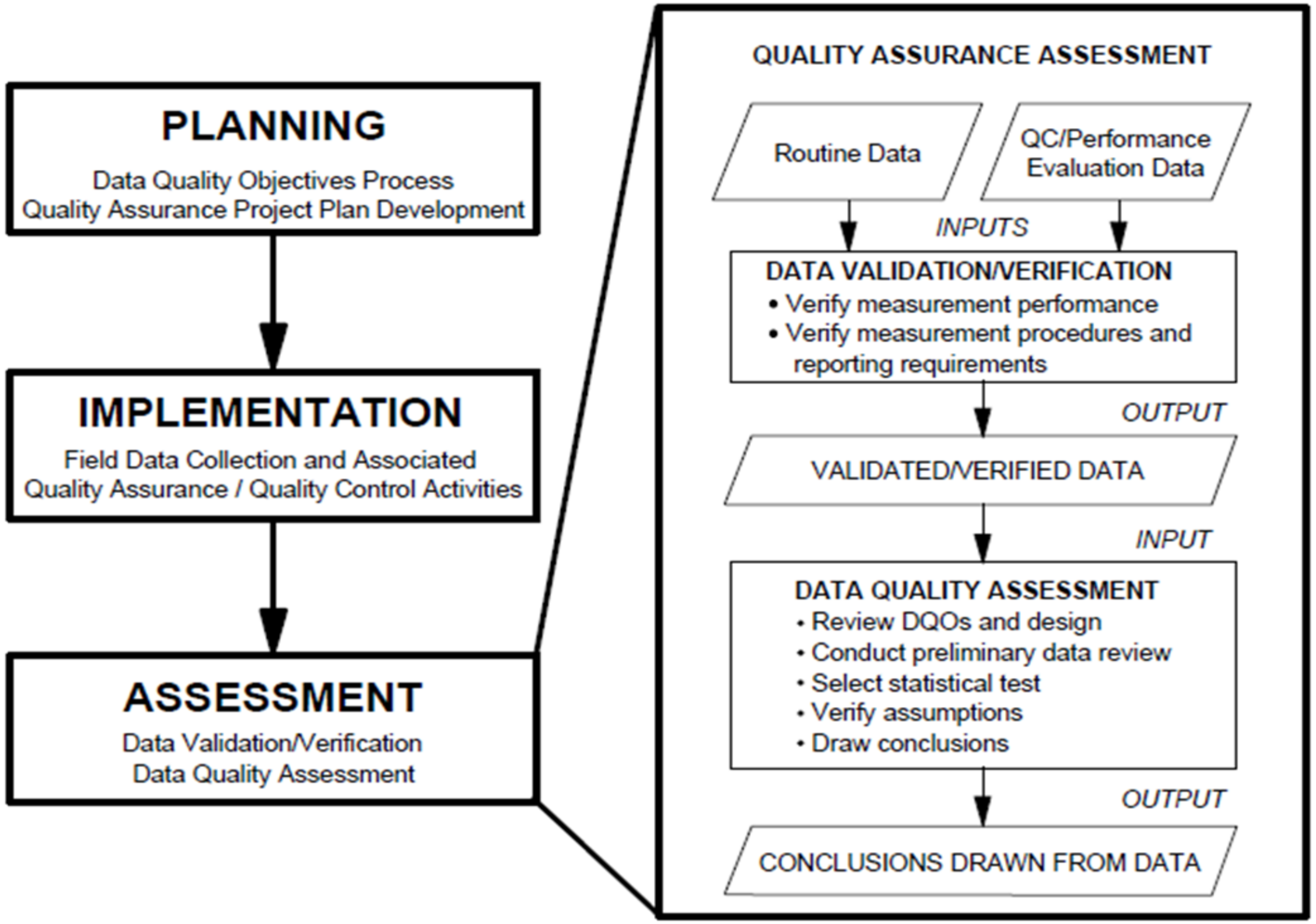
(ITRC 2015b) https://rmcs-1.itrcweb.org/4-adaptive-site-management/

Data Available for Survey Planning

Data source	Data set description(s)
Previous to RSSI	Engineering drawings (facilities, structures, etc.), operations logs, GIS maps, background geophysical data (surface/subsurface), water resource characterization and climate data for Conceptual Site Model (CSM) development
HSA	Risk assessment, hazard assessment, RCRA/CERCLA documentation (including soil/rock core sample data as appropriate), NEPA documentation (as appropriate), Source term quantification modeling/estimates for relevant sites, Contaminant fate and transport modeling
Scoping	RI/FS or FI/CM reports, updated CSMs, specification of sampling types/design/media/location, proposed statistical methods, identification and characterization of potential contaminant plumes
Characterization	Geologic maps, soil maps, drillers logs, maps of site infrastructure, collection of groundwater levels, hydraulic tests, soil or rock cores, and development of a GIS, visualizations, and maps for the site, Surveillance monitoring data from previous remediation activities (if applicable), geophysical and hydrogeological modeling results,
Remediation	Characterization of plume structure and composition, conceptual site model, possibly computer models of flow and transport for the site, feasibility studies or prior relevant work demonstrating the feasibility of amendments, ongoing monitoring data to assess performance of the remedy, including routine sampling of contaminant concentration and signatures of the remedy and its effects.
Geophysical data	Borehole, cross-hole, surface, or remote sensing collection of data through electrical techniques (e.g., electrical resistivity tomography, induced polarization), electromagnetic methods (e.g., frequency and time domain electromagnetic induction, magnetotellurics, ground penetrating radar), seismic methods (e.g., reflection seismology, seismic refraction, seismic tomography), gravity techniques (e.g., gravimetry and gravity gradiometry), magnetic techniques (e.g., magnetometers), thermal methods (e.g., infrared, fiber-optic distributed temperature sensing) or multi-spectral/hyperspectral methods.
Groundwater model	Deterministic or stochastic subsurface numerical models of flow and transport in the vadose zone, saturated zone, or a combination, including input files, model calibration results, and predictive results. Geo-framework model describing the hydrogeology and forming the basis for a Conceptual Site Model.
Authorized limit data	Authorized limit(s) based on DOE Order 458.1 (DOE 2011, 2017) or data required to translate regulatory limits to authorized limit(s), including hydrologic parameters (i.e. soil density, precipitation, irrigation) human health based from pre-described risk approach, and other default params in the RESRAD computer code.

Data Quality Assurance (DQA)

DQA steps applied to data collected prior to & from characterization survey

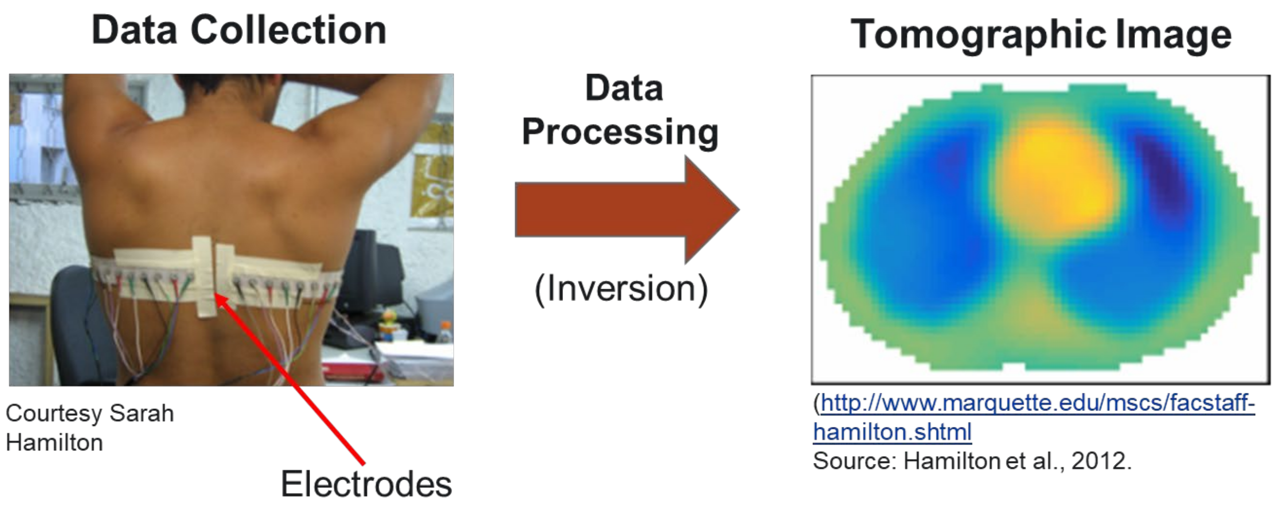


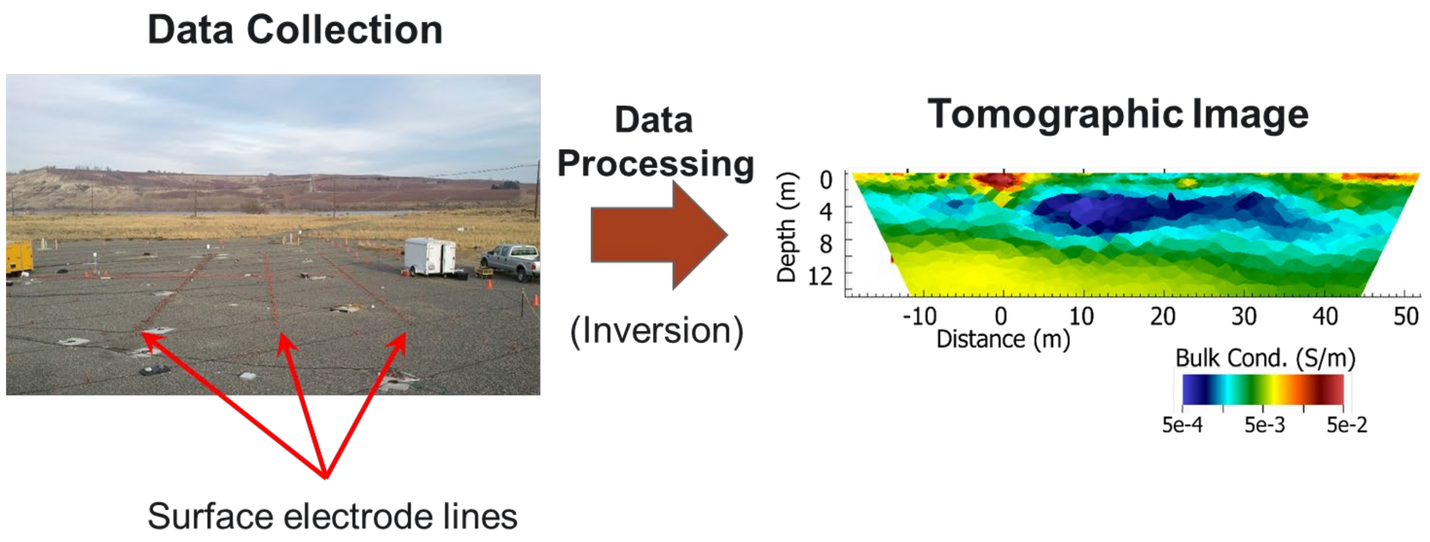
EPA QA/G-9 (https://www.epa.gov/sites/default/files/2015-06/documents/g9-final.pdf)

DATA ANALYSIS FOR CHARACTERIZATION

Geophysical Characterization

- Geophysical methods
  - Fill gaps in space (or time) between measurements
  - 2D or 3D imaging of subsurface properties
  - Indirect – requires petrophysical conversion or correlation
  - *Potentially valuable conditioning data for geostatistical methods*
    - ✓ *Quantitative estimation*
    - ✓ *Uncertainty reduction and quantification*





- Credit: Tim Johnson (ERT); Piyoosh Jaysaval (EM)

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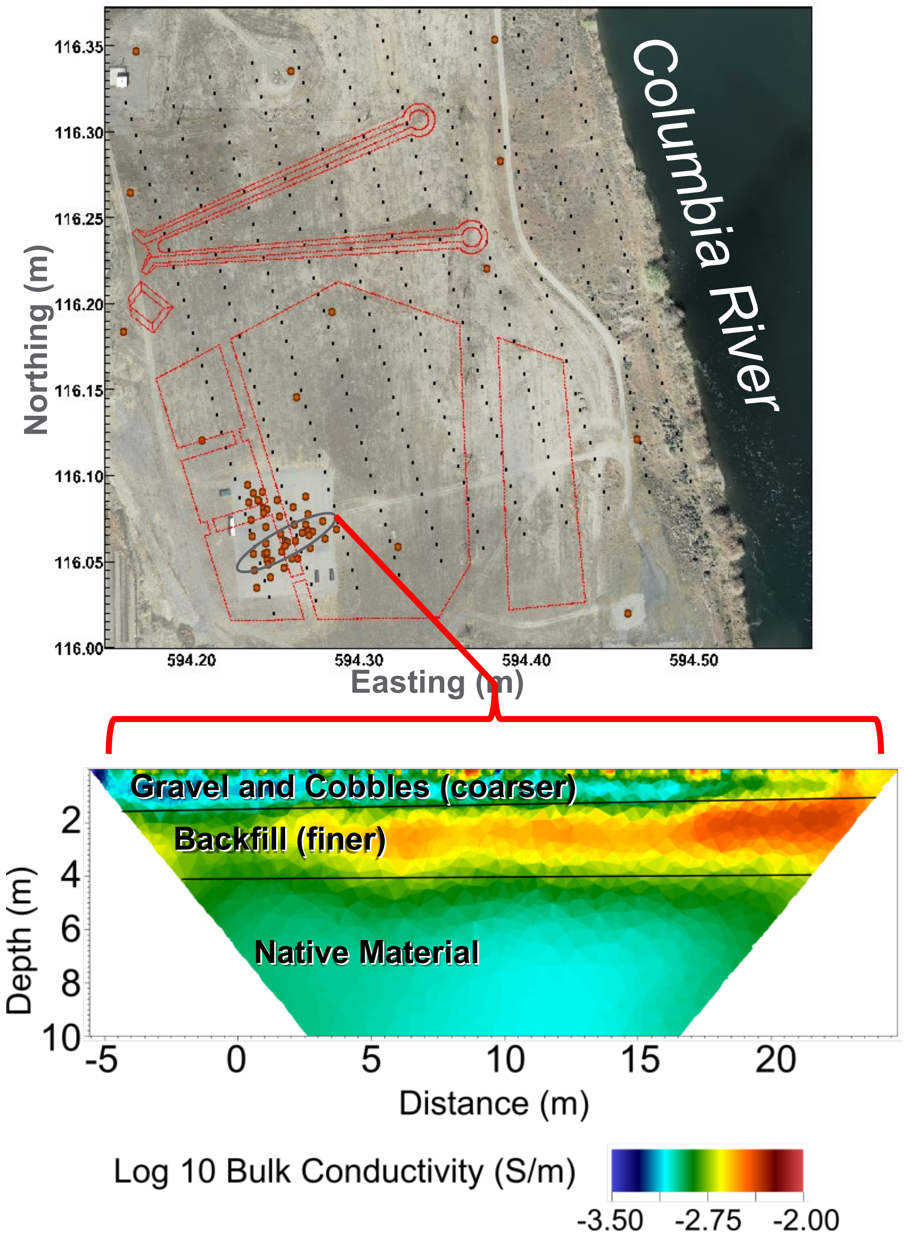
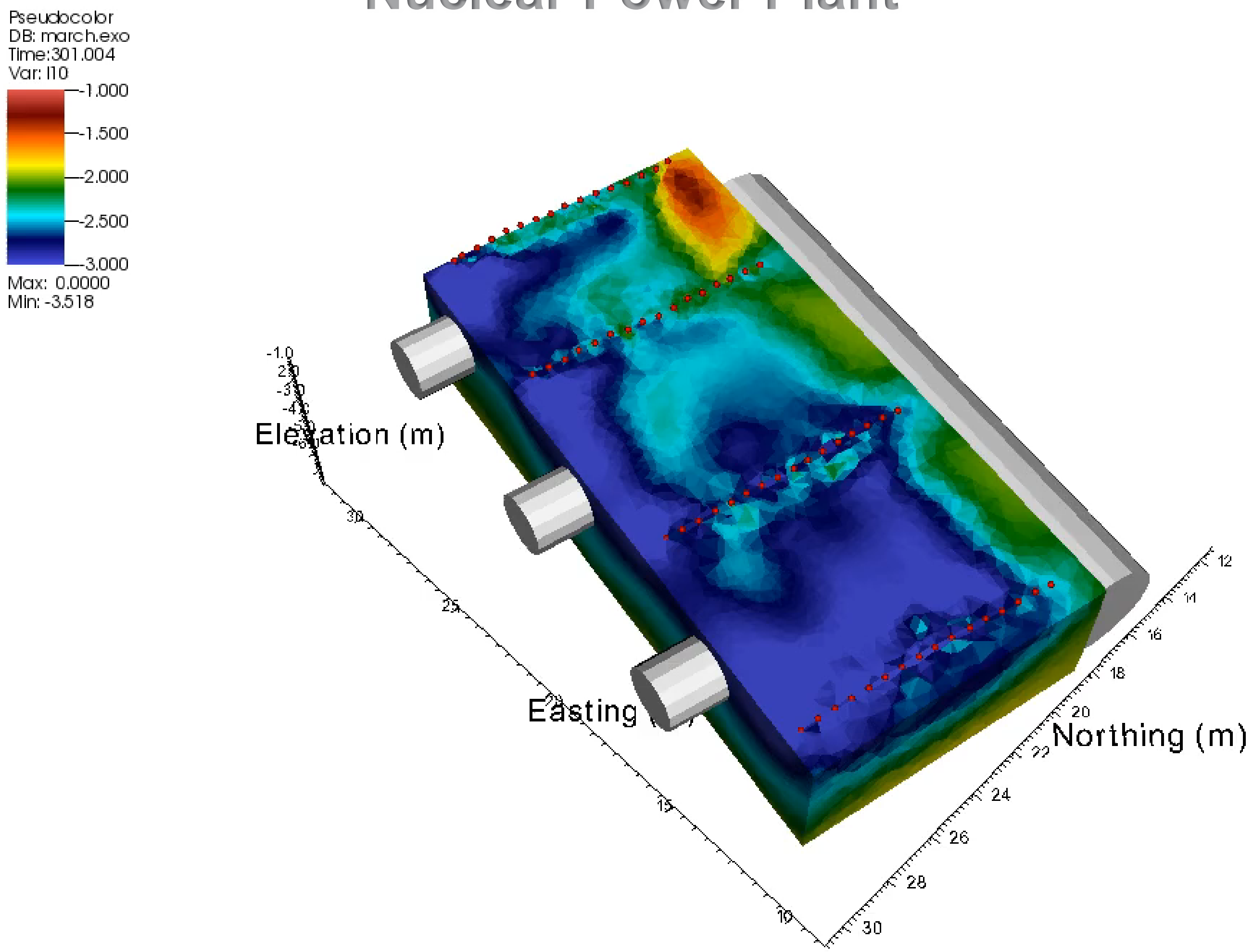
Example 1: Static ERT Imaging of Subsurface Structure

