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Statistical Methods for Subsurface Surveys to Support Decommissioning

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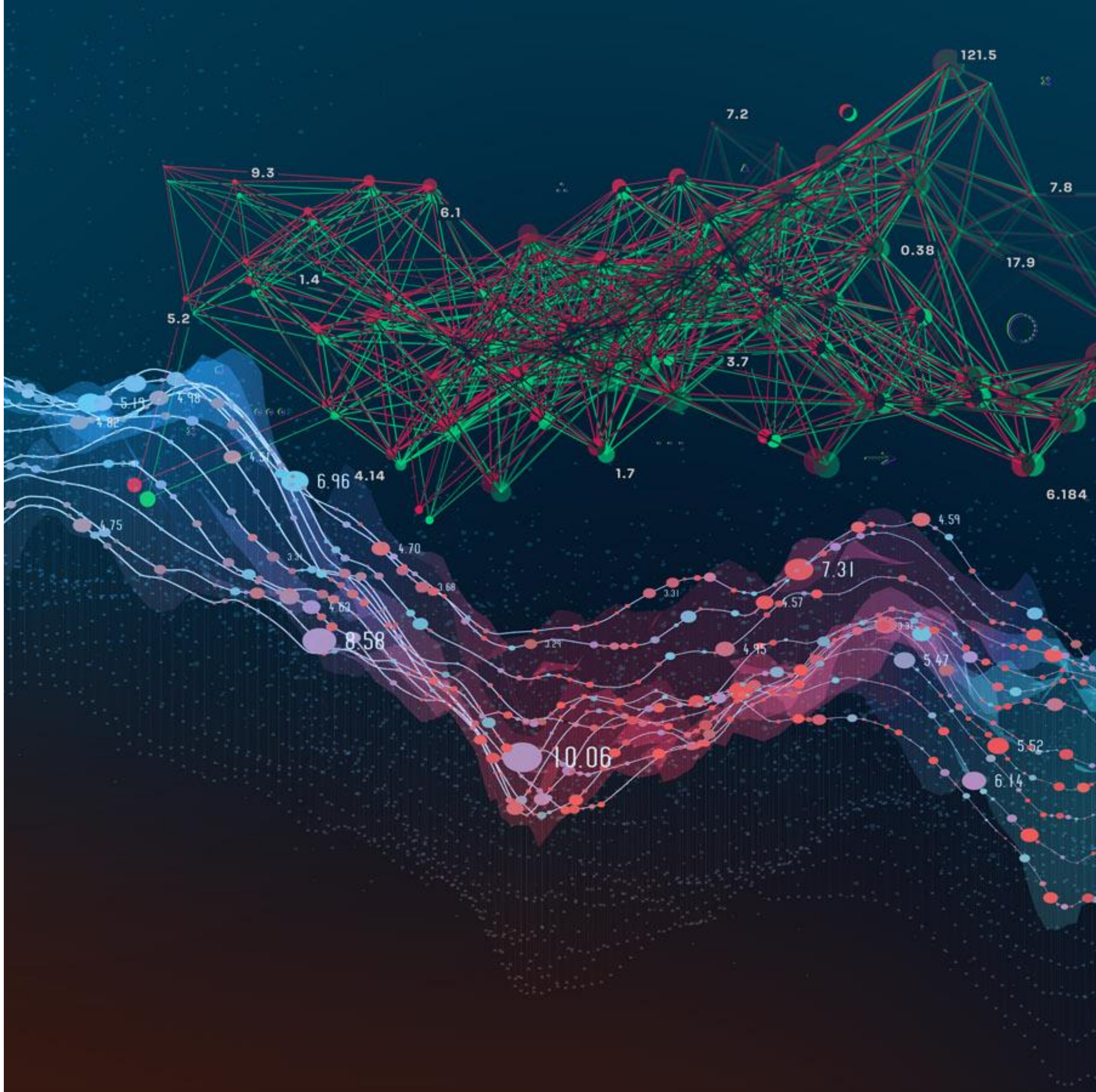
U.S. DEPARTMENT OF ENERGY   BATTELLE



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Nuclear Regulatory Commission (NRC)

Work presented today supported by the Nuclear Regulatory Commission Office of Nuclear Regulatory Research (nrc.gov)

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Office of Nuclear Regulatory Research

