SAND2010-3950C

Advanced Conceptual and Numerical Methods for Modeling Subsurface Processes Regarding Nuclear Waste Repository Systems

IAEA Network of Centers of Excellence

Sandia National Laboratories

Far-Field Modeling and Radionuclide Transport

Conceptual Model Development, Interface with Site Characterization, and Performance Assessment

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Outline

- Performance Assessment methodology
- Defining modeling objectives
- Conceptual model development
- Interface with site characterization
- Assessment of uncertainty and variability
- Numerical model implementation
- Interface with performance assessment and model abstraction

Performance Assessment Methodology

- There are three primary technical roles in the development of a nuclear waste repository:
  - Site characterization
  - Repository design
  - Performance Assessment
- Technical and programmatic integration among these groups is vitally important to successfully select and investigate a site, and license and operate a repository.

Performance Assessment Methodology

- There are numerous obstacles to successful integration between these groups.
  - Lack of consensus regarding the overall framework for completing the tasks of repository development
  - Contrasting cultures among the three groups (e.g., engineering perspective vs. scientific research perspective)
  - Organizational separation of the three groups
  - Physical separation of the three groups
  - Competing budgetary goals

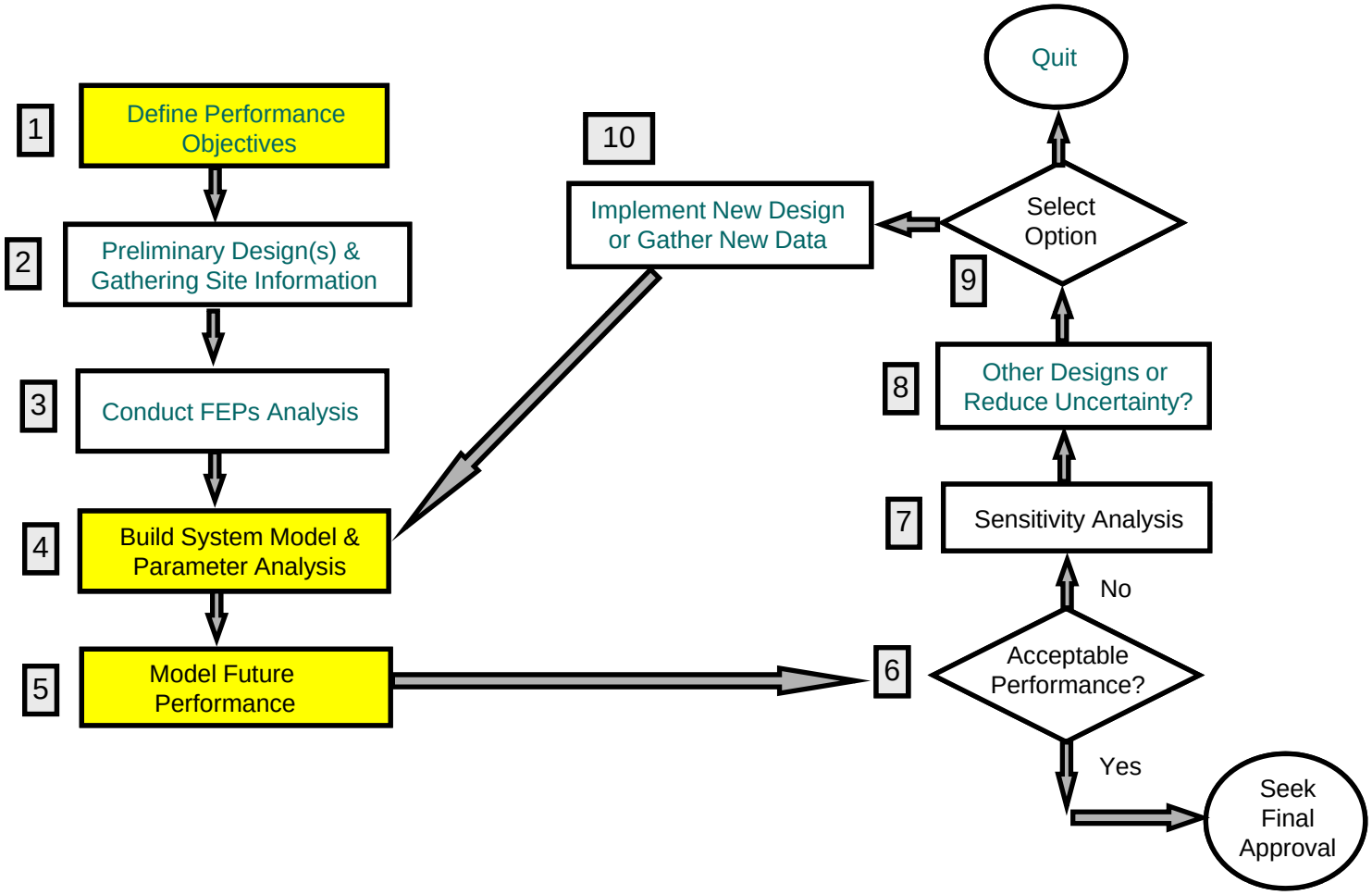
Performance Assessment Methodology

- Potential solutions to these obstacles can be both formal and informal in nature.
  - Interaction between managers from the three groups is necessary to negotiate goals, strategy, schedules, etc.
  - Formalized interactions between technical staff from the groups in the form of technical exchanges and workshops should be arranged
  - Collaborative work between groups should be encouraged wherever possible
  - Each group should have some expertise in other areas (e.g., uncertainty analysis in site characterization)

Performance Assessment Methodology

- Performance assessment (PA) methodology can form the framework around which integration among repository design, site characterization, and PA groups can be organized.
