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Characterization: Dealing With Uncertainty

KHNP Training Program
Module 4: Repository Siting and Characterization

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Outline

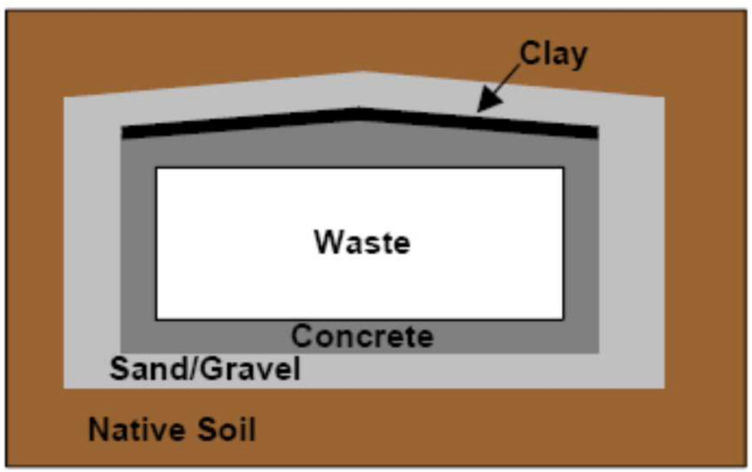
- Review of requirements for geologic disposal
- Key uncertainties and investigation techniques
- Brief tour of uncertainty
- Formal methods for dealing with uncertainty in model building
- Iterative refinement

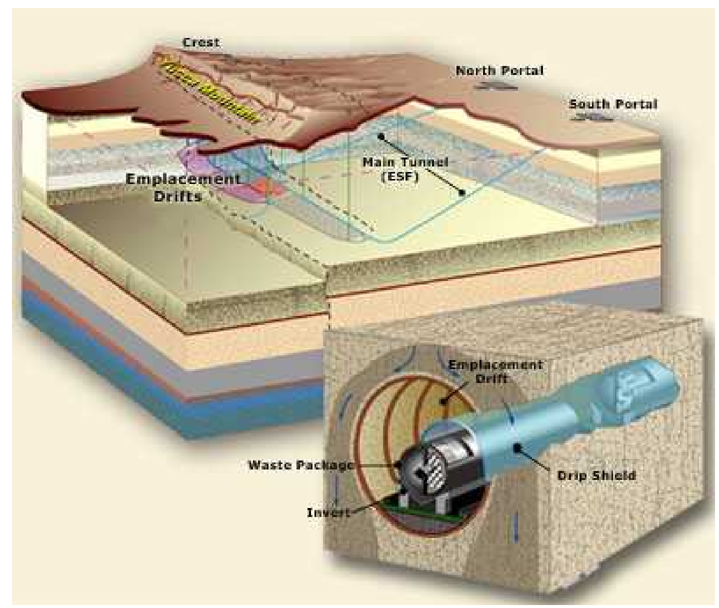
Functional Requirements for Geologic Disposal

- No releases (at hazardous levels) into biosphere
- Isolation for sufficient period of time
  - from human activity
  - from catastrophic natural events
- Disposal technology must be available at acceptable cost
- Retrieval technology must be feasible (optional)
- Processes that determine performance must be well-characterized
  - models and data sufficient to reliably demonstrate predicted performance
  - uncertainty reduced to manageable level

Defense-in-Depth: Multiple Barrier Concept

- Waste form (engineered)
- Waste container/canister (engineered)
- Backfill/buffer (engineered)
- Geosphere (natural)





Multiple Barriers: Functions

- Waste form
  - restricts releases
- Waste container/canister
  - prevent/reduce contact with water
  - favorable chemical environment (short-term)
- Backfill/buffer
  - prevent/reduce contact with water
  - delay/restrict release (diffusion)
  - favorable chemical environment (short-term)
- Geosphere
  - retard transport
    - slow flow/long travel times
    - diffusion and dispersion
    - Sorption/immobilization
  - favorable chemical environment (long-term)
  - stable geologic conditions

Key Uncertainty – Waste Form Performance

- Depends on materials and design
  - cements, ceramics, glass, SNF, polymer resins, bitumen
- Mechanical properties
  - fracture resistance, thermal properties
- Reactivity/stability
  - dissolution, weathering, leaching
- Typical characterization strategy
  - laboratory experiments to estimate material properties (surrogates for SNF), build models
  - underground investigations, modeling to estimate potential physical and chemical environments