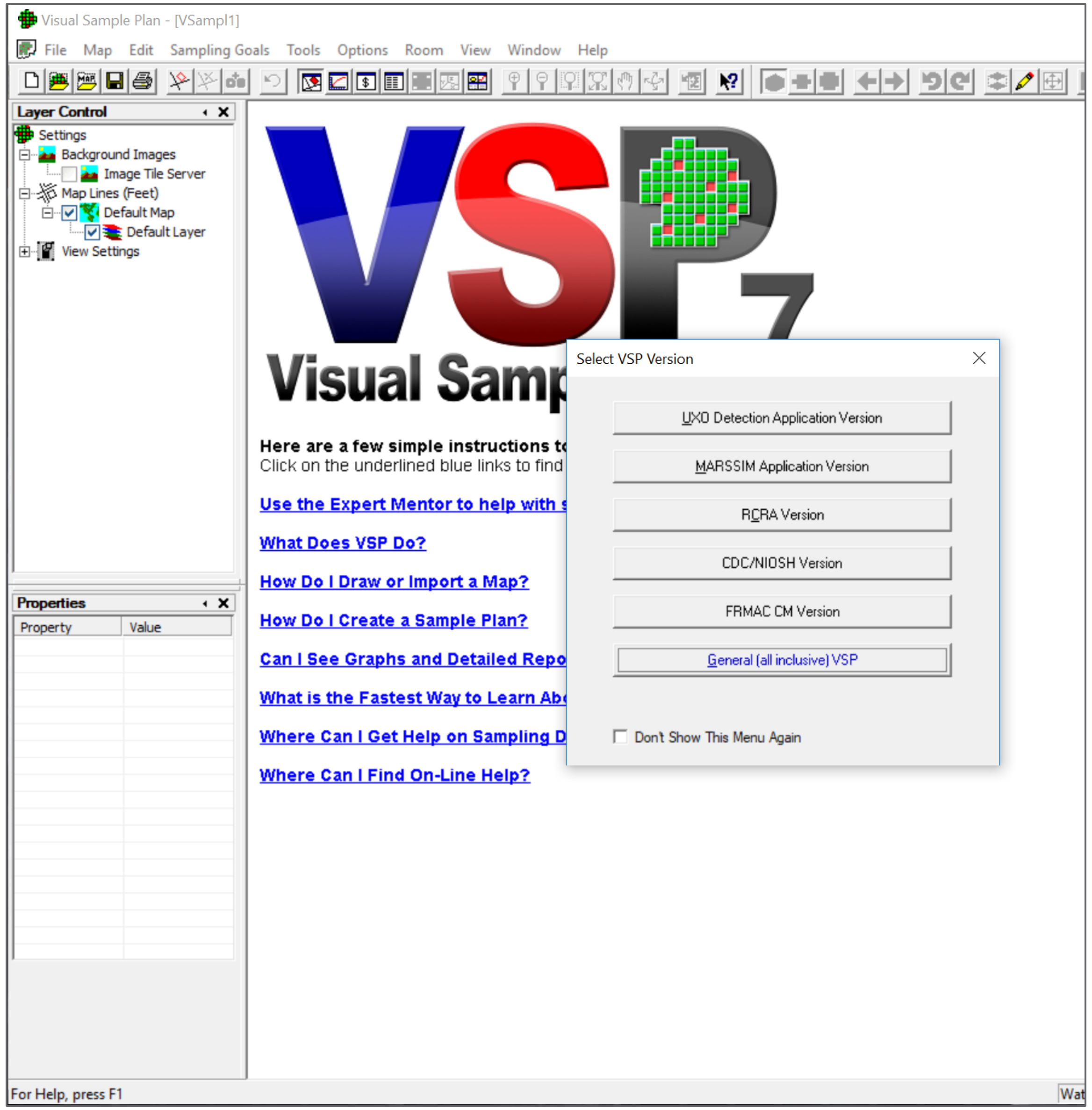
Decontamination & Decommissioning

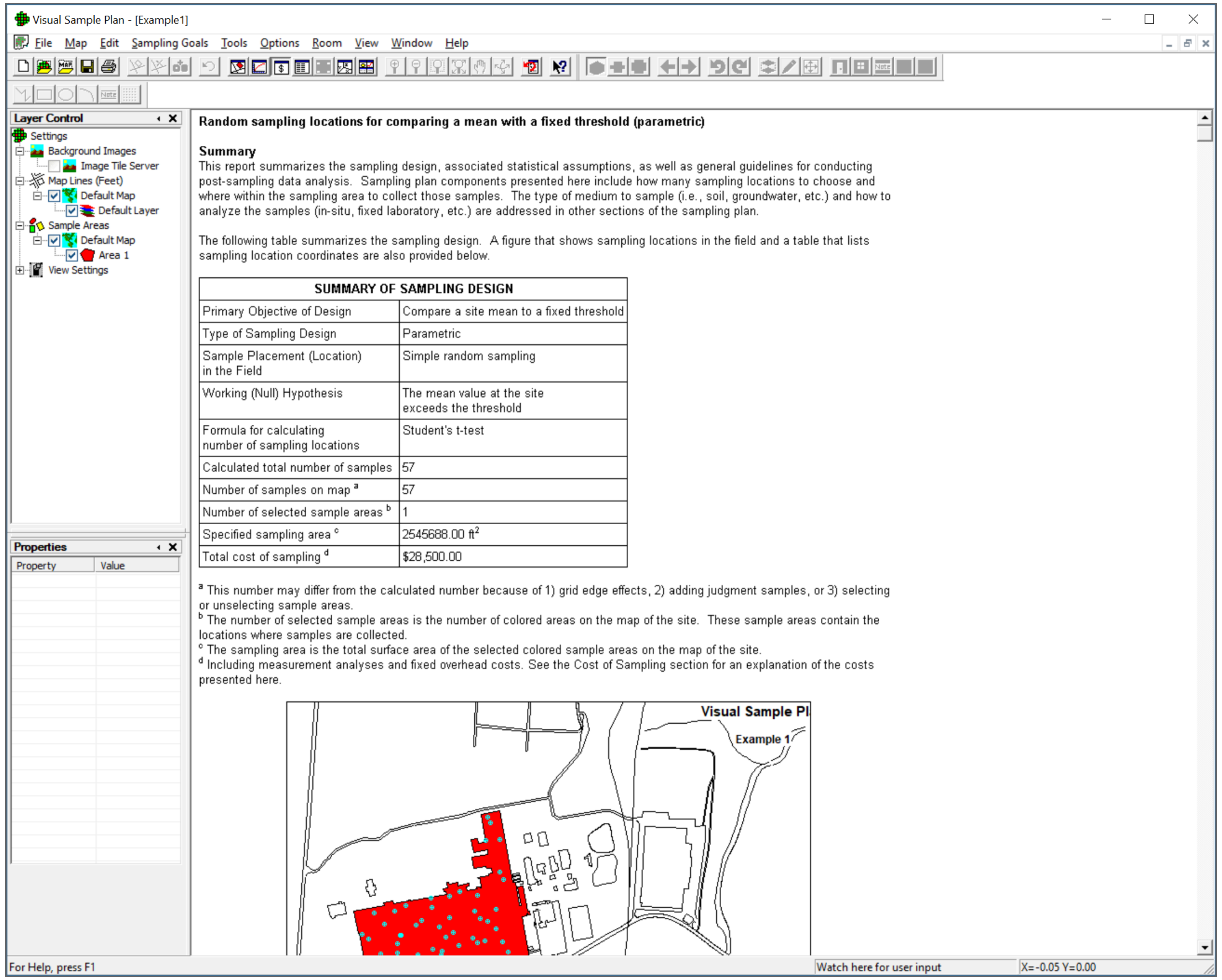
- Decommissioning: safely removing a [nuclear] facility or site from service and reducing residual radioactivity to a level that permits either:
  - Property release for unrestricted use and terminate the license
  - Property release under restricted conditions and terminate the license

- PNNL's role
  - Consider regulations, guidance, and communications
  - Develop methods and tools for survey sample design and statistical analyses to demonstrate compliance with decommissioning requirements

- Recent developments
  - Low altitude un-piloted

Visual Sample Plan (VSP)