- The iterative nature of the PA process provides an opportunity for collaboration and updating of information exchanged among the groups.
- The roles, responsibilities, and authorities for each of the three groups can be defined for each step in the PA process.

Performance Assessment Methodology



Defining Modeling Objectives

- Ideally, performance objectives are taken directly from legal regulations governing the repository.
- The performance assessment group designs the analyses to simulate the quantities specified in the regulations (e.g., radiological dose to the receptor group or maximum groundwater concentrations).
- The site characterization group should translate these performance objectives into surrogate, intermediate performance metrics at the sub-system level (e.g., transport time in the saturated zone).

Defining Modeling Objectives

- All participants must know the performance objectives and understand the relevance of their research or analyses to those objectives.
- In the earlier stages of a repository program specific regulations may not exist and participants can contribute to formulation of the regulations
  - The site characterization group can provide site-specific information that constrains regulations.
  - The performance assessment group can provide information on the technical feasibility of analyzing a particular performance metric

Conceptual Model Development

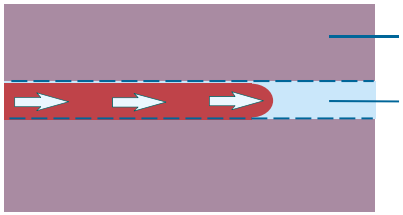
- Conceptual model development is one of the most important components of groundwater flow and radionuclide transport modeling because of the limits that may be placed on the resulting numerical model.
- The FEPs analysis is a way of formalizing the contents of the conceptual model of the repository system.
- The importance of the FEPs analysis and its relationship to conceptual model development, but may not be fully appreciated by the site characterization and repository design groups.

Conceptual Model Development

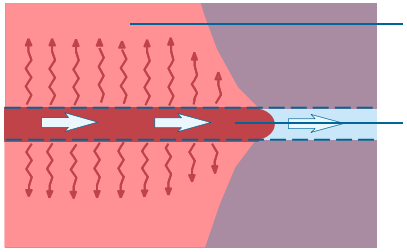
- Groundwater flow processes
  - Porous medium, fracture network, or dual permeability
- Radionuclide transport processes
  - Single porosity or dual porosity
  - Colloid-facilitated transport
- Boundary conditions
- Hydrogeologic framework model
- Dimensionality of the model
- Initial conditions
- Steady-state versus transient flow conditions
- Impacts of future climatic conditions