Hanford Site 300 Area
2D ERT Image



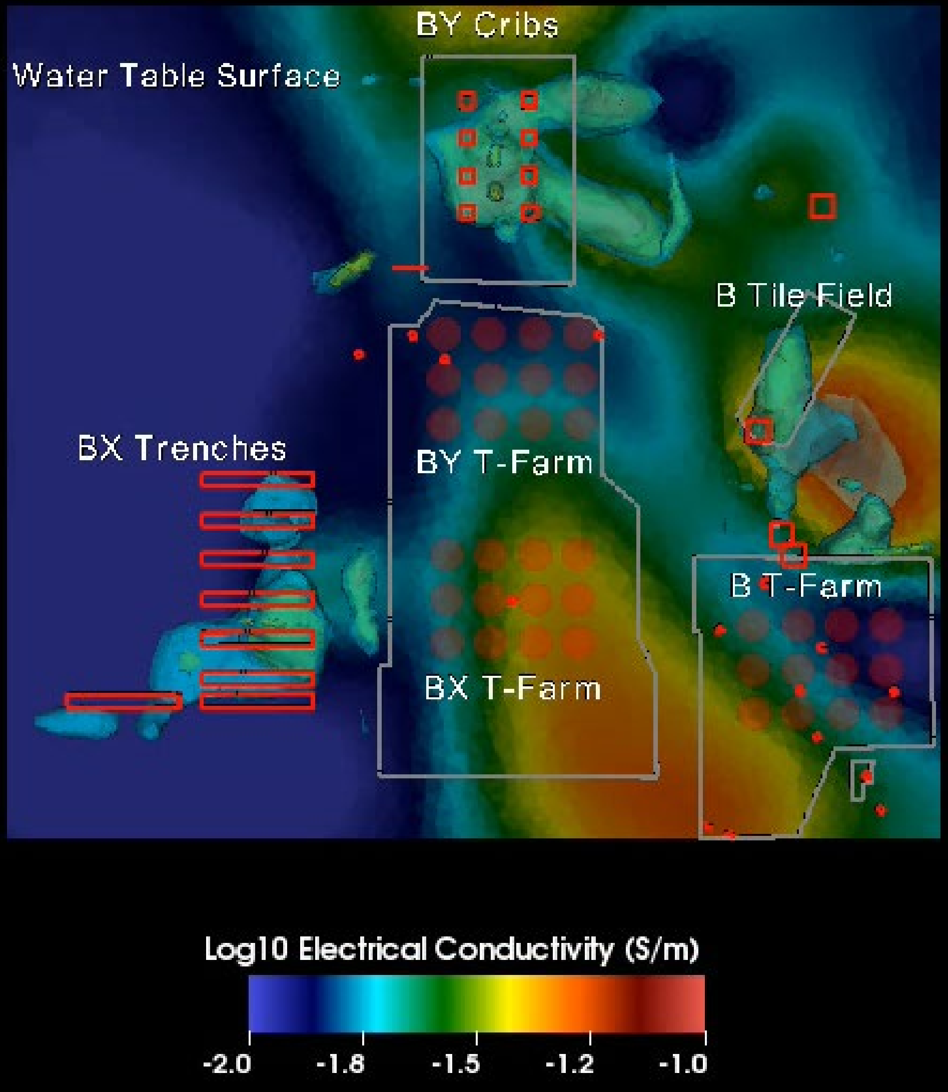
3D ERT Image Around Cooling Water
Discharge Pipes at an Operating Nuclear Power Plant



Example 2: Static Imaging of Vadose Zone Contaminant Plumes

Hanford Site B-Complex

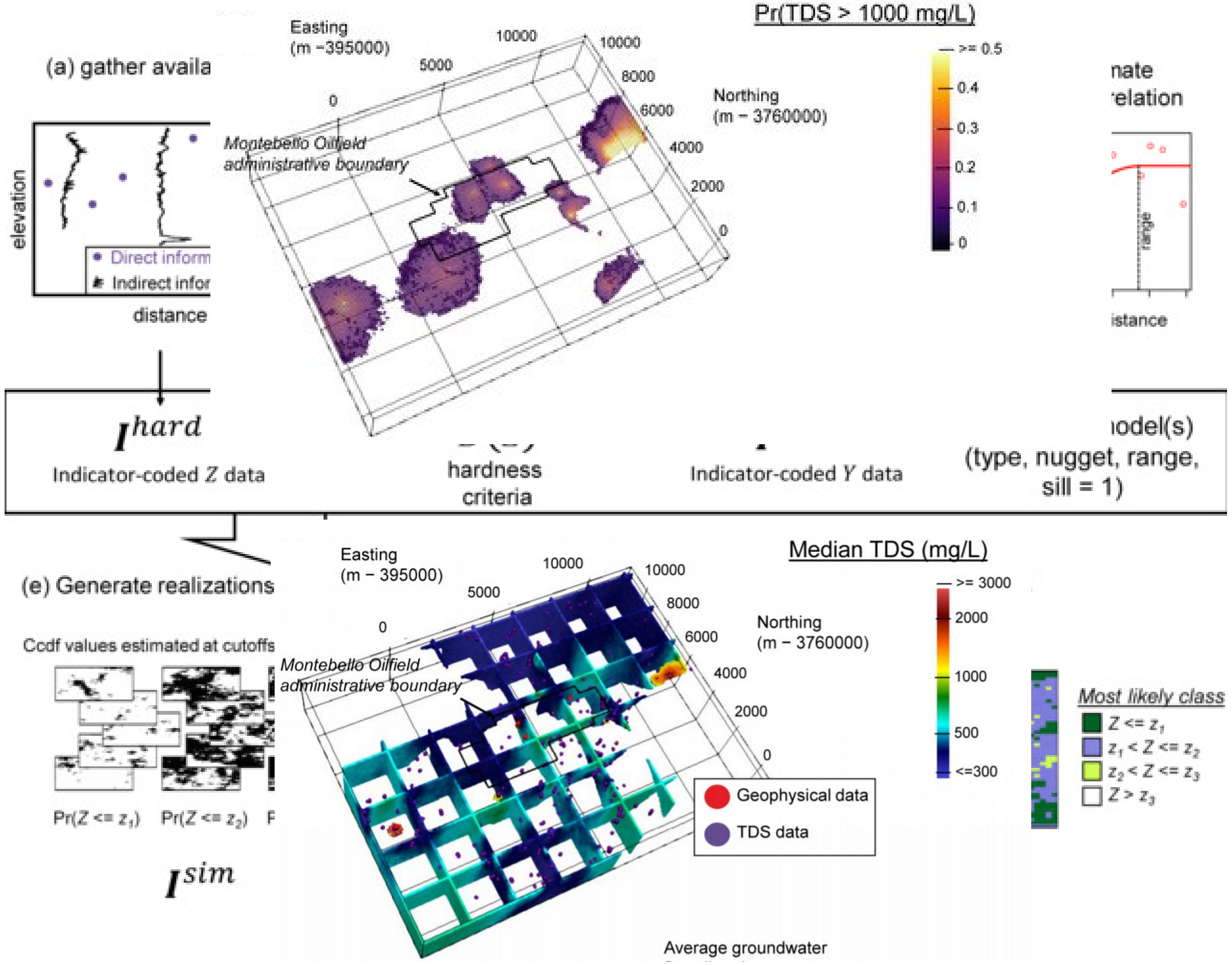
3D ERT Image Fly-around



Example 3: Using Geophysics for Estimation

Example: Water quality in areas of oil & gas development in CA

- Indicator simulation of TDS based on:
  - Hard data
  - Soft geophysical data (EM logs)
- Framework can:
  - Combine different data types
  - Use prior probabilities based on ML analysis

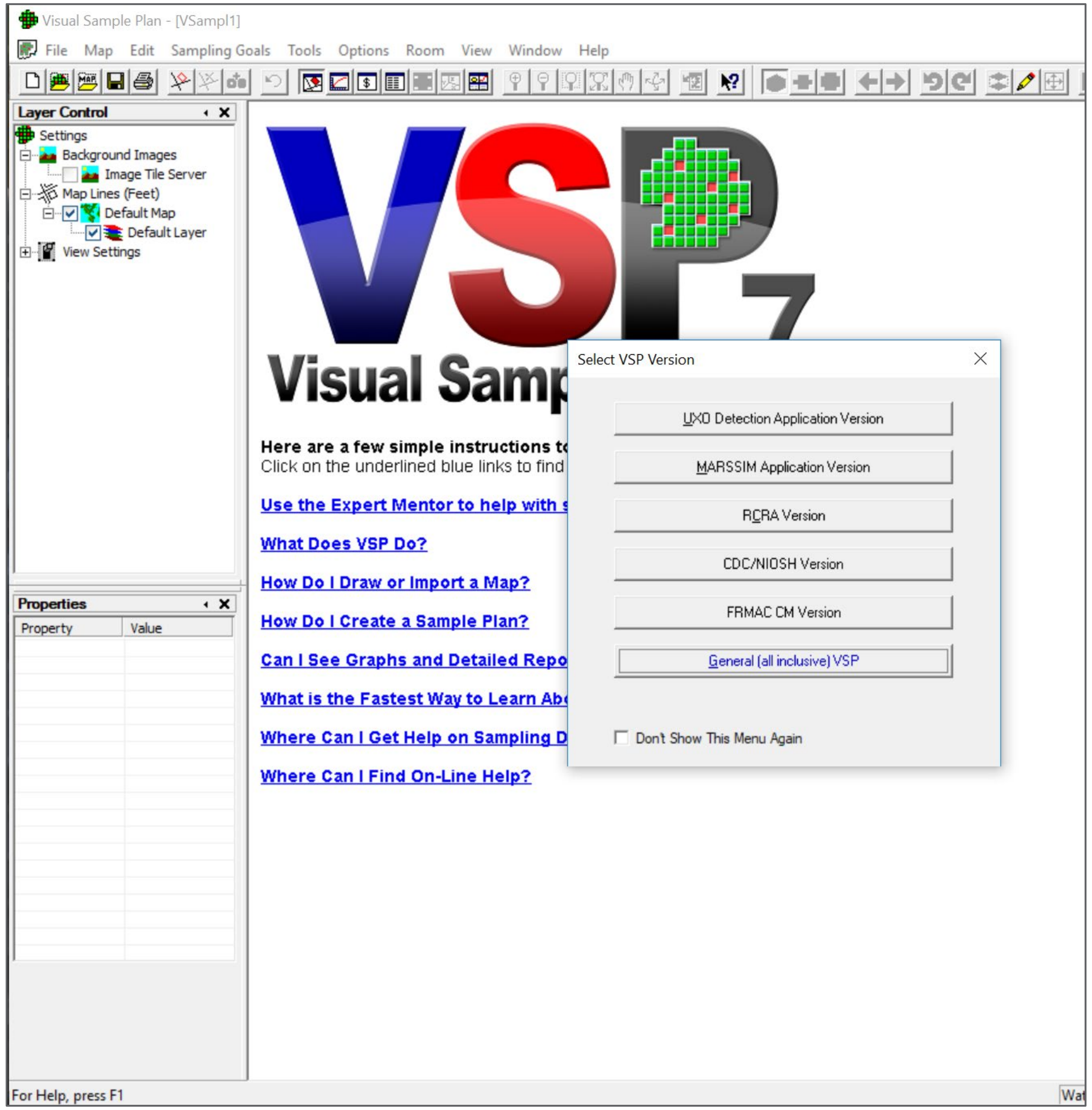


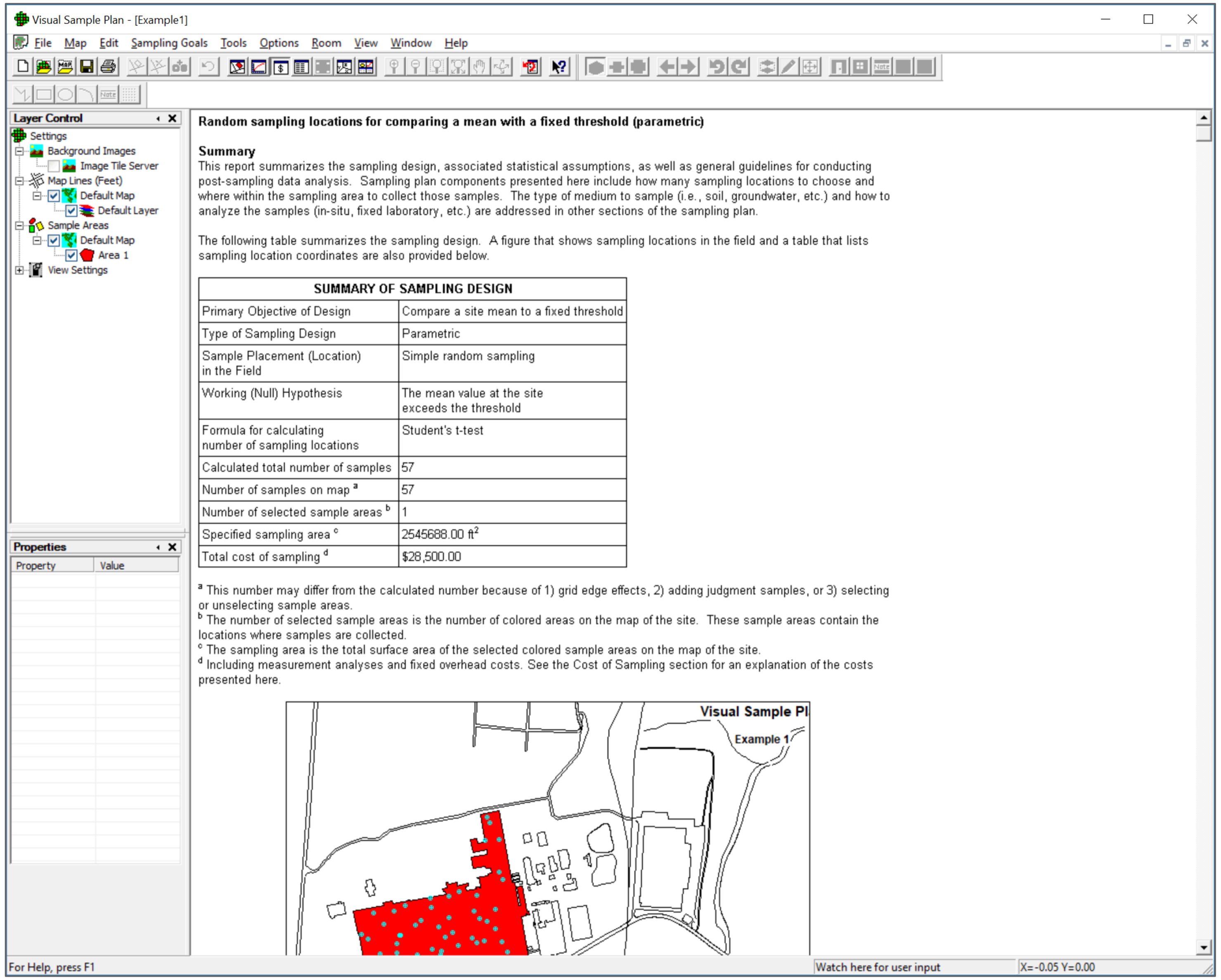
Terry, Day-Lewis et al., 2022, Groundwater.