Key Uncertainty – Waste Container Performance

- Depends on materials and design
  - alloy, wall thickness, welds
- Mean time to containment failure
- Distribution of containment failure over time
- Mode of containment failure
  - general corrosion
  - localized corrosion (pitting, stress corrosion cracking, inter-granular corrosion
  - other (seismic?)
- Typical characterization strategy
  - laboratory experiments to estimate material properties, build models
  - underground investigations, modeling to estimate potential physical and chemical environments

Key Uncertainty – Backfill Performance

- Depends on materials and design
  - cements, clays, crushed rock
  - barrier, divert water, reduce settling/motion, conduct heat
- Mechanical properties
  - swelling, plasticity, bearing capacity, thermal conductivity
- Hydraulic properties
  - Hydraulic conductivity, filtration coefficient
- Chemical properties
  - Retardation/sorption, buffering capacity
- Typical characterization strategy
  - laboratory experiments to estimate material properties, build models
  - underground investigations, modeling to estimate potential physical and chemical environments

Key Uncertainties – Geosphere

- Depends upon type of geologic formation
  - crystalline (granite), salt dome, bedded salt, mudstone/shale, basalt, volcanic tuff
- Hydrogeologic conditions
  - "dry", saturated (diffusion), saturated (fracture flow)
- Chemical conditions
  - active control of oxidation potential, buffering of oxidation potential and/or pH, no buffering
- Near-field environment
  - behavior influenced by presence of repository and/or waste
- Far-field environment
  - behavior controlled by natural conditions

Near-Field Investigation

- **Underground Research Laboratory**
- **Detailed characterization of rock mass within repository volume**
- **Large-scale *in situ* experiments**
  - **groundwater flow experiments**
  - **geochemical and transport experiments**
  - **measure response of host rock to excavation**
  - **measure response of host rock to waste emplacement (thermal stress)**

Far-Field Investigation (I)

- Groundwater flow and radionuclide transport typically area of greatest of uncertainty
- Complexity
  - fractures, fracture zones, faults
  - lithology/mineralogy changes
- Heterogeneity/spatial variability
  - hydraulic conductivity
  - dispersion
  - retardation

Far-Field Investigation (II)

- Field investigations
  - geologic mapping
  - surface geophysical surveys
  - exploratory drilling
  - borehole geophysical investigation
  - groundwater flow mapping, age dating
  - groundwater sampling
  - aquifer testing
  - tracer tests
- Laboratory investigations
  - detailed lithology/mineralogy
  - geochemistry
  - core-scale hydraulic and transport
- Model building

Brief Tour of Uncertainty

- **Aleatory uncertainty**
  - irreducible uncertainty, inherent randomness, future events
  - examples: future climate, precipitation, human activities

- **Epistemic uncertainty**
  - reducible uncertainty, lack of knowledge about system
  - examples: material properties, model structure, model parameters, heterogeneity

Aleatory Uncertainty

- Characterize/model uncertainty in process
  - investigate natural analogs
  - investigate past behavior
- Multiple models
  - develop alternative scenarios
    - human activities
    - climate
  - develop alternative models
    - undisturbed behavior
    - disturbed behavior

Epistemic Uncertainty

- Model structure (governing equations)
  - correct processes correctly modeled?
- Model domain and discretization
  - system well-defined?
  - appropriately resolve key processes?
  - layering?
- Model boundary and initial conditions
  - influence of boundaries?
  - how well are initial conditions known?
- Model inputs (parameters)

Quantifying and Reducing Uncertainty

- Sensitivity Analysis
  - determine appropriate spatial and temporal resolution
  - investigate sensitivity to initial and boundary conditions
  - identify sensitive parameters
- Model Calibration
  - hand calibration
  - automated parameter estimation via inverse problem (PEST)
  - generalized Likelihood Uncertainty Estimation (GLUE)
- Monte Carlo Simulations
  - forward simulations with models that meet calibration criteria

Epistemic Uncertainty

- For a given model
  - uncertainty/Sensitivity analysis
    - guide collection of new data
  - model calibration
    - reproduce observed behavior at site/regional scale
- What about uncertainty in model structure?
  - generalized likelihood uncertainty estimation (GLUE)
  - multi-model ranking and inference (MMRI)
  - model averaging