Conceptual Model Development

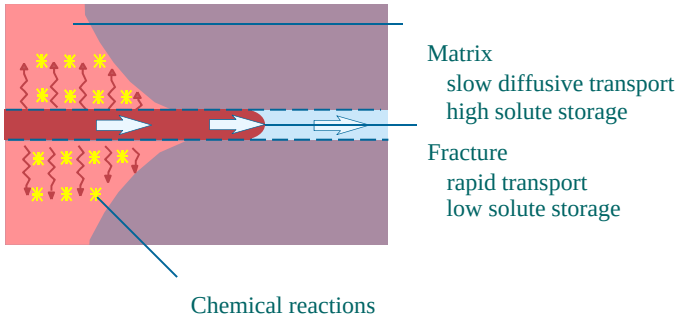
Fracture-Only Transport



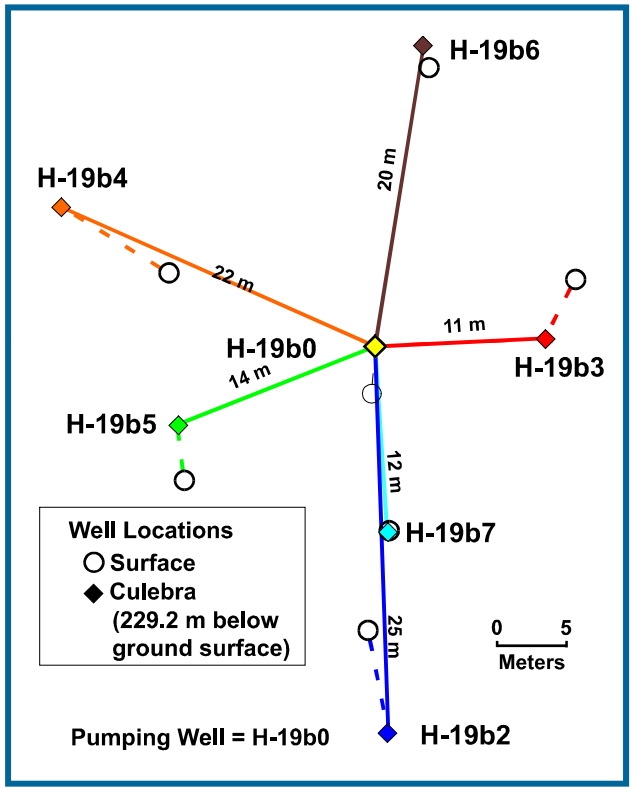
Double-Porosity Nonreactive Transport (Physical Retardation)



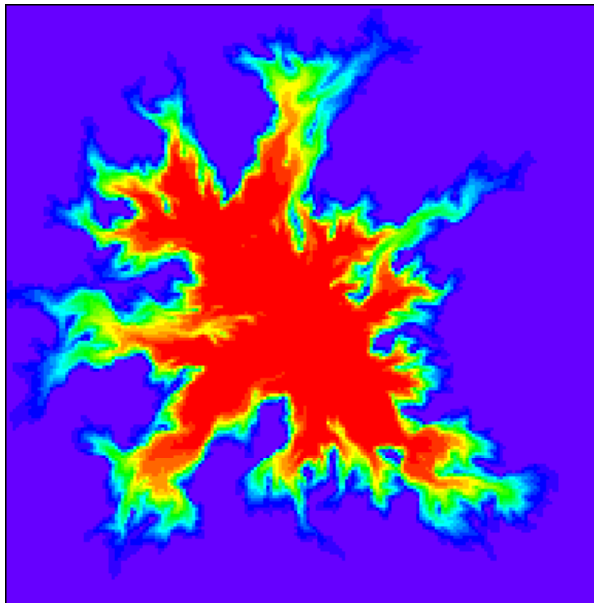
Double-Porosity Reactive Transport (Physical and Chemical Retardation)