SITE STATISTICAL ANALYSIS FOR CHARACTERIZATION

Visual Sample Plan (VSP)

VSP available on PNNL website (link)

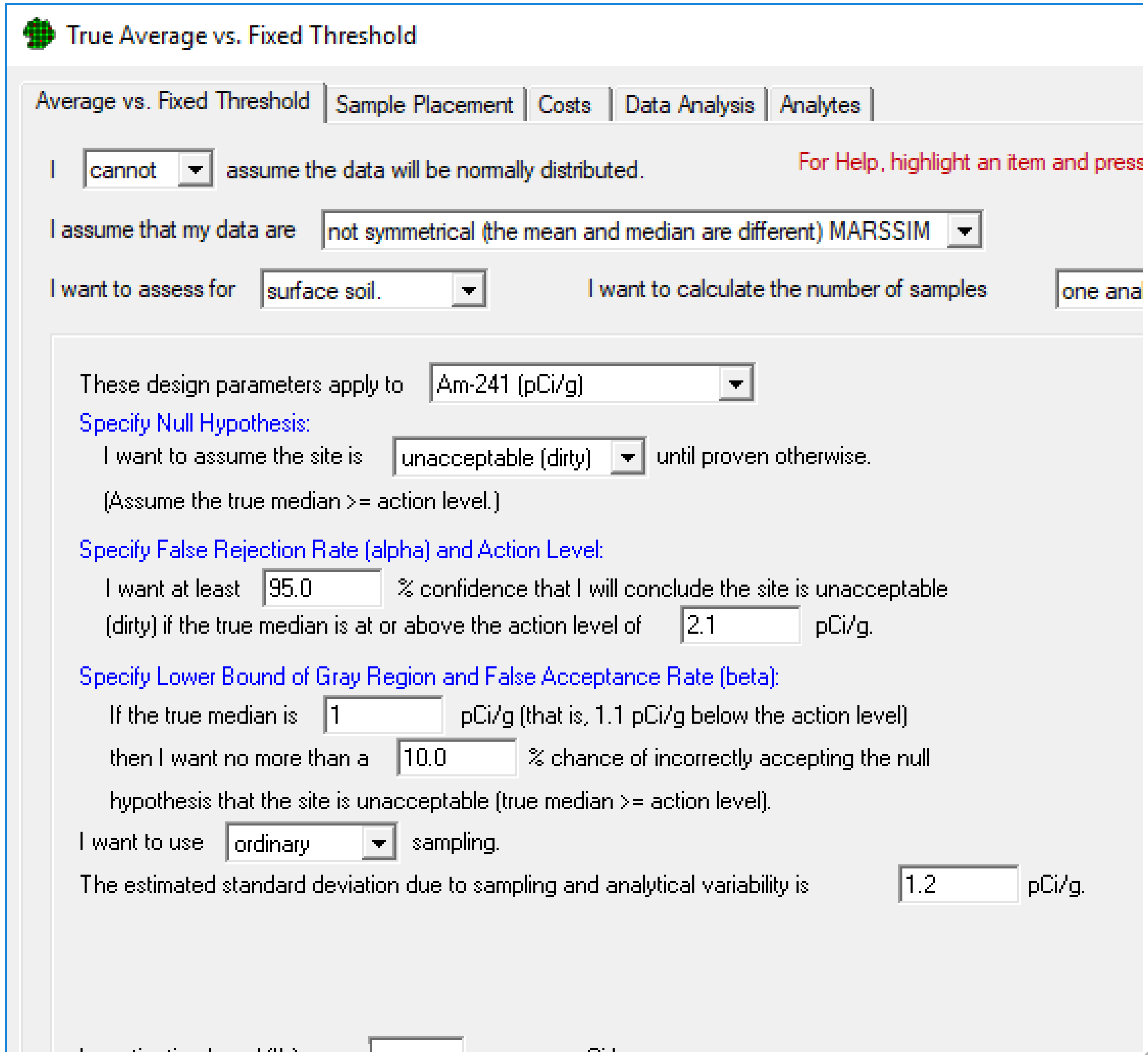




Screenshots from Visual Sample Plan

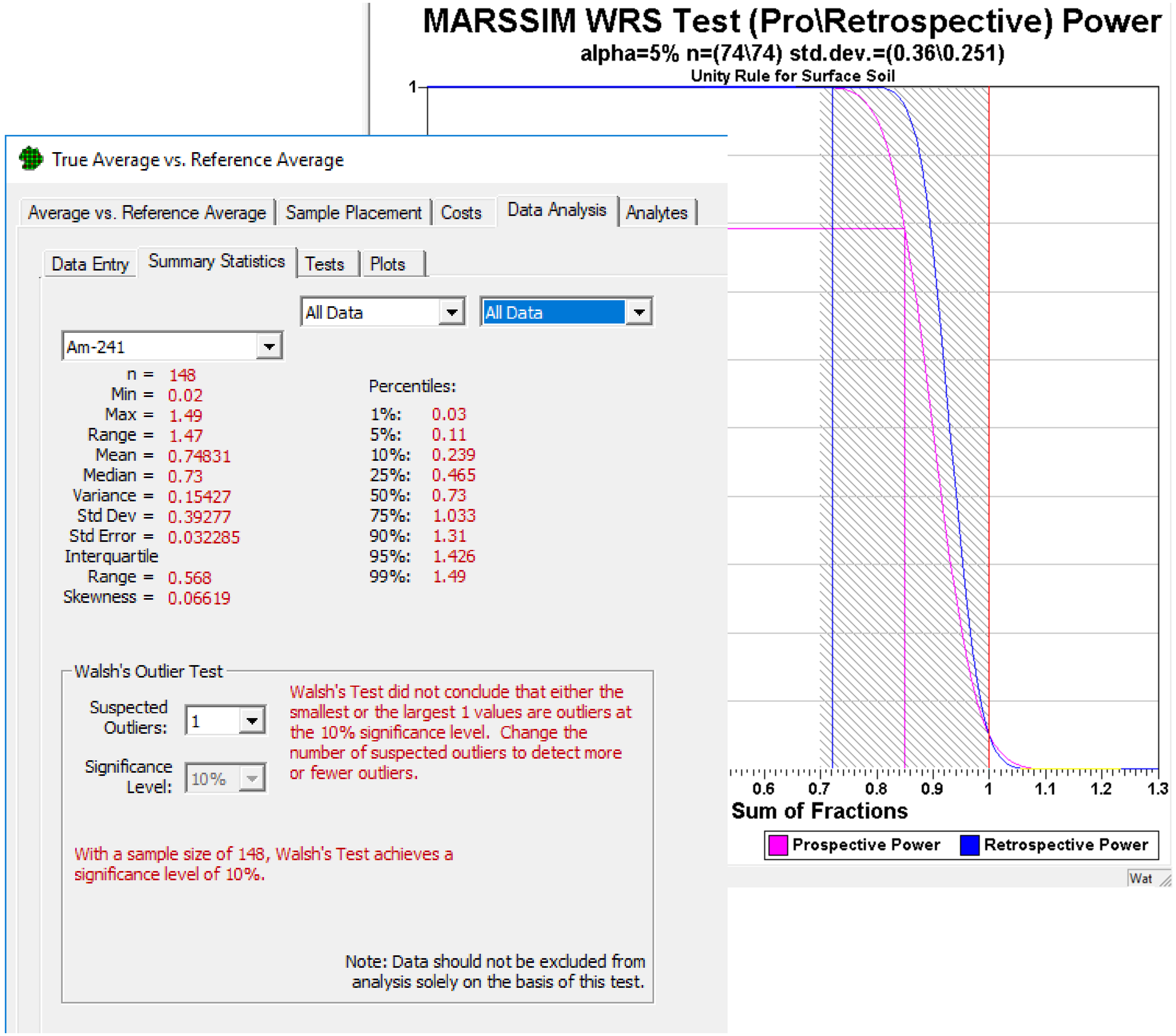
What is Visual Sample Plan (VSP)?

- VSP is a software tool to…
  - **Design** a statistically-based sampling strategy
    - ✓ How many samples should be collected, and where?
    - ✓ Based on the Data Quality Objectives (DQO) process



What is Visual Sample Plan (VSP)?

- VSP is a software tool to…
  - **Design**
  - **Analyze** data to support decisions
    - ✓Statistical tests
    - ✓Graphs, plots and summary statistics



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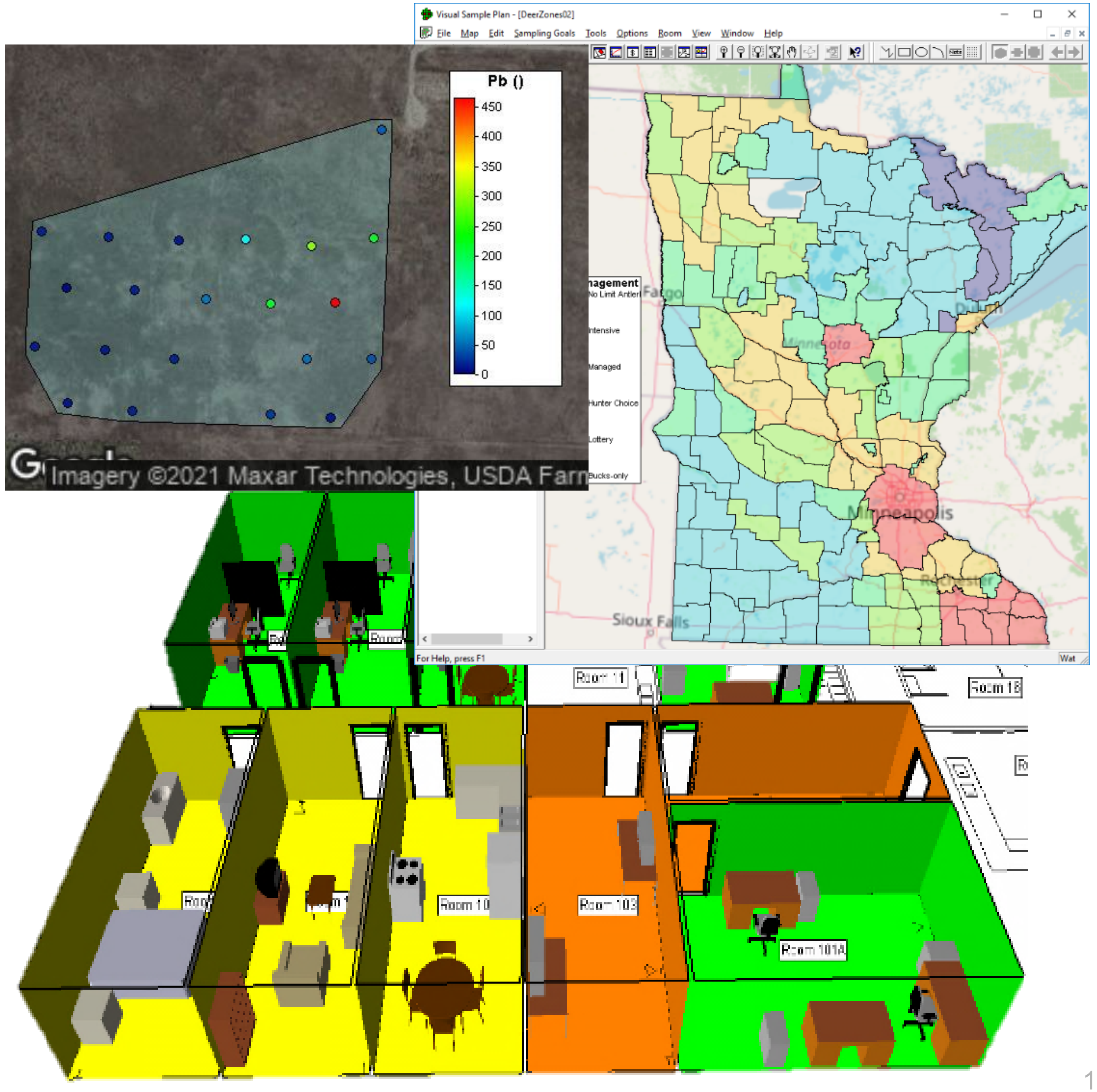
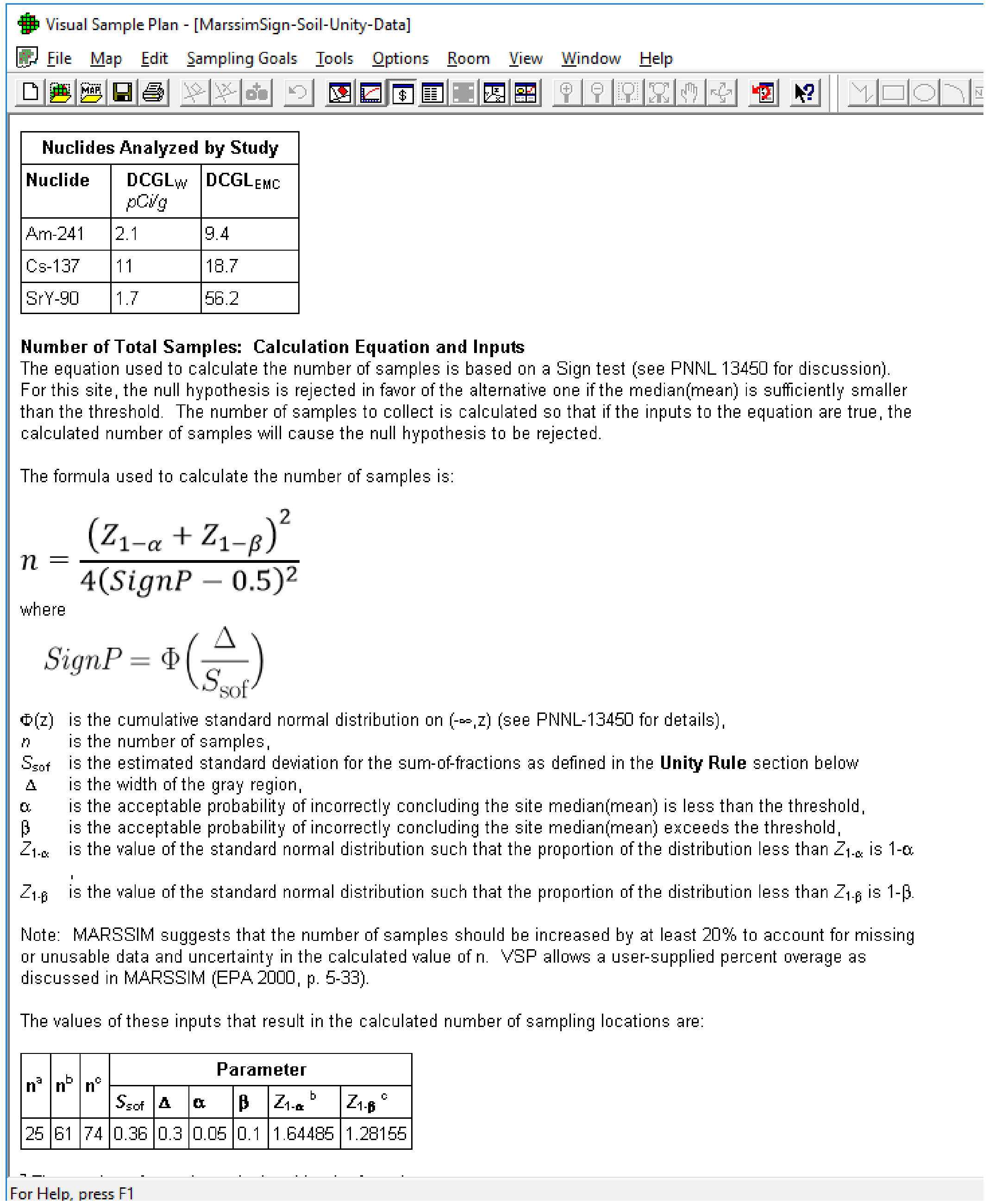
What is Visual Sample Plan (VSP)?

- VSP is a software tool to…
  - **Design**
  - **Analyze**
  - **Visualize** maps, buildings, planned sample locations, and results
    - ✓CAD and GIS file import
    - ✓Map imagery download
    - ✓3D room and equipment modeling and visualization



What is Visual Sample Plan (VSP)?