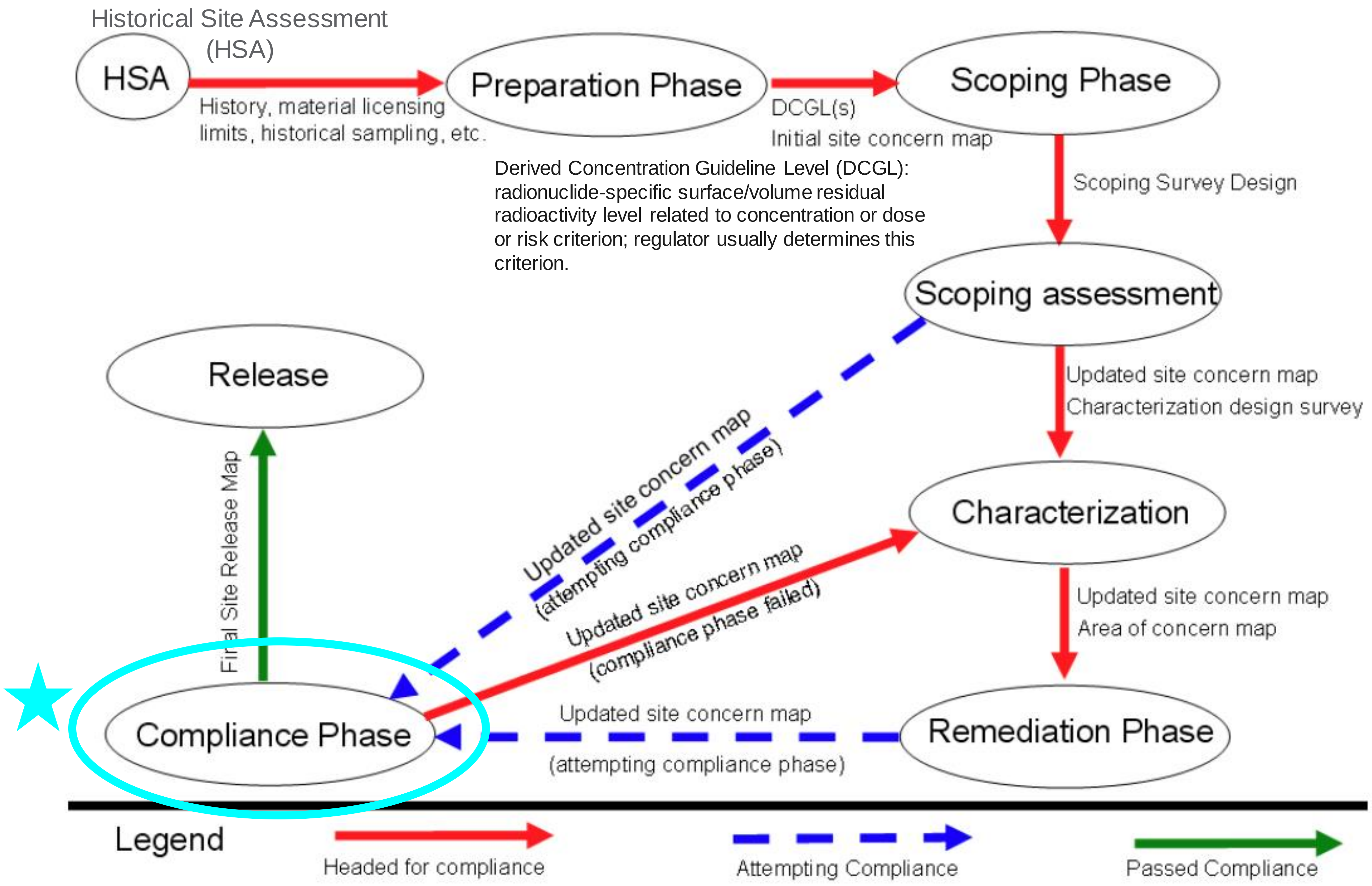




VSP is available at: https://www.pnnl.gov/projects/visual-sample-plan

Screenshots from Visual Sample Plan

Flow Diagram



Derived Concentration Guideline Level (DCGL): radionuclide-specific surface/volume residual radioactivity level related to concentration or dose or risk criterion; regulator usually determines this criterion.