Conceptual Model Development



Well layout for 7- well convergent flow tracer test

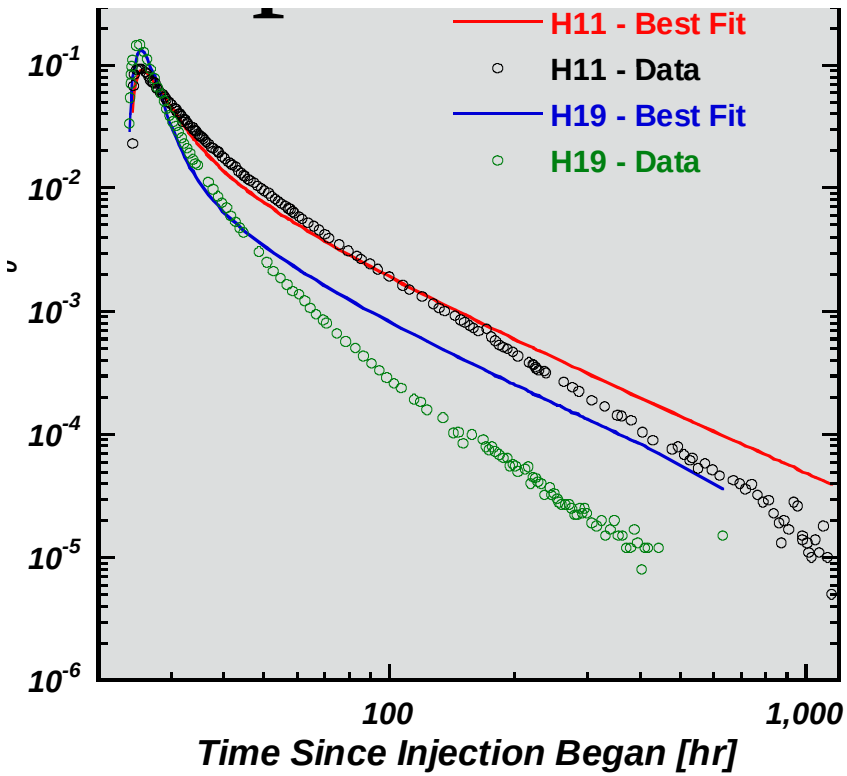


Numerical simulations for design of single-well injection/withdrawal tracer test

Conceptual Model Development

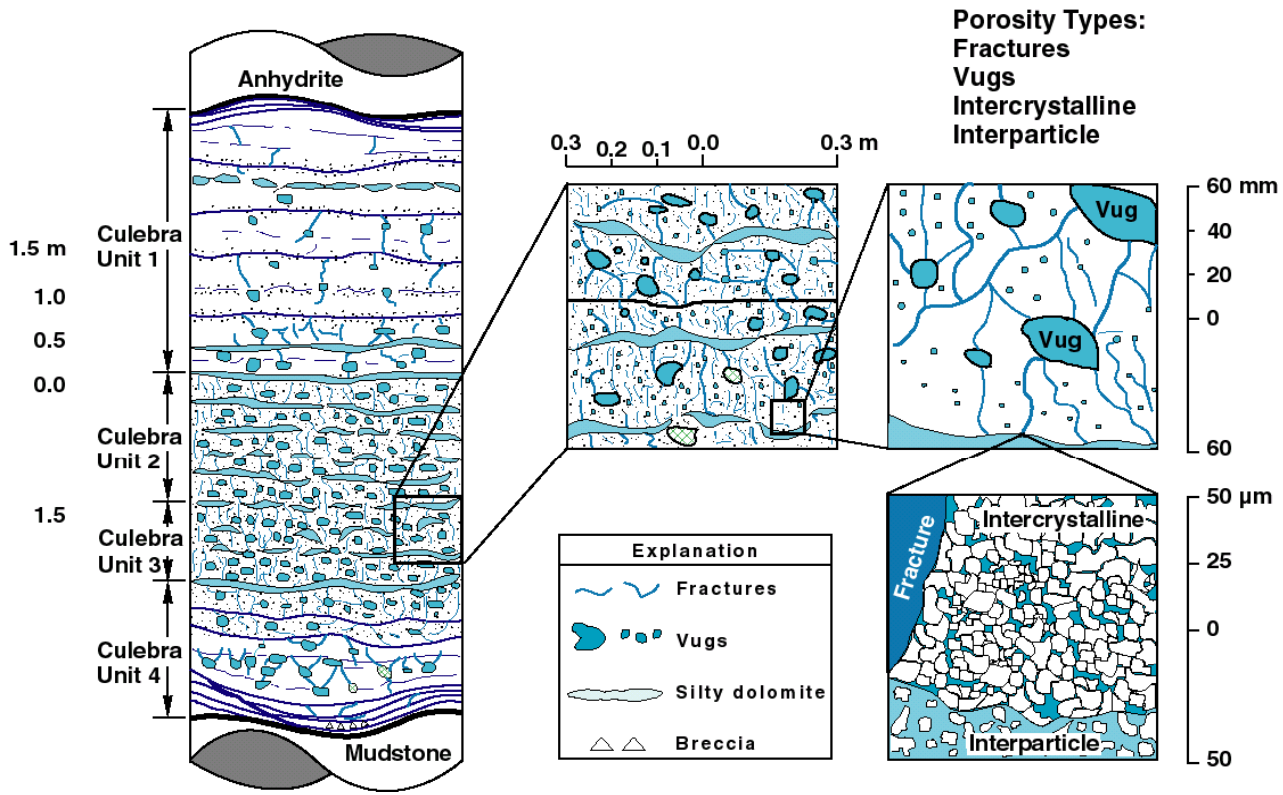
Single-Well Injection-Withdrawal tracer tests proved most effective for characterizing diffusion parameters