- VSP is a software tool to…
  - **Design**
  - **Analyze**
  - **Visualize**
  - **Guide** users who don't have statistical expertise
    - ✓Decision-driven and plain (jargon-free) language
    - ✓Automatically generated reports documenting steps and assumptions
    - ✓Thorough documentation and references



Nuclides Analyzed by Study		
Nuclide	DCGL$_W$ pCi/g	DCGL$_{EMC}$
Am-241	2.1	9.4
Cs-137	11	18.7
SrY-90	1.7	56.2

Number of Total Samples: Calculation Equation and Inputs

The equation used to calculate the number of samples is based on a Sign test (see PNNL 13450 for discussion). For this site, the null hypothesis is rejected in favor of the alternative one if the median(mean) is sufficiently smaller than the threshold. The number of samples to collect is calculated so that if the inputs to the equation are true, the calculated number of samples will cause the null hypothesis to be rejected.

The formula used to calculate the number of samples is:

$$n = \frac{(Z_{1-\alpha} + Z_{1-\beta})^2}{4(SignP - 0.5)^2}$$

where

$$SignP = \Phi\left(\frac{\Delta}{S_{\mathrm{sof}}}\right)$$

$\Phi(z)$ is the cumulative standard normal distribution on (-∞,z) (see PNNL-13450 for details),
n is the number of samples,
S_{sof} is the estimated standard deviation for the sum-of-fractions as defined in the **Unity Rule** section below
Δ is the width of the gray region,
α is the acceptable probability of incorrectly concluding the site median(mean) is less than the threshold,
β is the acceptable probability of incorrectly concluding the site median(mean) exceeds the threshold,
$Z_{1-\alpha}$ is the value of the standard normal distribution such that the proportion of the distribution less than $Z_{1-\alpha}$ is 1-α,
$Z_{1-\beta}$ is the value of the standard normal distribution such that the proportion of the distribution less than $Z_{1-\beta}$ is 1-β.

Note: MARSSIM suggests that the number of samples should be increased by at least 20% to account for missing or unusable data and uncertainty in the calculated value of n. VSP allows a user-supplied percent overage as discussed in MARSSIM (EPA 2000, p. 5-33).

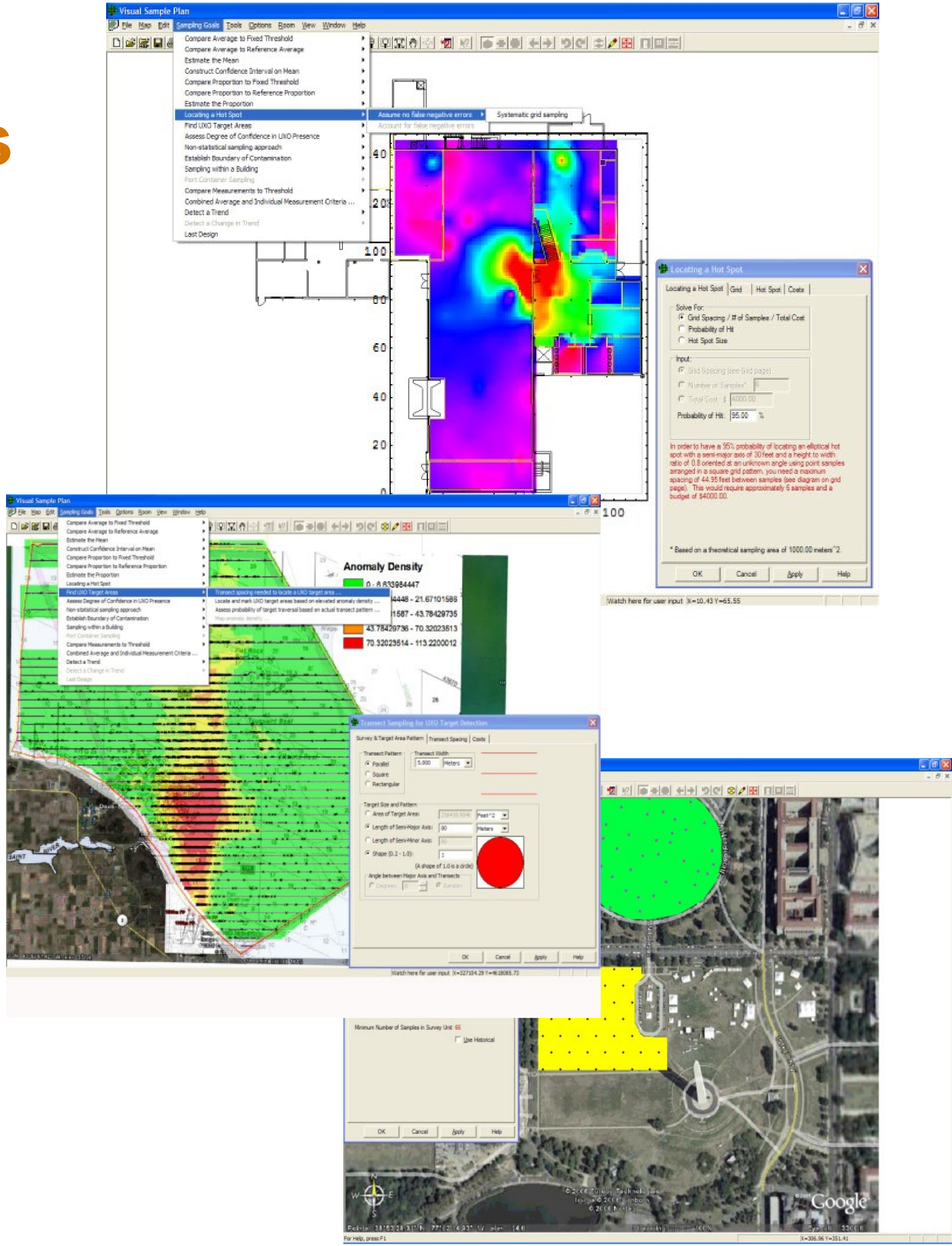
The values of these inputs that result in the calculated number of sampling locations are:

n[a]	n[b]	n[c]	Parameter					
			S_{sof}	Δ	α	β	$Z_{1-\alpha}$ [b]	$Z_{1-\beta}$ [c]
25	61	74	0.36	0.3	0.05	0.1	1.64485	1.28155

For Help, press F1

Current VSP Applications

- Environmental Characterization and Remediation
- Decontamination and Decommissioning
- Indoor or Outdoor Bio/Chem/Rad Terrorist Event
- Long-Term Legacy and Groundwater Monitoring
- Identification, Delineation, and Remediation of UXO Sites
- Natural Disaster Assessments
- Clean-Room Verification
- Item Audits and Surveillance



Wherever Sampling Is Used to Support Decisions

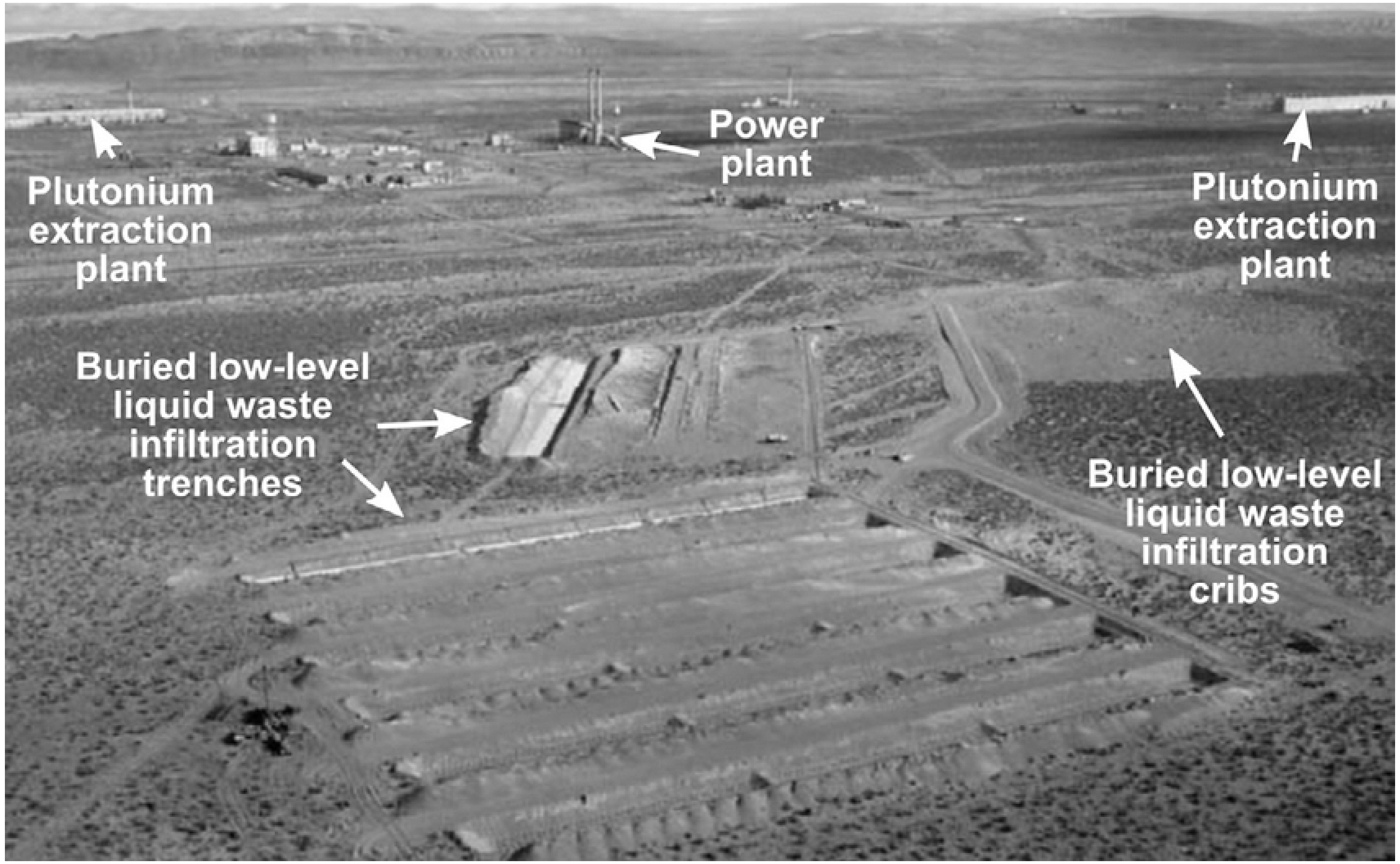
History and Sponsors

- Development sponsored by multiple agencies since the 1990s
  - U.S. Nuclear Regulatory Commission (NRC)
  - U.S. Dept. of Energy (DOE)
  - U.S. Dept. of Defense (DoD)
  - U.S. Dept. of Homeland Security (DHS)
  - U.S. Centers for Disease Control (CDC/NIOSH)
  - U.S. Environmental Protection Agency (EPA)
  - UK Atomic Weapons Establishment
  - UK Government Decontamination Services
  - UK Department of Food and Rural Affairs
- Integrated development into a single freely available tool means investments are effectively leveraged into multiple spaces by varied users

Data Quality in VSP

- Current capabilities
  - Outlier detection
  - Tests of distributional assumptions
  - Retrospective power curves for Sign and Wilcoxson Rank Sum (WRS) tests
  - Data visualization
  - Interpolated maps and contours
  - Area delineation
  - Remediation estimation

Site Characterization Scenario: Hanford BC Controlled Area



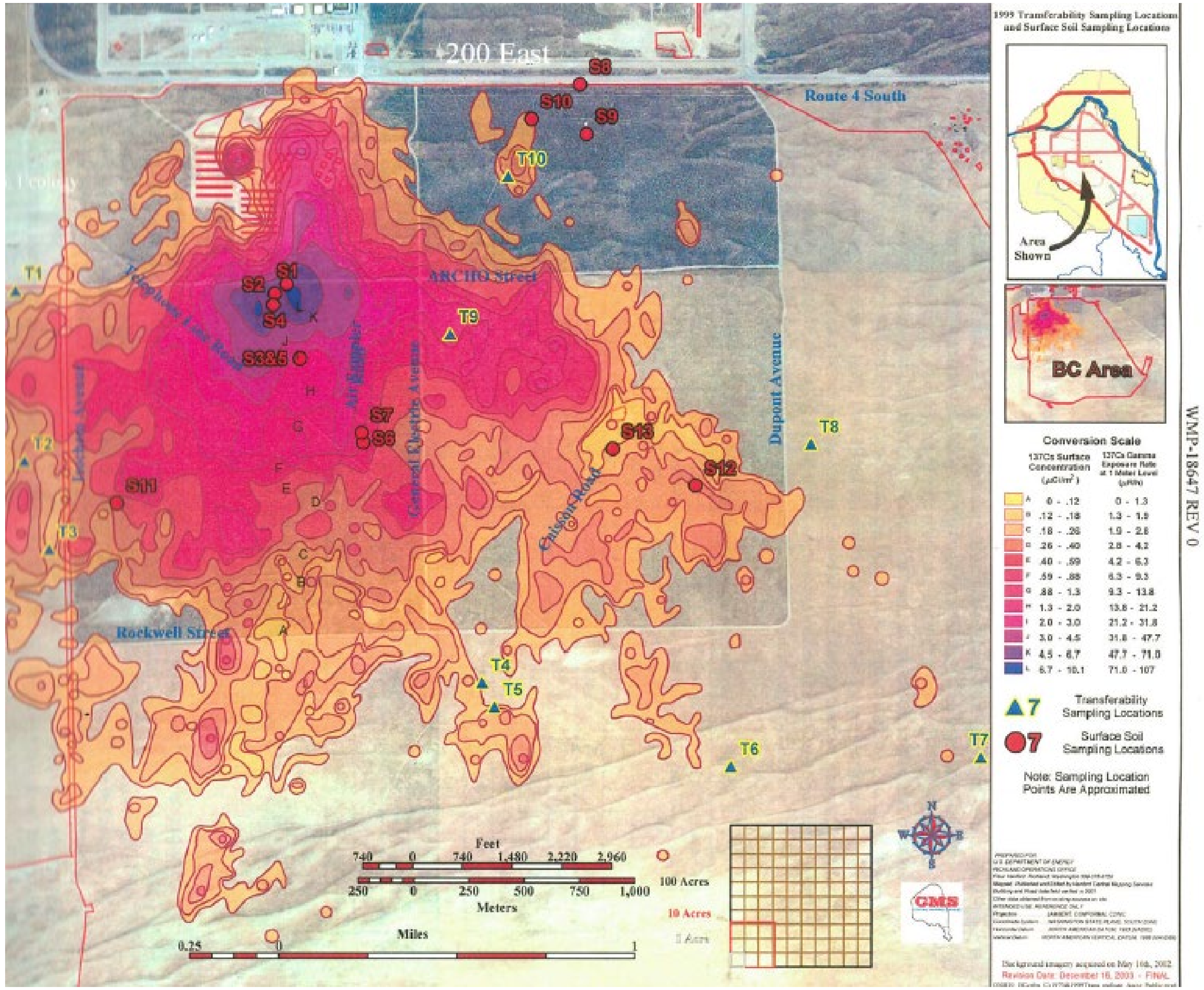
Historical Site Assessment of the Surface Radioactive Contamination of the BC Controlled Area; WMP-18647

Contamination Events

- The trenches were covered with soil, but initially, burrowing native animals intruded into the trenches and used the waste as a “salt lick”
  - Badgers, rodents, primarily jackrabbits
  - The animals defecated and urinated in the vicinity
  - Predators (coyotes) also ate the rabbits and further spread scat and urine
  - Also, deep-rooted tumbleweeds and subsequent grasses added to the distribution
- This was discovered in 1958-1960; the holes were filled in 1965 and the trenches covered with asphalt. Additional gravel was added in 1969
- A total of ~10 km^2 (4 square miles) was directly impacted

Historical Site Assessment of the Surface Radioactive Contamination of the BC Controlled Area; WMP-18647

The Extent of the Contamination



Historical Site Assessment of the Surface Radioactive Contamination of the BC Controlled Area; WMP-18647

Characterization Examples

- The following examples show possible sampling and analysis objectives before remediation via soil removal
- Specific details, contamination values and the sampling plans created are for illustrative purposes and have been simplified / modified

On Scene Coordinator Report FY2010 and FY2011;
DOE/RL-2011-101

Decision Units

- Zone A (orange): Region of elevated contamination prior to remediation
- Zone B (green): Some areas of elevated contamination but lower risk