GLUE Methodology

- Choose model structure(s) for the system
- Choose ranges and prior distributions for the parameters to be identified
- Use Monte Carlo simulations to choose feasible parameter sets
  - use sampling to construct parameter sets
  - run simulations for all feasible parameter sets
- Evaluate a likelihood measure comparing simulation results with available knowledge of observations (i.e. match with present landscape)
- Reject nonbehavioral models and parameter sets
- Use likelihood weights associated with each model retained to form nonparametric distribution functions for predicted variables

Multi-Model Ranking

- **Akaike Information Criteria**

$$AICc = n\log(\sigma^2) + 2k + \left(\frac{2k(k+1)}{n-k-1}\right)$$

n = # of observations; *s2* = residual variance = *WSSR/n;* *k* = # of parameters

- **Ranking by simple difference, model probabilities, or evidence ratios**
- **Questions:**

1. **What if one model is not overwhelmingly best?**
2. **What if all models show high variability around a prediction?**

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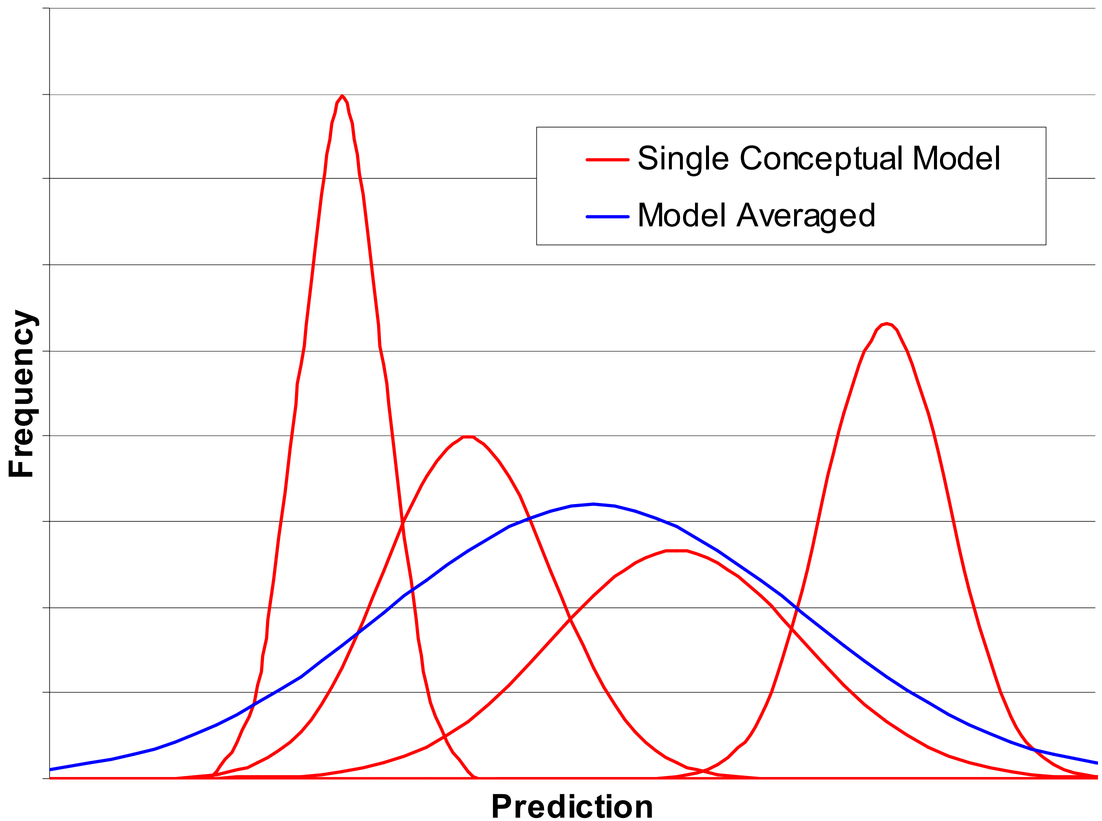
Multi-Model Averaging

- **Compute an estimate of the predicted and parameter values by weighting the model predictions:**

$$\hat{\bar{y}} = \sum_{i=1}^{R} w_i \hat{y}_i \qquad \hat{\bar{\beta}}_j = \sum_{j=1}^{R'} w'_j \hat{\beta}_{j,i}$$