Single-diffusion rate model cannot capture tailing behavior



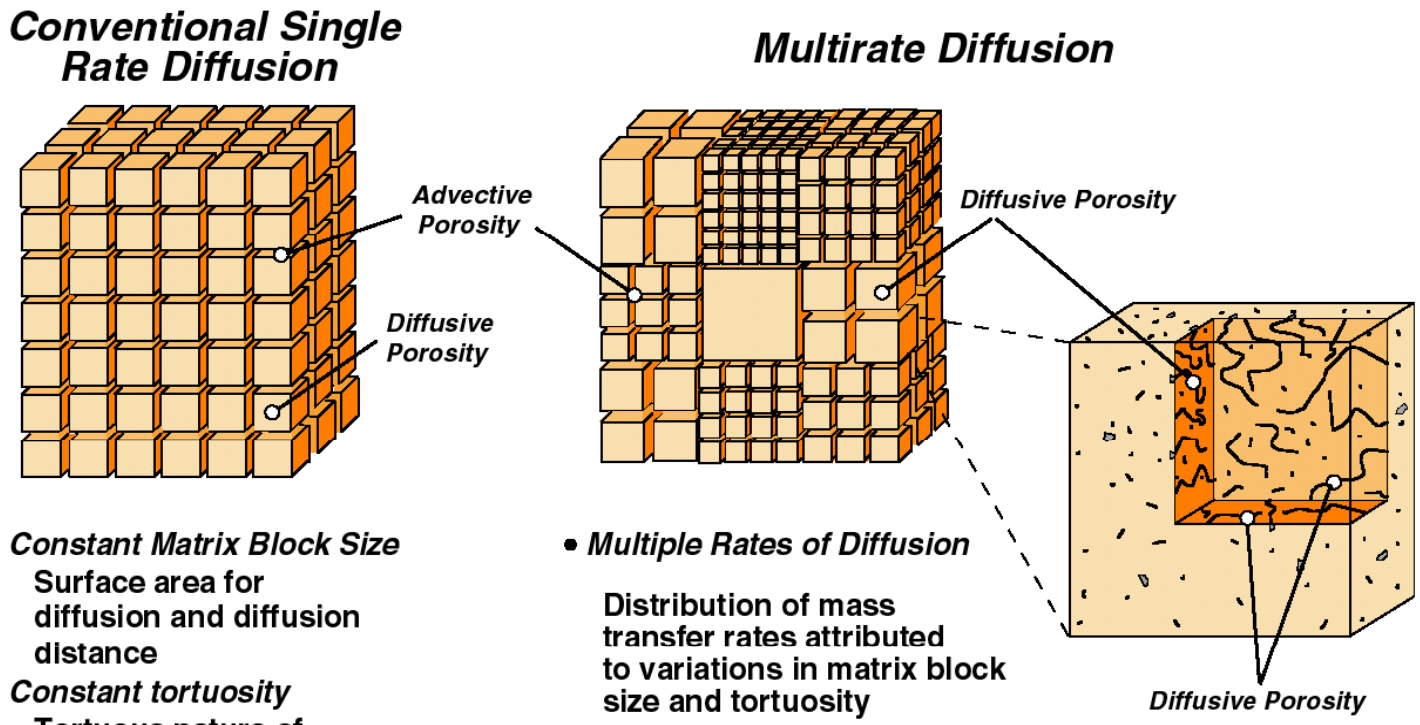
Conceptual Model Development

Refined Conceptual Model of Geology



Conceptual Model Development

Multirate Diffusion Model Conceptualization

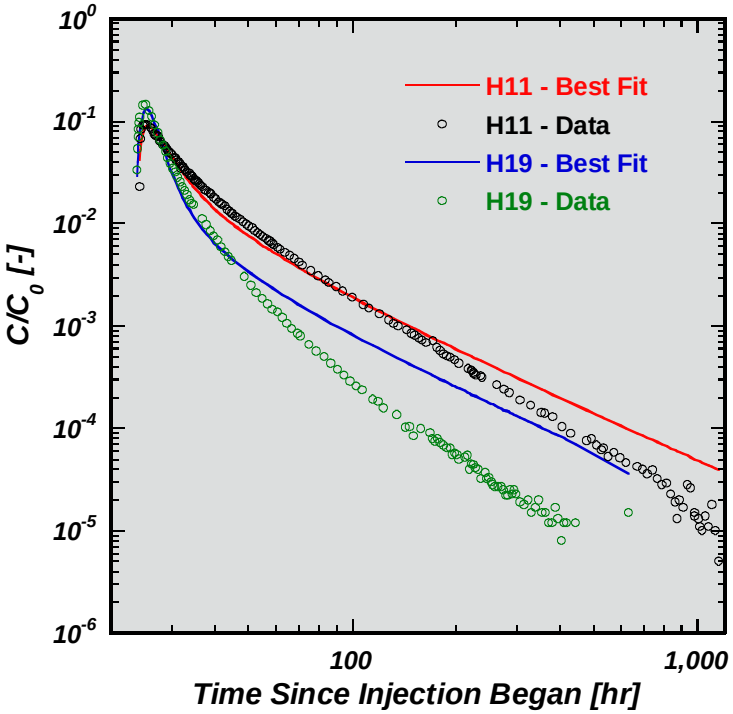