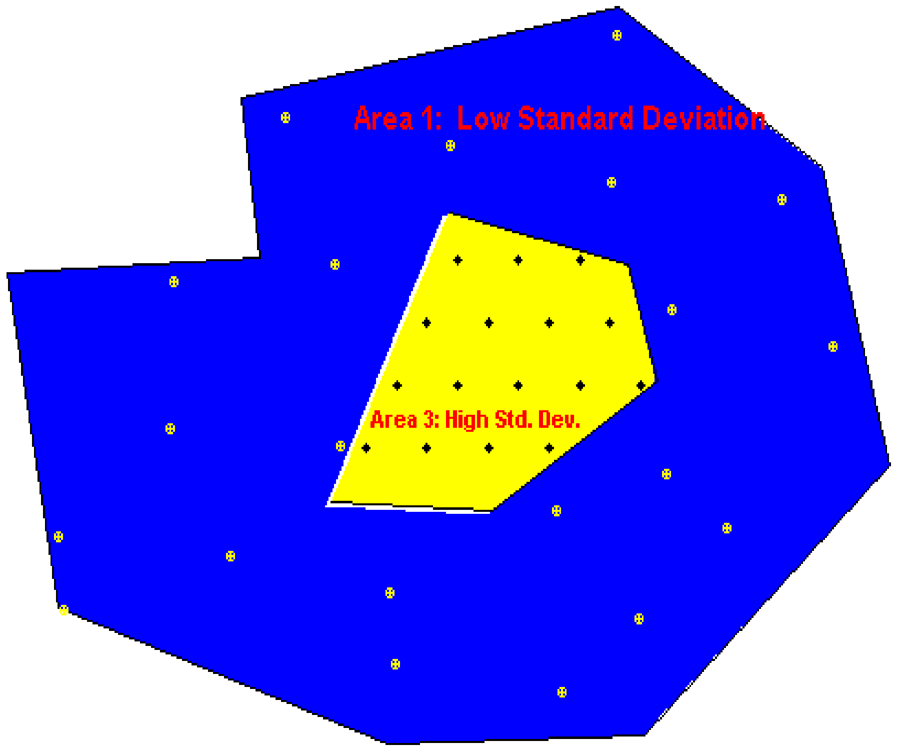
Example 1: Unbiased Mean Estimation for Differing Strata

- Suppose that prior to remediation, stakeholders want estimate the overall Cs-137 average for both Zone A and Zone B
  - Planning for handling and disposal of removed soil
- The two zones differ in
  - Average concentration
  - Standard deviation of concentration
  - Size

	Zone A	Zone B
Area	230 acres	3,970 acres
Average concentration	950 pCi/g	200 pCi/g
Standard deviation	475 pCi/g	100 pCi/g

Stratified Sampling

- What is Stratified Sampling?
  - Divide a heterogeneous population into non-overlapping groups (strata) that are internally more homogeneous
  - Use random or systematic sampling in each stratum
- Advantages
  - Provides more accurate estimates of the mean or percentiles of the heterogeneous population than if simple random sampling is used over the entire site without stratification
  - Better allocation of samples

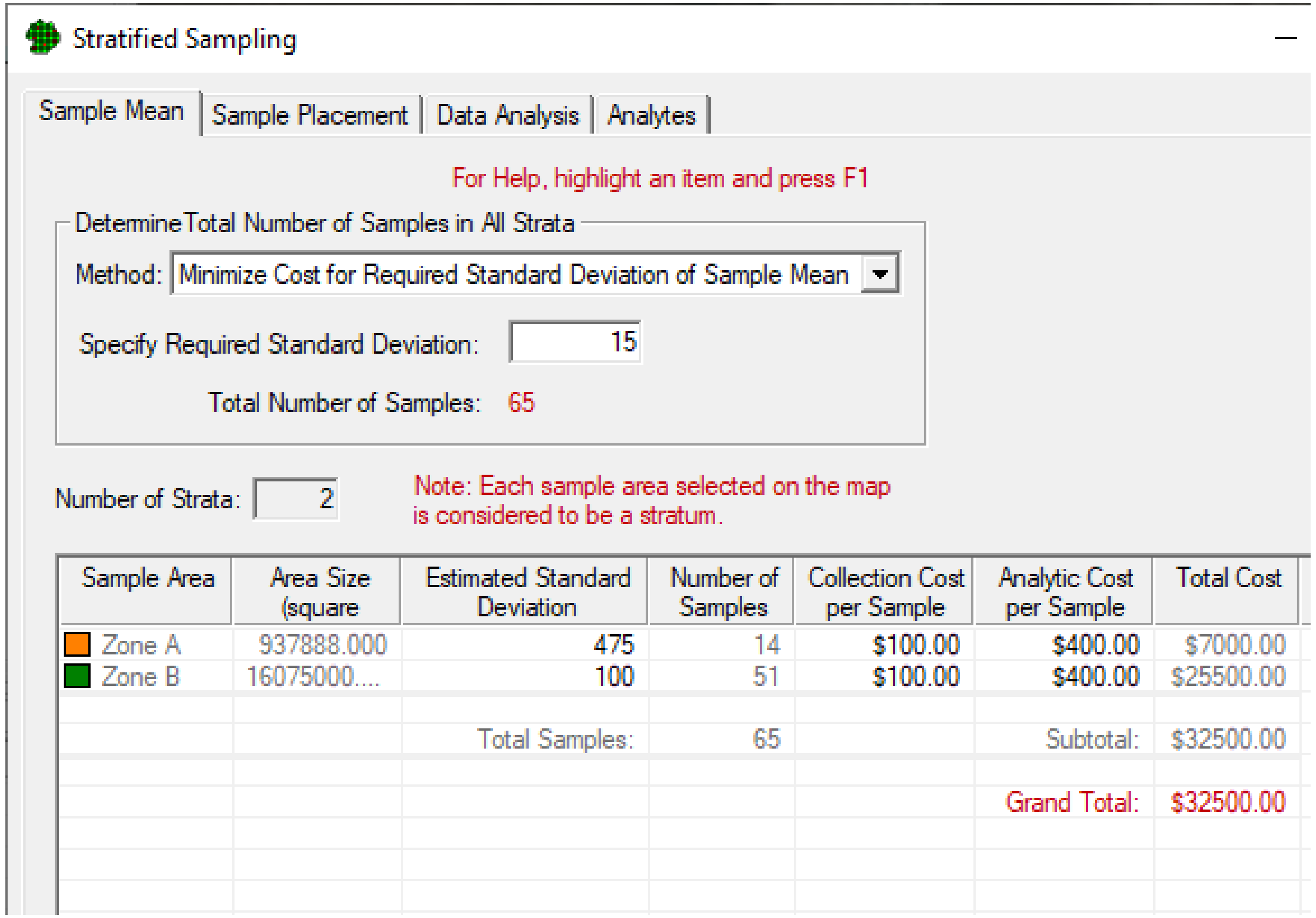


Stratified Sampling: Mean Estimation

- Objective is to obtain an unbiased, sufficiently precise estimate of the mean
- Allocates samples by size of area and standard deviations
- Provides weighted estimate of mean and standard error

Stratified Sampling Design Dialog

- Enter strata parameters
- Select optimization method
- Sample size, distribution and total cost calculated
- 65 samples total
  - 14 in Zone A
  - 51 in Zone B



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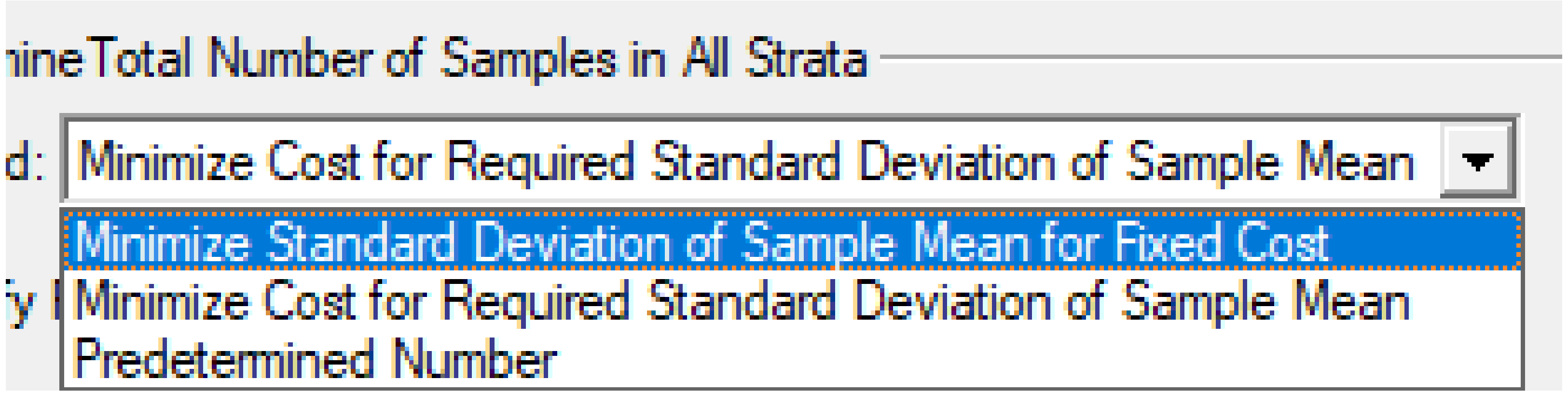
Optimization Methods

- Minimize Standard Deviation of Sample Mean for Fixed Cost
  - Fixed budget, minimize uncertainty on mean estimate
- Minimize Cost for Required Standard Deviation of Sample Mean
  - Fixed required uncertainty on mean, minimize overall cost
- Predetermined Number
  - Fixed number of samples, optimize allocation across strata



Cost Information

- Cost per sample and per analysis can be specified for each stratum
- Example: Suppose collection costs were greater for Zone A (due to radiological controls, PPE, etc.)
  - If optimizing cost, total sample size and sample allocation will be adjusted (shown on next slide)

Cost Information

Sample Area	Area Size (square	Estimated Standard Deviation	Number of Samples	Collection Cost per Sample	Analytic Cost per Sample	Total Cost
Zone A	937888.000	475	14	$100.00	$400.00	$7000.00
Zone B	16075000....	100	51	$100.00	$400.00	$25500.00
		Total Samples:	65		Subtotal:	$32500.00
					Grand Total:	$32500.00

Sample Area	Area Size (square	Estimated Standard Deviation	Number of Samples	Collection Cost per Sample	Analytic Cost per Sample	Total Cost
Zone A	937888.000	475	11	$600.00	$400.00	$11000.00
Zone B	16075000....	100	56	$100.00	$400.00	$28000.00
		Total Samples:	67		Subtotal:	$39000.00
					Grand Total:	$39000.00

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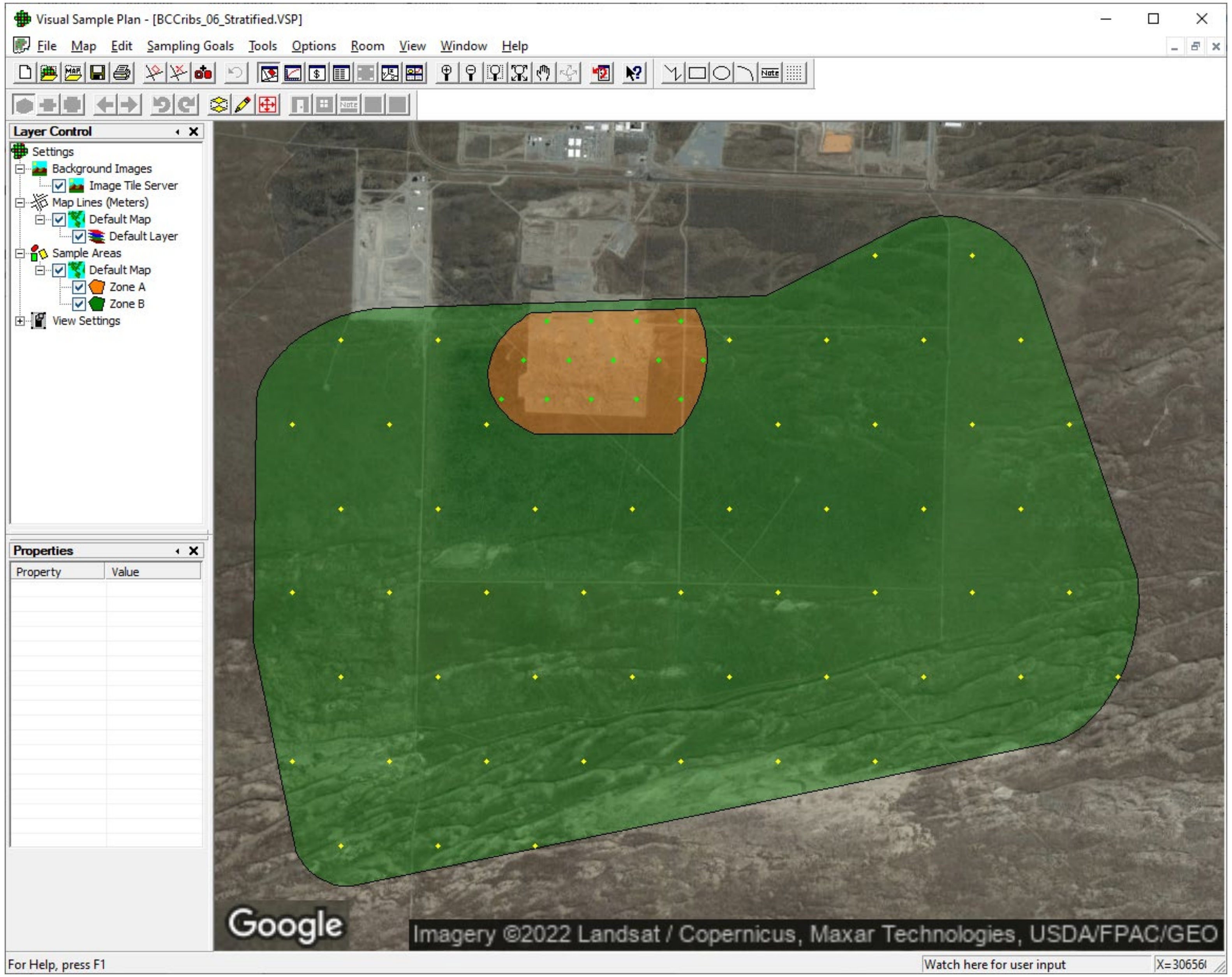
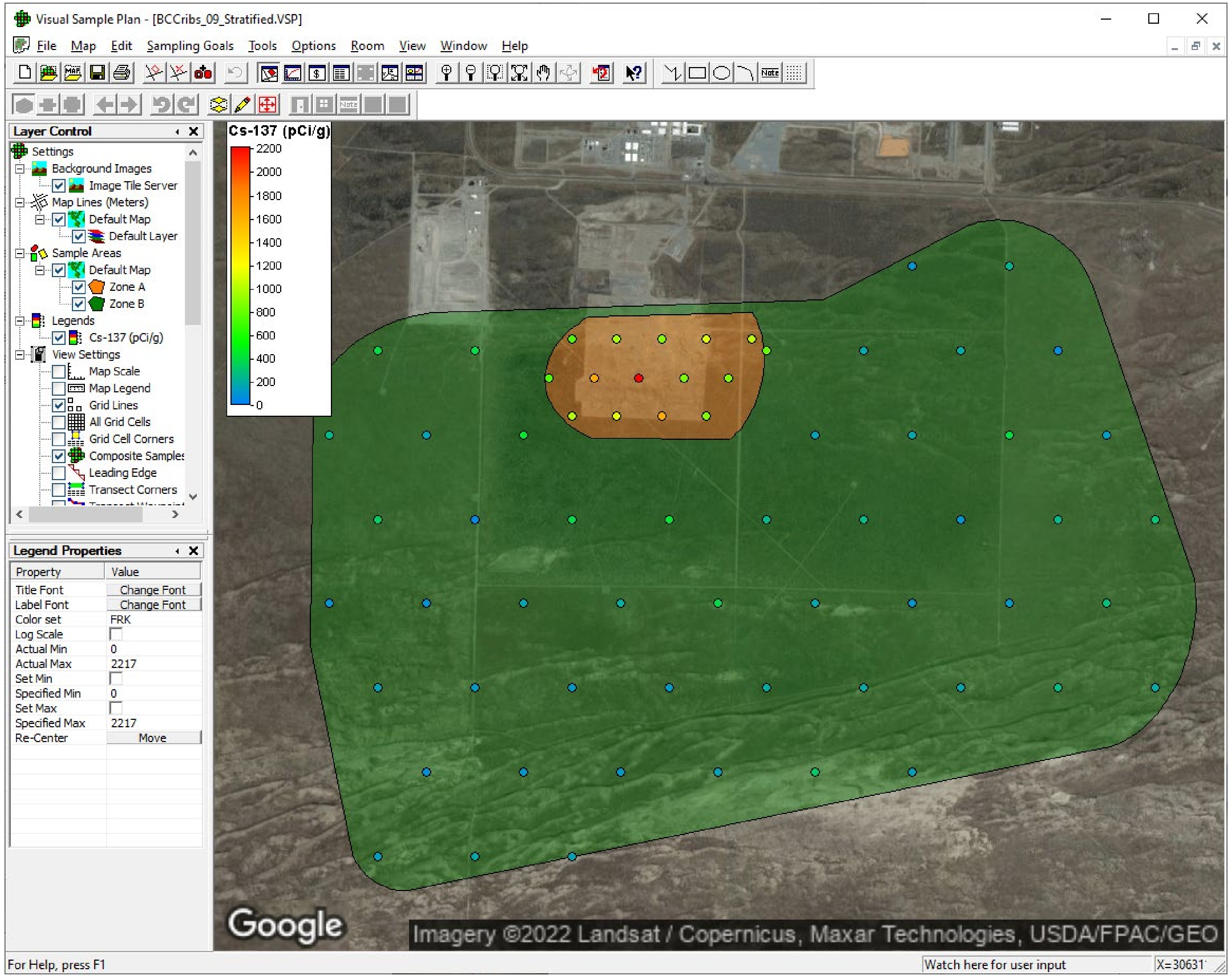
Sampling Plan