Figure from NUREG-7021

Preparation through Remediation Phases

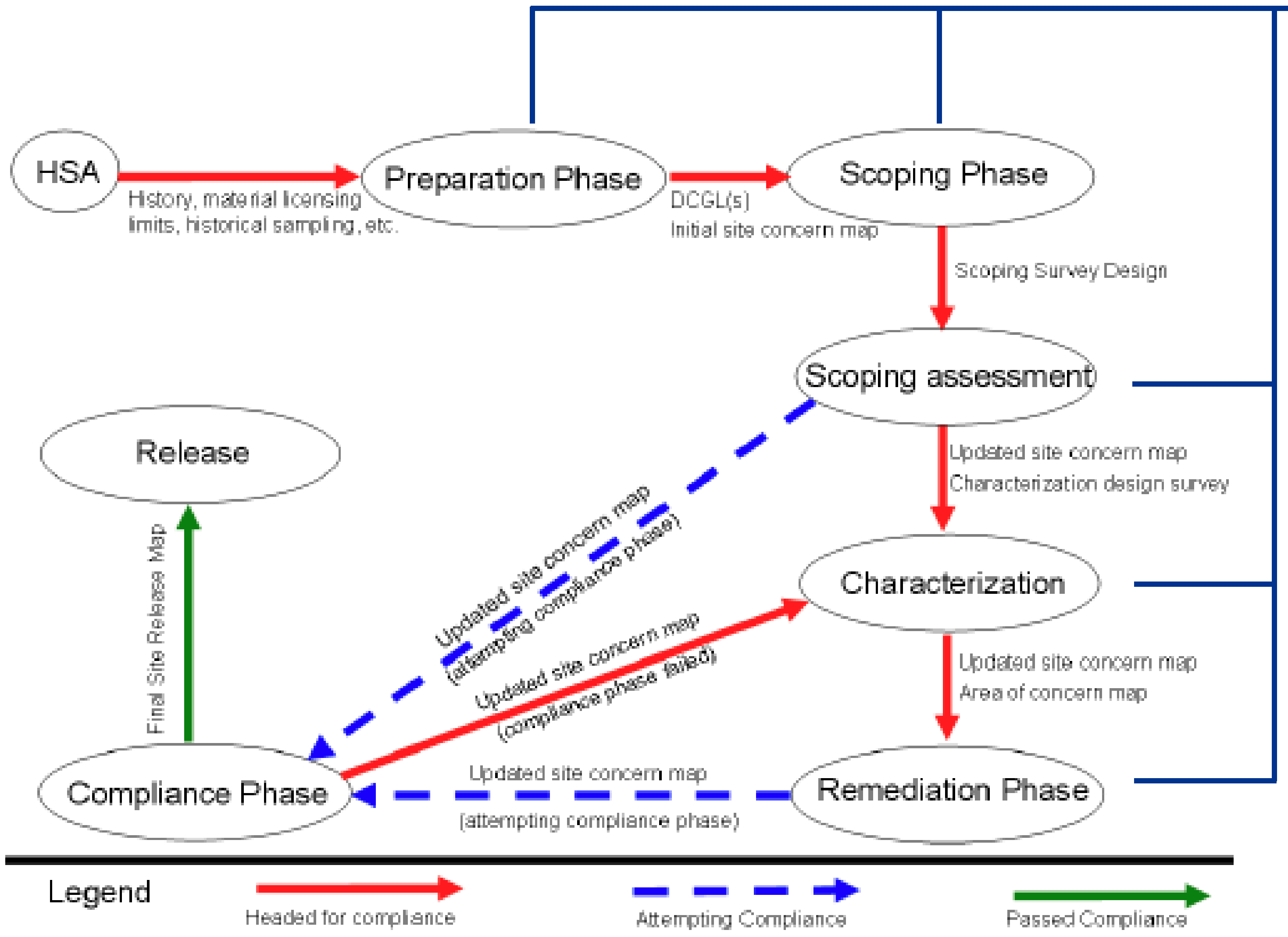
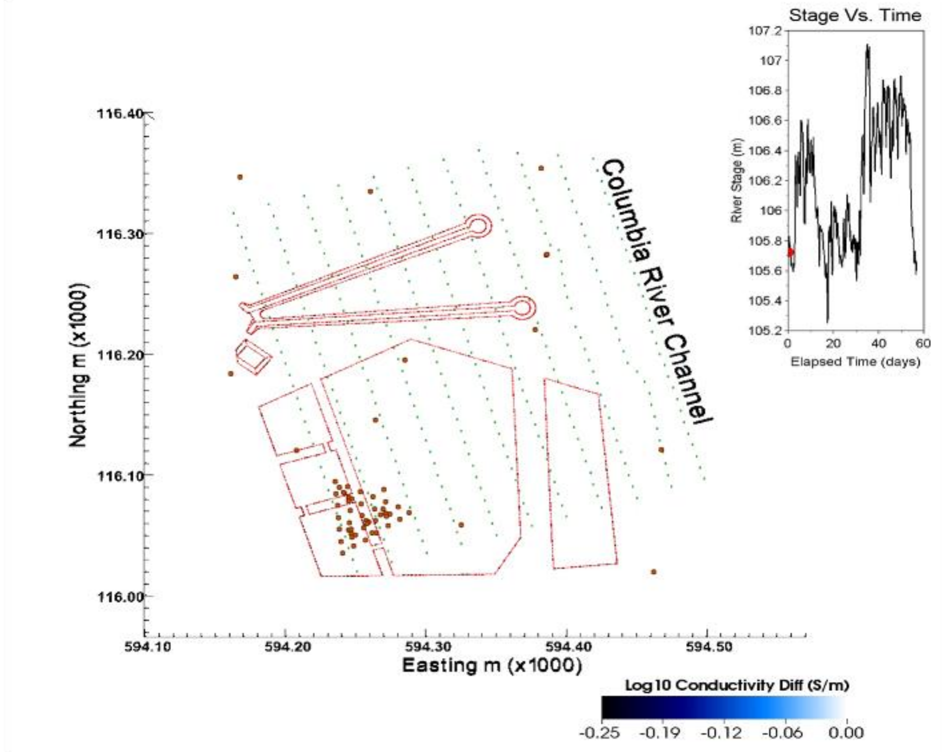