- *Constant Matrix Block Size*
  Surface area for diffusion and diffusion distance
- *Constant tortuosity*
  Tortuous nature of "matrix" pores

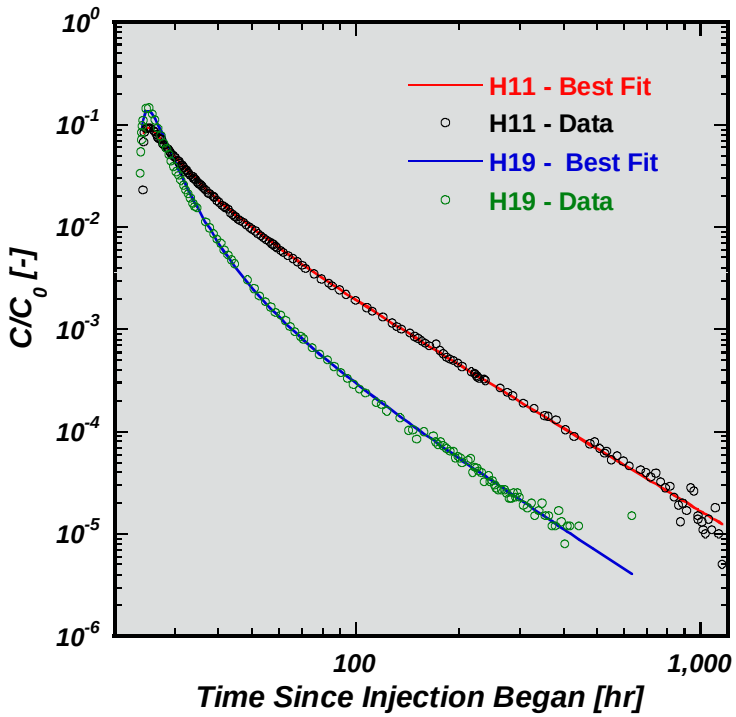
- *Multiple Rates of Diffusion*
  Distribution of mass transfer rates attributed to variations in matrix block size and tortuosity