- **Allows estimation of optimal parameter values and predictions from multiple models**
- **Can predict multi-model variance**
  - **provides bounds on possible parameter values**
  - **can compute confidence intervals**

Multi-Model Averaging

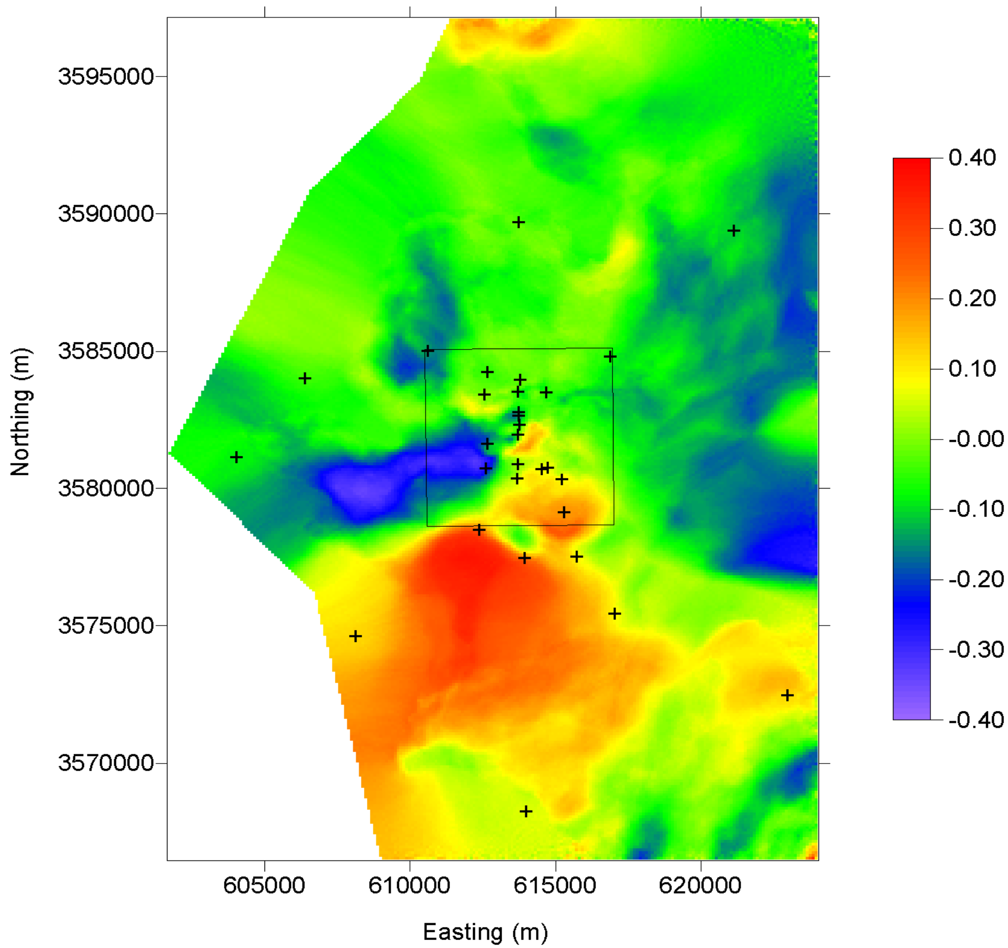


Iterative Refinement: Big Picture

- Phased site selection and characterization
  - site selection program
    - 1 or more sites selected
  - phase 1 site characterization
    - regional scale
      - climate, geology, groundwater hydrology
  - phase 2 site characterization
    - local scale
      - precipitation patterns, detailed stratigraphy and structure, infiltration, groundwater paths, flow velocities
  - phase 3 site characterization
    - repository scale
      - interaction of repository and waste with local conditions

Iterative Refinement: WIPP Hydrology Example

- Given existing site information and models, investigate sensitivity of travel-time predictions to key model inputs (sampling-based sensitivity)
- The sign of the rank correlation coefficient (RCC) indicates the sign of the correlation between head and travel time
- Regions of greatest sensitivity of travel-time to head estimates are to south of WIPP site and to west of WIPP site
- Use as a guide to collecting additional head data



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