Data Results (notional)



Data Analysis: Calculating Estimated Mean

- Estimated site mean (all strata combined)

$$\bar{x}_{st} = \sum_{h=1}^{L} W_h \bar{x}_h$$

where $\bar{x}_h$ = estimated mean of data in stratum h

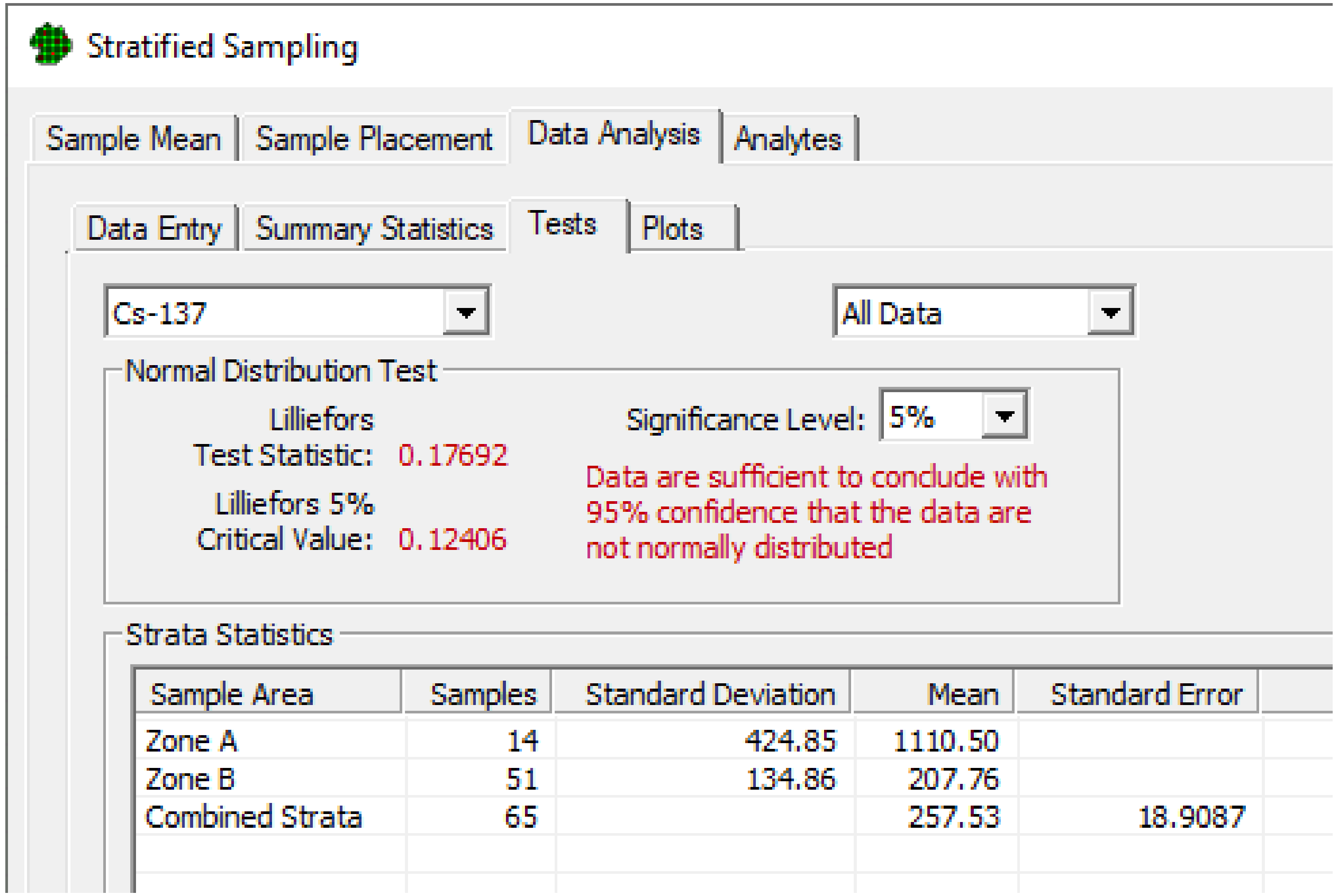
W_h = proportion of site in stratum h

- Standard error (standard deviation of estimated site mean)

$$s(\bar{x}_{st}) = \sqrt{\sum_{h=1}^{L} W_h^2 S_h^2 / n_h}$$

Data Analysis: Calculating Estimated Mean

- Unbiased estimate of mean: 257.53 pCi/g
  - Simple average of all values: 402.2 pCi/g



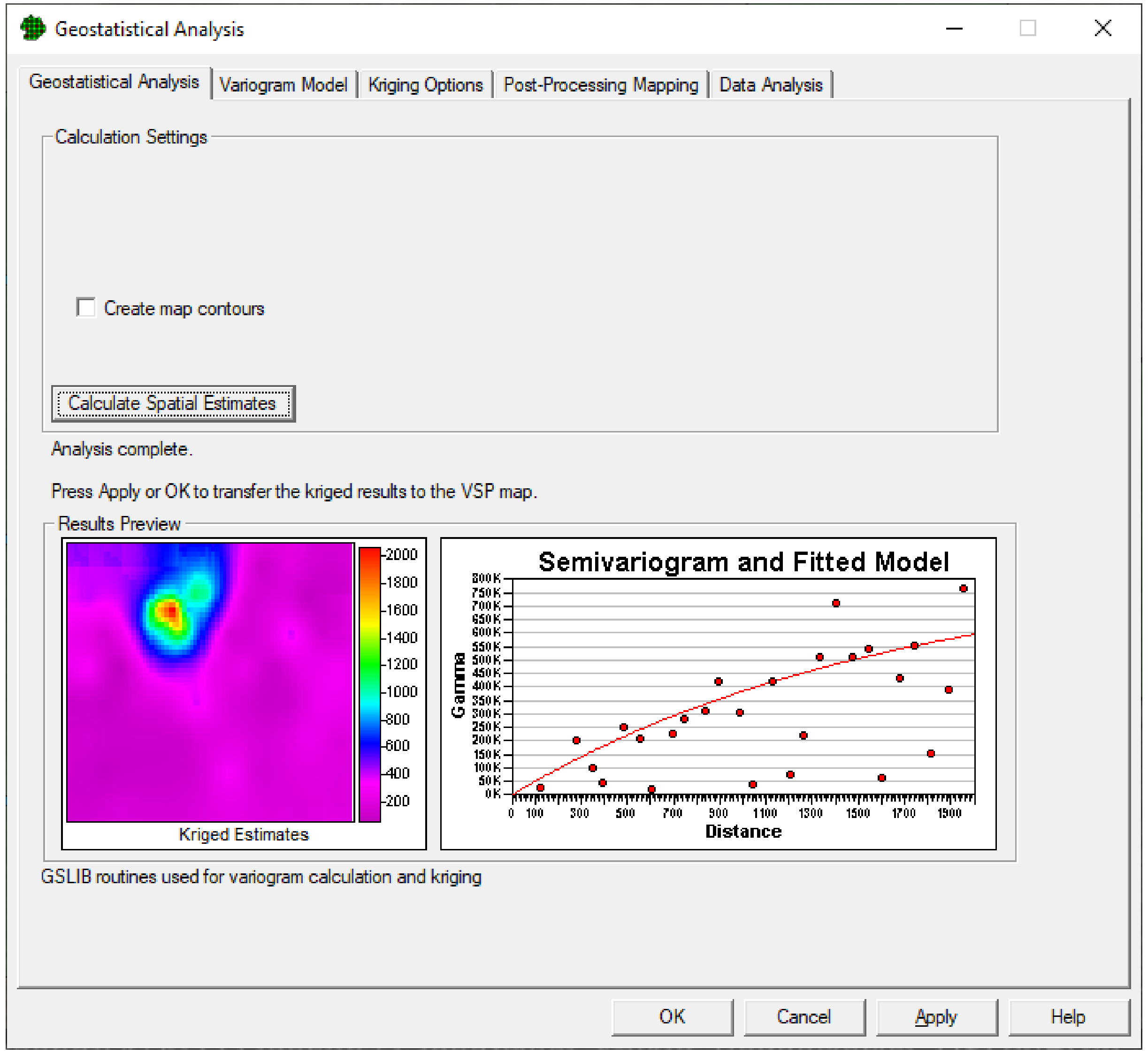
Sample Area	Samples	Standard Deviation	Mean	Standard Error
Zone A	14	424.85	1110.50	
Zone B	51	134.86	207.76	
Combined Strata	65		257.53	18.9087

Example 2: Spatial Analysis

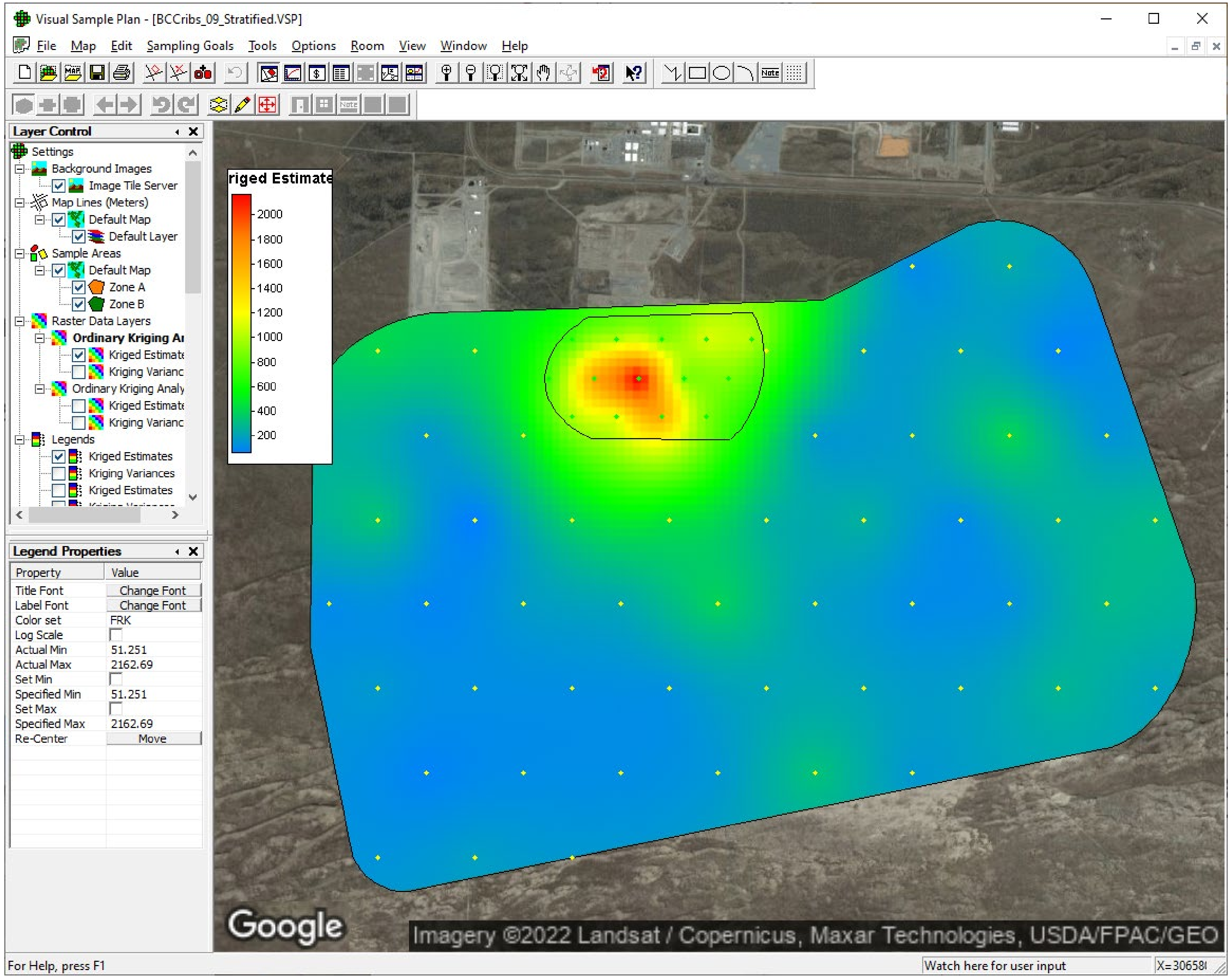
- **Analysis Objective:** Create a spatial estimate of radiological contamination across both areas
- Use geostatistical analysis (kriging) to create an estimate map and delineate contours

Geostatistical Analysis in VSP

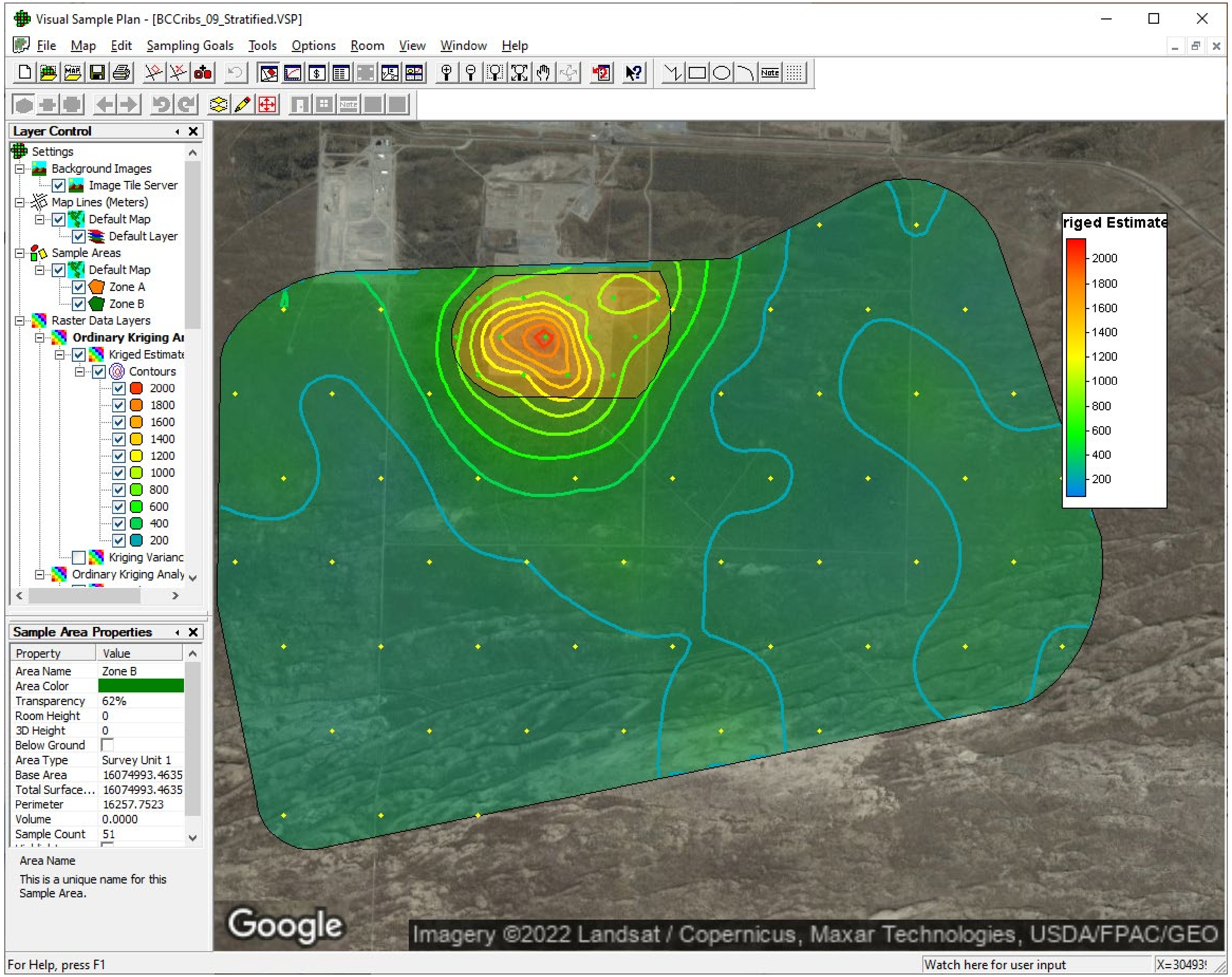
- “Easy Button” one-click analysis
- Many options for refining and improving estimates