Conceptual Model Development

Single-Well Injection Withdrawal Test Results



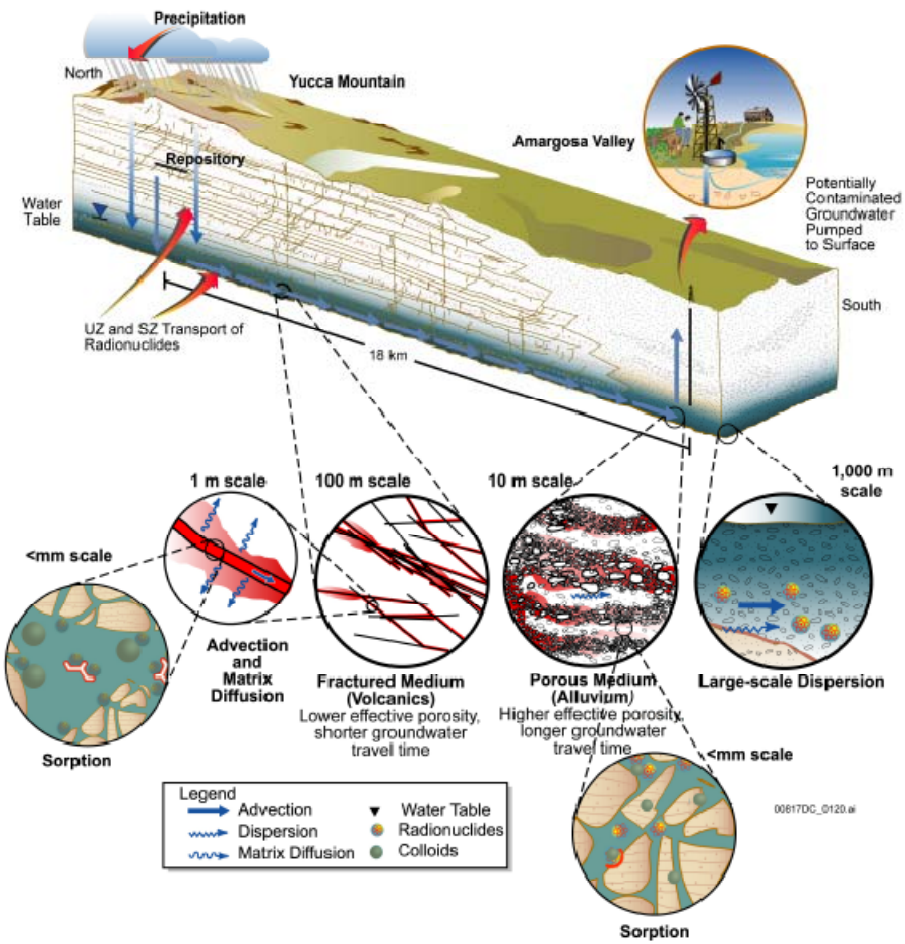
Single-diffusion rate model cannot capture tailing behavior