Figure 3.3 from NUREG/CR-7021

Dynamic Conceptual Site Model

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



Johnson, et al, 2015

COPC = contaminant(s) of potential concern

Compliance Phase

Information needed to show end-state is achieved
- Surface & subsurface matrix samples
- Fate & transport of COPCs on-/off-site are understood
- COPC spatiotemporal concentrations meet release criteria

Assumptions
- Data from HSA, preparation, and scoping phases will be available
- Data from characterization and remediation phases <u>may</u> be available
- Variation in how much/what type

What tools are needed in VSP to support compliance phase?
- Data visualization
- Data collection/survey planning
- Analysis of collected data
- Uncertainty quantification, confidence bounds and hypothesis testing for end-state decisions

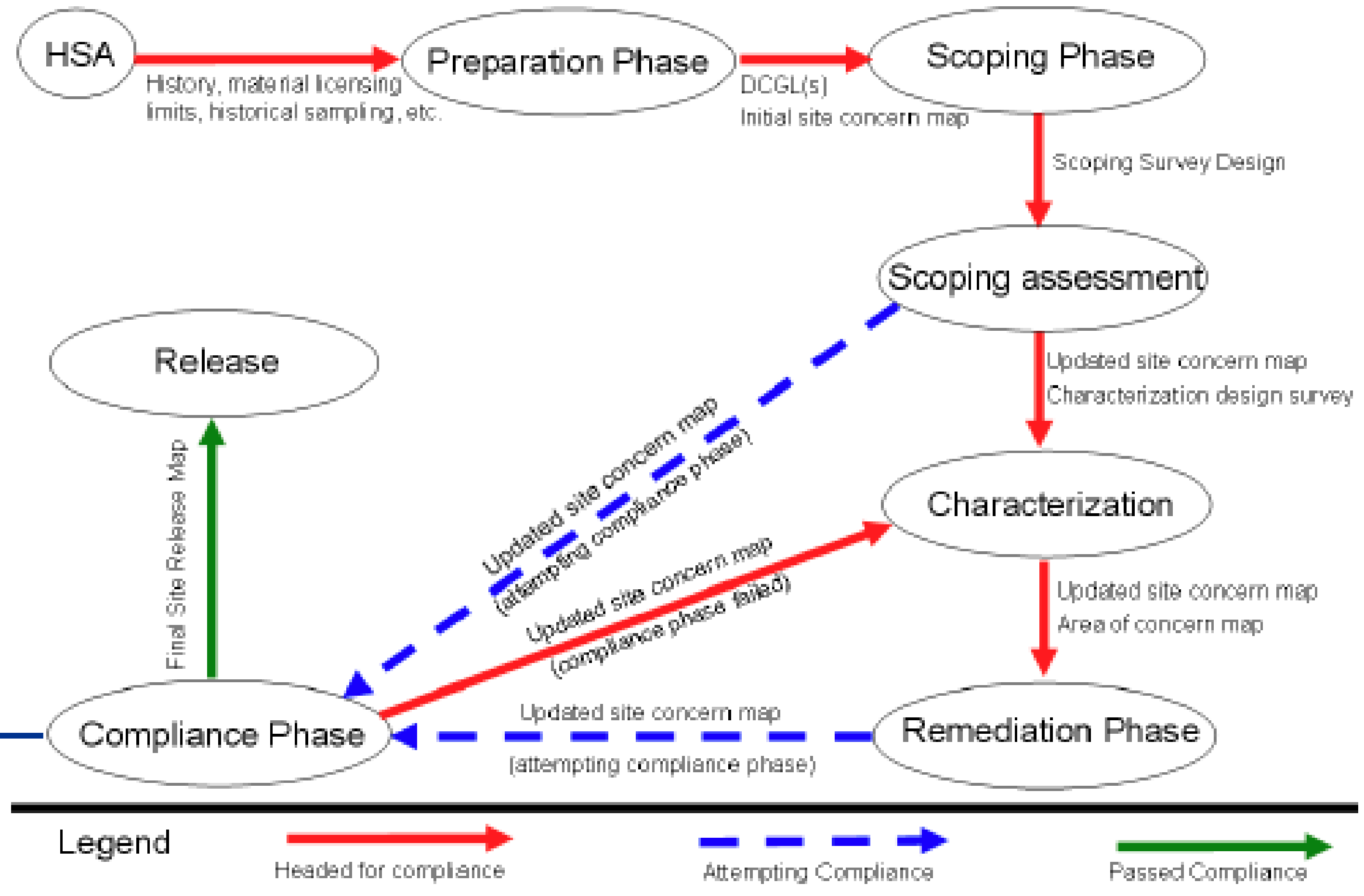


Figure 3.3 from NUREG/CR-7021

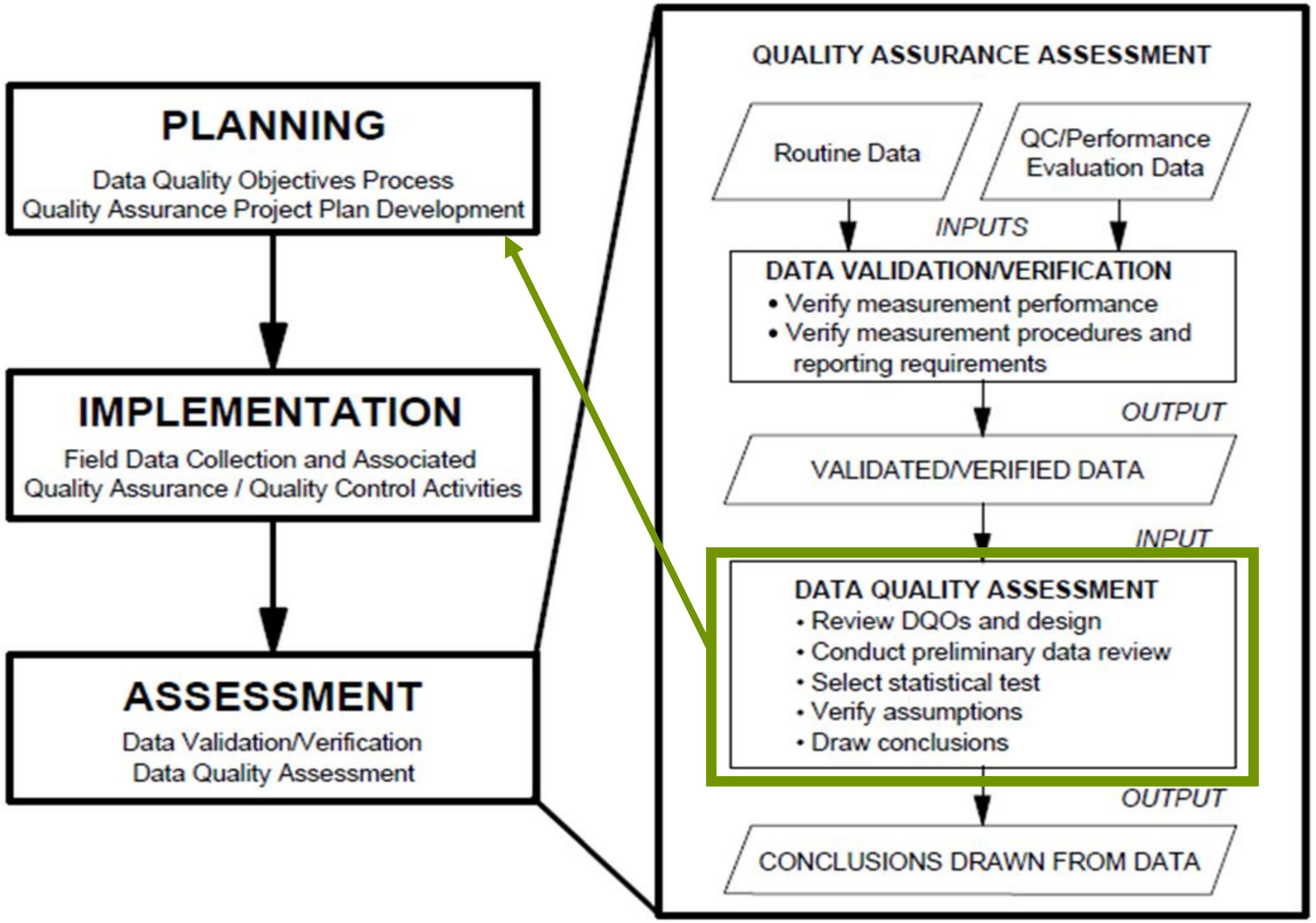
Data Available for Compliance Survey Planning