Viewing Estimate on Map

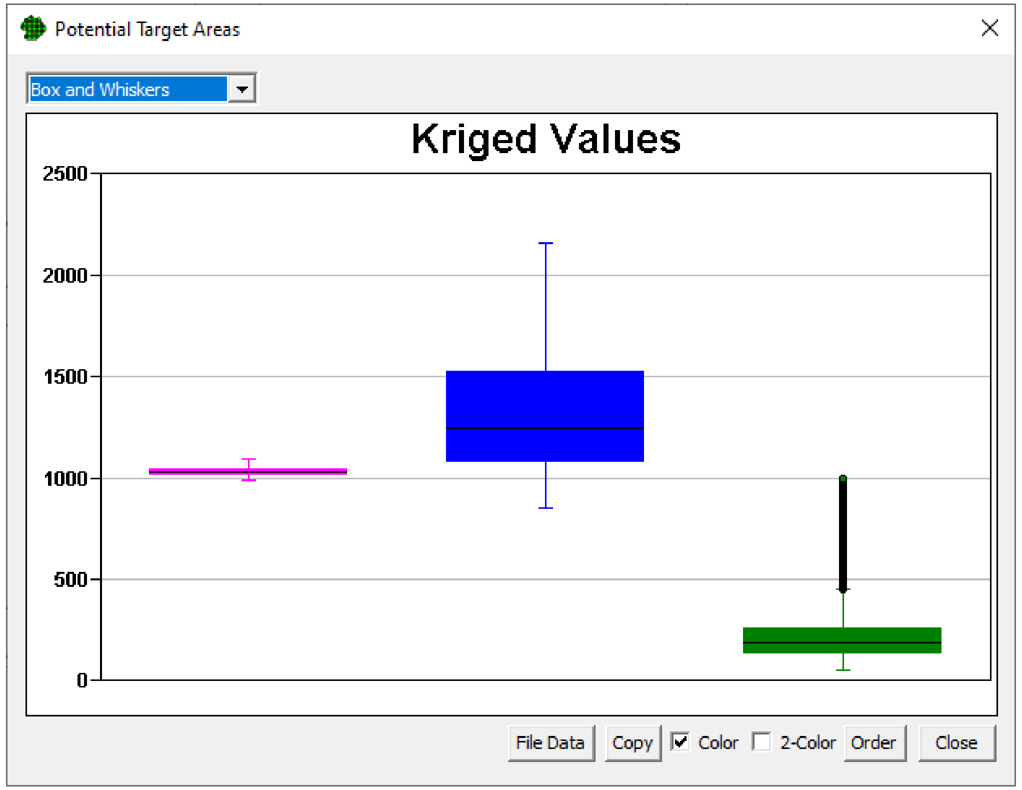


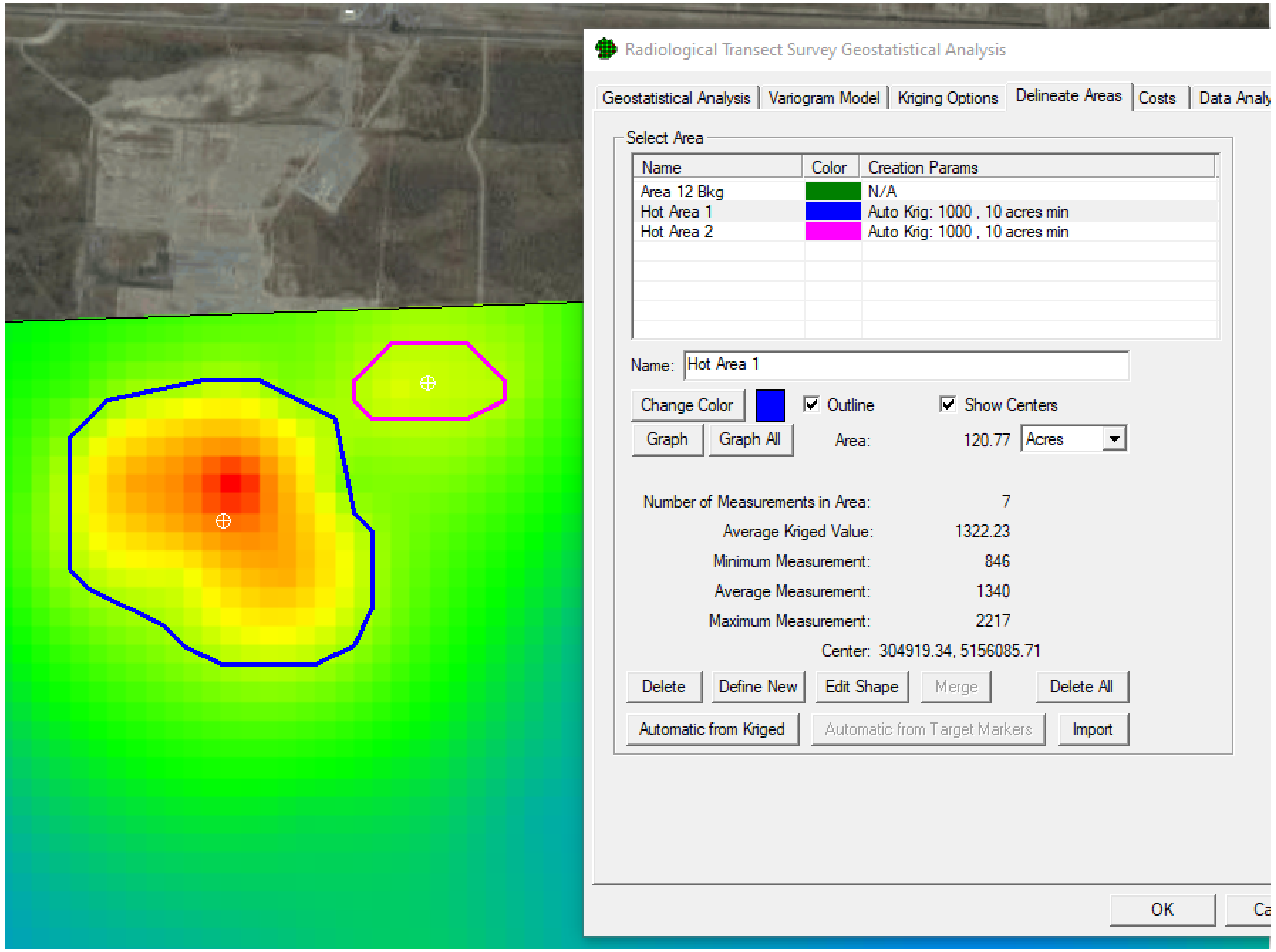
Delineating Contours



Area Delineation

- Delineate Areas: Identify elevated regions
  - Automatic from kriged data
  - Manually
- Statistics and graphs of delineated areas vs. background





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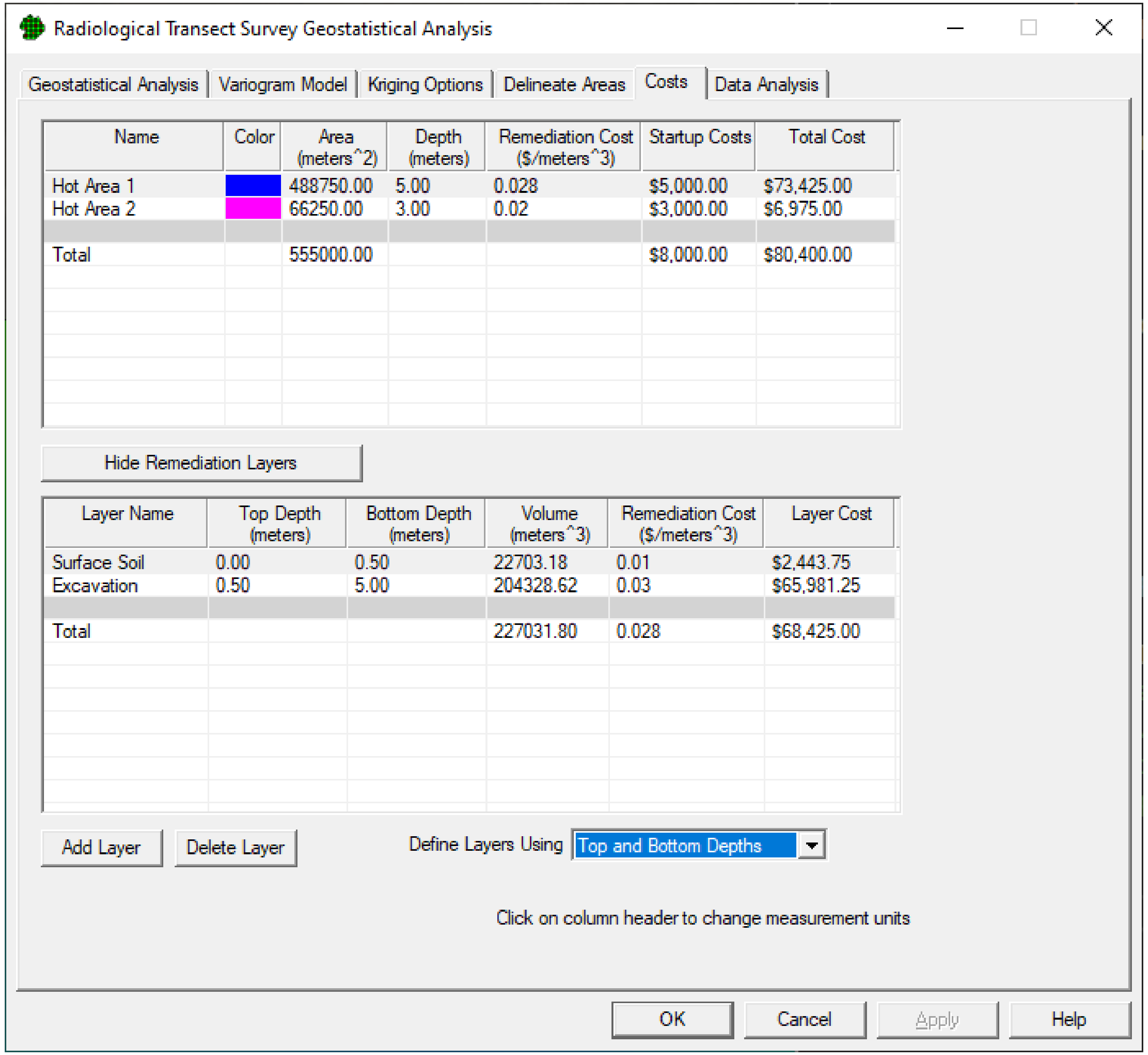
Remediation Costs Estimation

- Tool for estimating remediation costs based on area size and parameters
  - Depth
  - Remediation cost / volume
  - Fixed startup costs
- Defining remediation layers allows specifying differing costs for portions of the area to be remediated

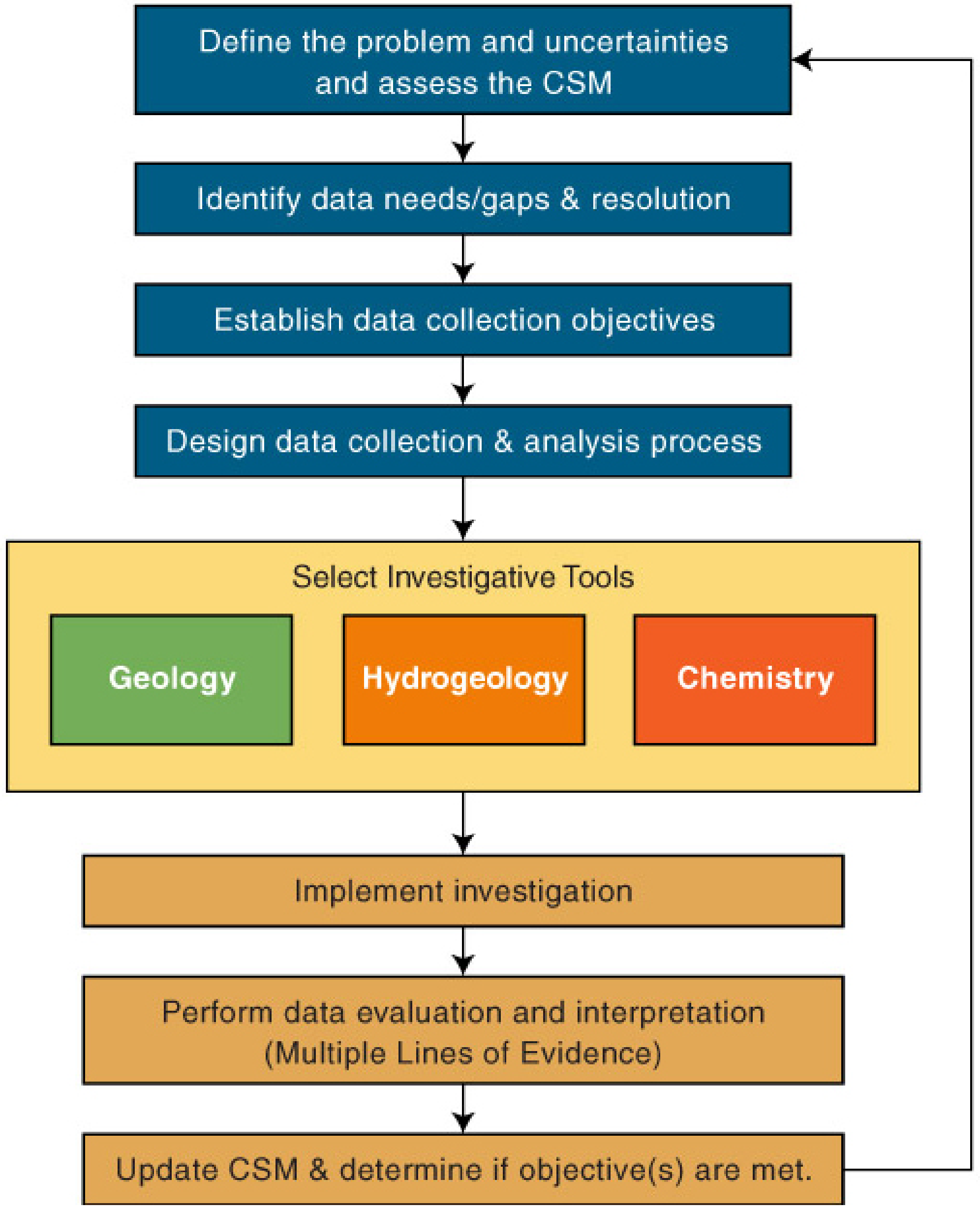


Name	Color	Area (meters^2)	Depth (meters)	Remediation Cost ($/meters^3)	Startup Costs	Total Cost
Hot Area 1		488750.00	5.00	0.028	$5,000.00	$73,425.00
Hot Area 2		66250.00	3.00	0.02	$3,000.00	$6,975.00
Total		555000.00			$8,000.00	$80,400.00

Layer Name	Top Depth (meters)	Bottom Depth (meters)	Volume (meters^3)	Remediation Cost ($/meters^3)	Layer Cost
Surface Soil	0.00	0.50	22703.18	0.01	$2,443.75
Excavation	0.50	5.00	204328.62	0.03	$65,981.25
Total			227031.80	0.028	$68,425.00

Conclusion

- Areas of Interest for Future Work
  - Further development of statistical models to assist with implementing quantitative, objective characterization methods
  - Implement advanced and 3D geophysical analysis capabilities in VSP
- Support for integrated site characterization:
  - sample design
  - analysis and conceptual understanding
  - uncertainty quantification
  - ….repeat as needed



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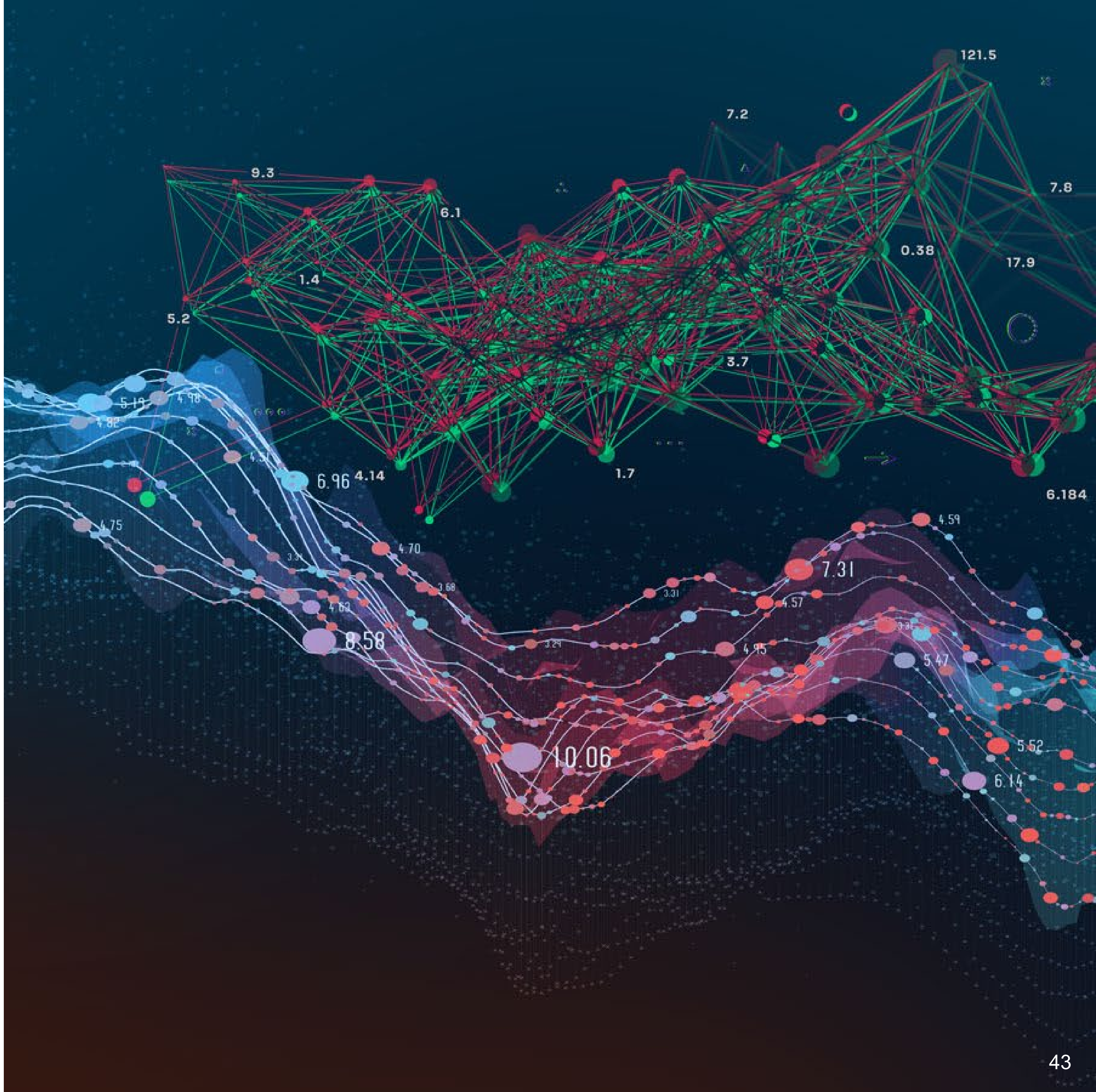
Thank you



Site Investigation Flow Diagram

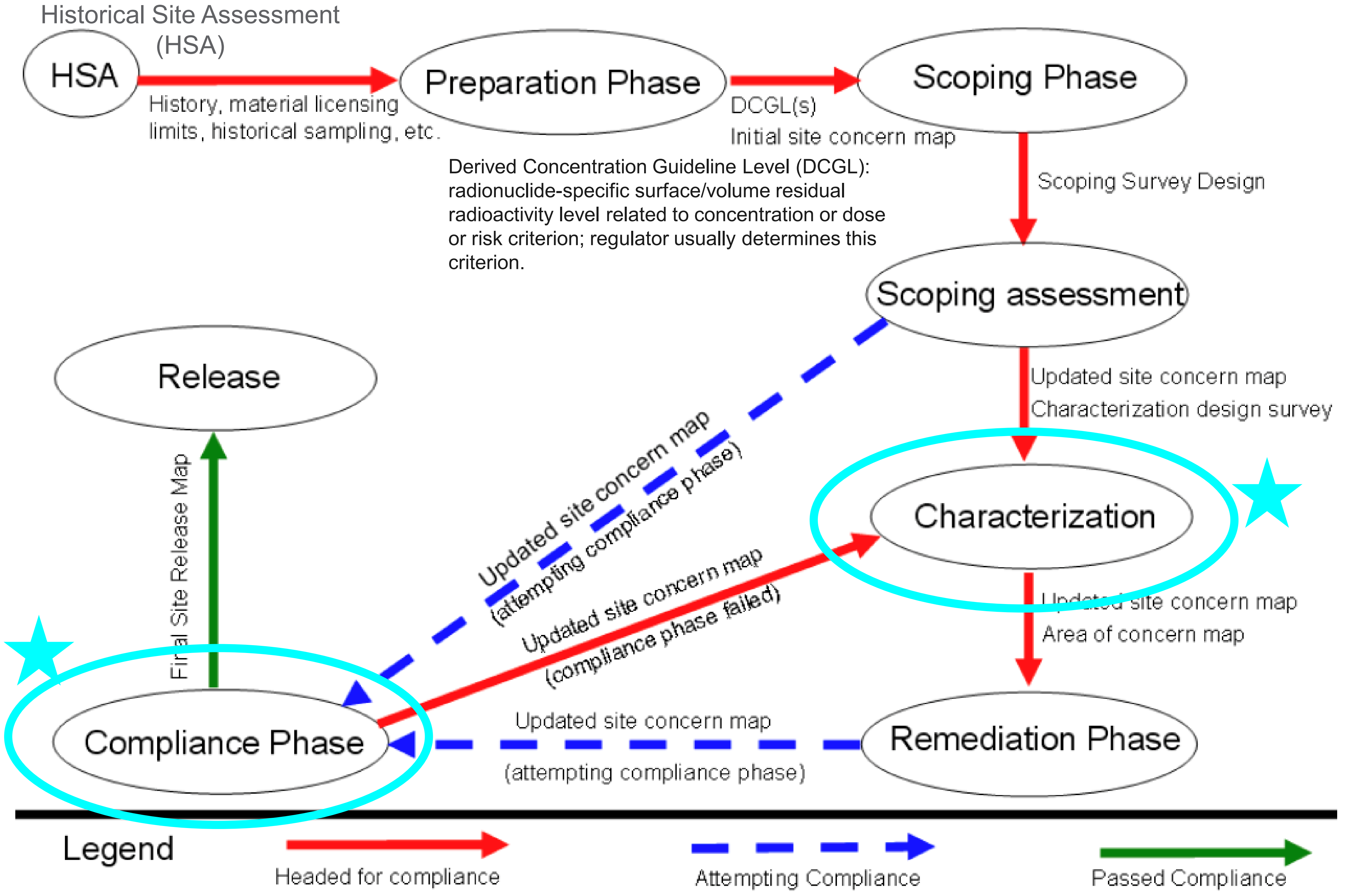


Figure from NUREG-7021

Preparation through Remediation Phases

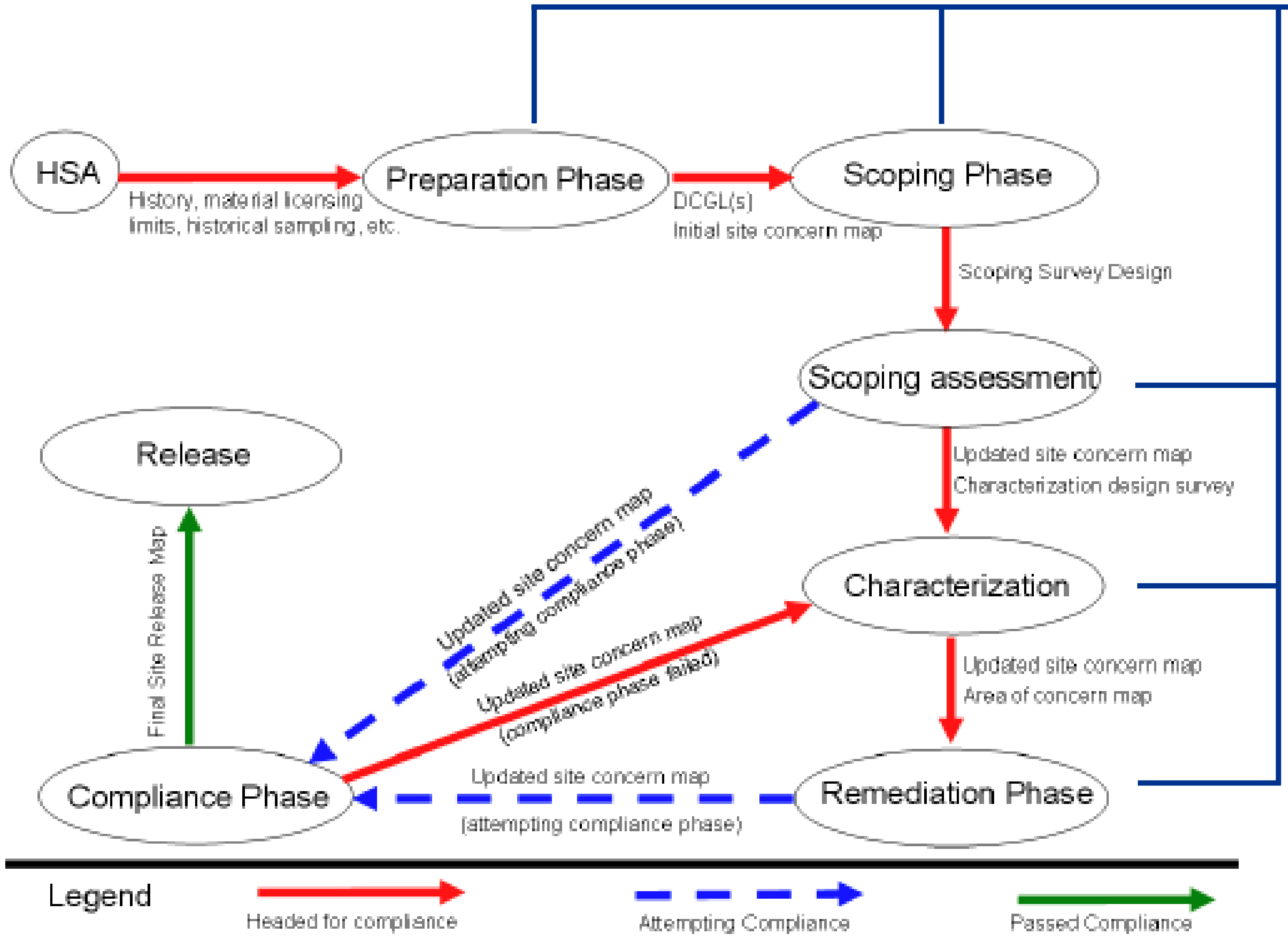
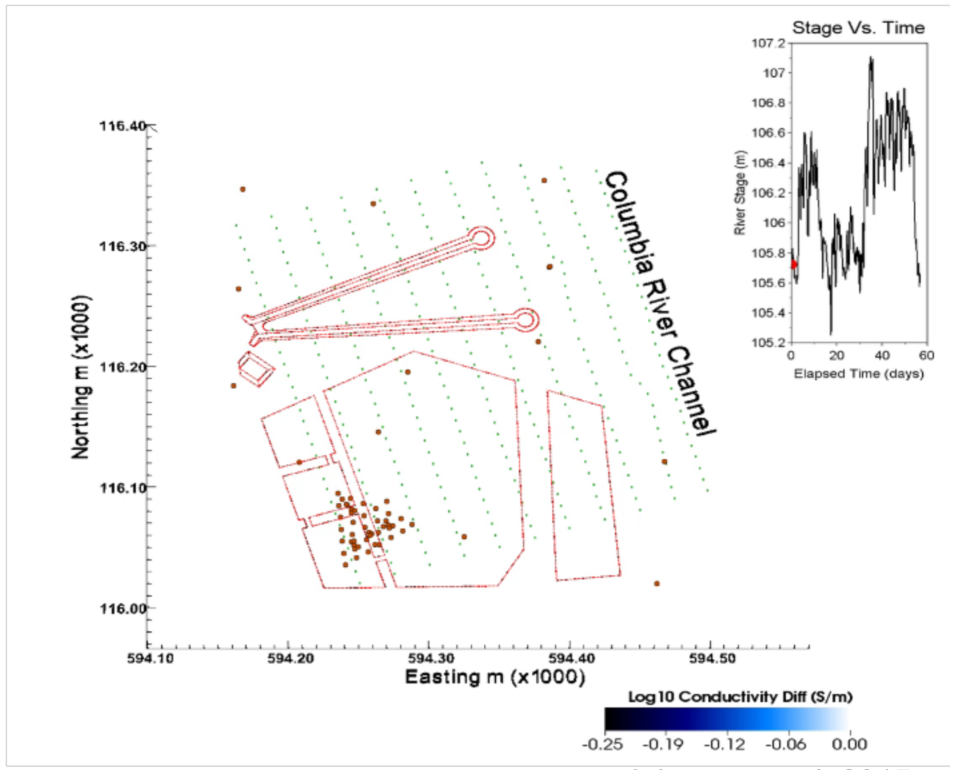


Figure 3.3 from NUREG/CR-7021

Dynamic Conceptual Site Model

- Co-mingled COPCs
- 4D spatio-temporal dynamics
- Groundwater/surface water interactions
- Vadose zone/groundwater interactions
- End-state objective



Johnson, et al, 2015

COPC = contaminant(s) of potential concern

Dimensionality of Approach

- **Layered approach:** model homogeneous 2D/3D layers
  - Use when
    - ✓ Layers are well-defined and homogeneous in geophysical properties governing contaminant fate and transport
    - ✓ Layers can be considered as separate decision units, potentially with unique acceptable limits
    - ✓ Use geophysical and dose models to identify layers and DCGL for each layer (and whether each layer needs to be considered)
  - Considerations
    - ✓ Layered approach ignores spatial dependence between layers—should not use if vertical correlation present/impacts result
    - ✓ Sample sizes governed by layer with highest sample size due to physical constraints of sampling
    - ✓ Alternative actions when results differ from layer to layer (e.g., above/below acceptable limits in different layers)

Dimensionality of Approach (cont.)

- **Volume approach:** model the complex 3D volume
  - Use when
    - ✓ Intra (between) layer dependence exists
    - ✓ Layers are not well-defined
    - ✓ Heterogeneity in effects of geophysical properties on contaminant fate and transport
    - ✓ Layers cannot be considered separate decision units
  - Considerations
    - ✓ Models are more complex—to implement, understand, and communicate
    - ✓ Sample sizes governed by layer with highest sample size due to physical constraints of sampling

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Survey Planning

- Leverage historical wells/boreholes in survey design
  - Start with convenience, judgmental, prior information
  - Consider additional locations based on uncertainty
  - Add randomly sampled locations based

Classical approaches (parametric or non-parametric)

- Stratified random/systematic: use risk & geophysical models to identify stratification
  - Vertical strata represent geophysical layers
  - Horizontal (or vertical) based on risk model
  - Allocate samples based on relative exposure risk and/or proportion of total volume

Geostatistical approaches

- Determine mathematically where to locate samples based on geostatistical uncertainty
- Incorporate geophysics input through
  - Bayesian methods
  - Geospatial/kriging methods that combine various data types
    - Fixed rank kriging to include data from different sensor properties
    - Generalized least squares (GLS) to include geophysical information through covariates
- Uncertainty from such models can guide sample placement
  - Identification of strata, sample allocation across strata
  - More sample locations allocated to regions of higher uncertainty and/or boundaries between high/low contamination

State of AI & ML in Subsurface Applications

- Challenging to collect sufficient data to accurately describe **subsurface** complexities
  - Traditional (point-source based & destructive sampling) methodologies are costly and present potential risk for human exposure
  - Borehole sampling represents state of the system at specific location(s) and time(s) – potentially not representative of whole area of concern
  - Large uncertainty in forecasting subsurface system evolution
- Few-shot machine learning in conjunction with remote subsurface sensing techniques and high-performance forward prediction
  - Reliably estimate subsurface property distributions, including permeability, porosity, and hydraulic conductivity, that control transport and fate of radioactive material
  - Address paucity of characterization data and complexities of heterogeneous subsurface systems
  - Advancements will reduce uncertainty of system-scale characterization and radiation rose assessments, minimize costs, and increase worker safety and protection of human health and the environment
- Expect these advancements to be most applicable in characterization & earlier phases

Data Quality in VSP

- Current capabilities
  - Outlier detection
  - Tests of distributional assumptions
  - Retrospective power curves for Sign and Wilcoxson Rank Sum (WRS) tests
  - Data visualization
  - Interpolated maps and contours
  - Area delineation
  - Remediation estimation

Geostatistical Analysis

- In environmental settings, often observe spatially correlated data; samples obtained close to each other are more correlated than samples farther apart.
  - Classical test of hypothesis approaches ignore spatial correlations.
  - Geospatial methods estimate and account for those spatial correlations.

Example 4. Mobile EM Geophysics

- Covers large areas rapidly
- Ground, waterborne or airborne
- Non-invasive

Vertical cross section of the inverted resistivity image along FloaTEM profile B-B'