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 from previous phases as part of <u>compliance survey planning</u>

QA Assessment and DQA applied to data collected during compliance phase



Data Quality in VSP

- Current capabilities
  - Outlier detection
  - Tests of distributional assumptions
  - Retrospective power curves for Sign and Wilcoxson Rank Sum (WRS) tests
- Additional tools for subsurface (code base, user interface, plots, etc.)
  - Activating the z-coordinate
    - ✓ Track borehole/well labels as well as location and time (label, x, y, z, t)
    - ✓ Identify or import vertical dimension data associated with dose/risk models for subsurface volumes (e.g., soil and rock stratum boundaries, aquifer locations and dimensions, and layers)
  - Data processing
    - ✓ Unit conversion capability
    - ✓ Allow data from disparate sensor platforms to be labeled as such & combined for analysis
  - Data visualization & analysis
    - ✓ Identify instrument and field of view to combine data from multiple sensor platforms and/or sensors
    - ✓ Identify sample matrices (e.g., groundwater, surface water, soils)
    - ✓ Identify sensor platforms (e.g., type & source of subsurface geophysical survey data)

SUBSURFACE SURVEY PLANNING & ANALYSIS

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

Compliance Survey Planning

- Leverage historical locations in compliance survey design
  - Start with convenience, judgmental, geophysical model-based locations
  - Add randomly sampled locations based on statistical models

Classical approaches (parametric or non-parametric)

- Stratified random/systematic: use risk & geophysical models 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
- Check & cover: convenience + random
  - Specify the number of convenience locations
  - VSP provides random locations

Geostatistical approaches

- Determine mathematically where to locate samples based on geostatistical uncertainty
- Incorporate geophysics input through
  - Bayesian methods
  - Geospatial/kriging methods combine data with different fields of view or uncertainty
    - Fixed rank kriging
    - Generalized least squares (GLS) models include geophysical information through covariates
- Uncertainty from these models can guide sample placement
  - Identification of strata, sample allocation across strata
  - More sample locations allocated to regions of higher uncertainty

Compliance Survey Planning (cont.)

- Geostatistical approaches
  - Determine mathematically where to locate samples based on geostatistical uncertainty
  - Incorporate geophysics input through
    - ✓ Bayesian methods
    - ✓ Geospatial/kriging methods that combine data with different fields of view or uncertainties
      - Fixed rank kriging
      - Generalized least squares (GLS) models that include geophysical information in covariates
  - Uncertainty from such models guides sample placement
    - ✓ Identification of strata, sample allocation across strata
    - ✓ More sample locations allocated to regions of higher uncertainty

Statistical Analysis for Compliance

- Subsurface volume mean concentration (or other metrics) estimation and hypothesis testing to compare estimates to a threshold
- "Classical" approaches
  - Independence assumption violated
  - Increases Type II error if spatial correlation is not incorporated
    - ✓ Type II error = incorrectly concluding a clean site is dirty
    - ✓ Leads to increased/unnecessary remediation
- Mathematically model the spatial correlation
  - If not present, use "classical" approaches
  - Parametric and non-parametric methods to model spatial correlation

Statistical Analysis for Compliance (cont.)

- Geostatistical methods to identify and determine boundaries of elevated residual activity
  - Integrate geophysical data into analysis and hypothesis testing
    - ✓ GLS
  - Determine if spatial correlation exists
    - ✓ Moran’s I and Local indicator of spatial association (LISA) statistic
  - Kriging
    - ✓ Indicator, Empirical Bayes, Fixed rank kriging (FRK)
  - Geostatistical simulation

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 fully representative
  - 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 & other early phases more so than compliance phase
  - To the extent that such AI/ML models can be updated with new assumptions after remediation phase, predictions can play a part in compliance phase survey planning

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Thank you