Multirate-diffusion model provides excellent fits throughout time range

Conceptual Model Development

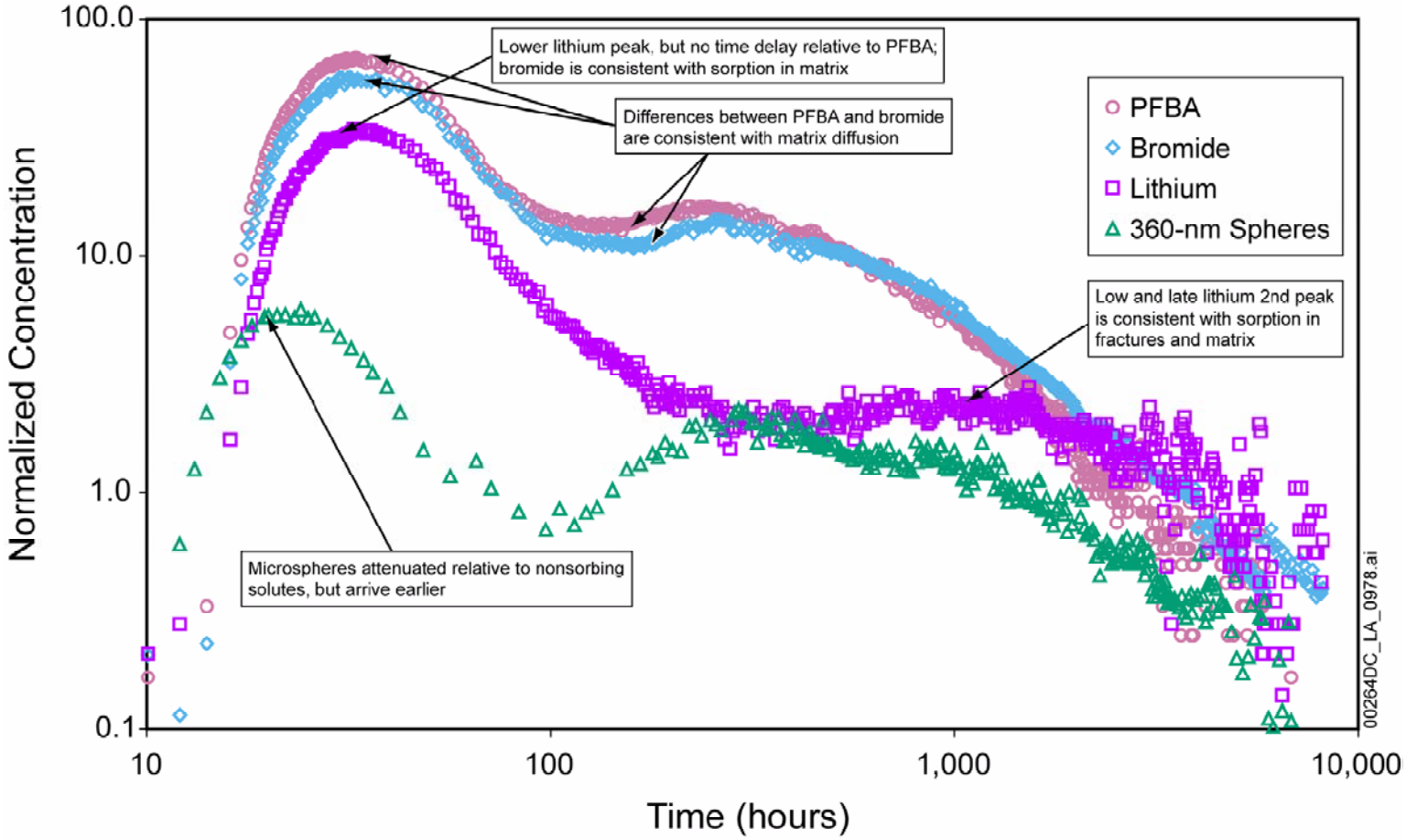
- Potential radionuclide releases enter the saturated zone at the water table beneath the repository
- Primarily horizontal groundwater flow would carry contaminants about 18 km for hypothetical discharge to the accessible environment via pumping
- Conceptual model of radionuclide transport includes the processes of advection, dispersion, matrix diffusion, sorption, colloid-facilitated transport, radioactive decay, and ingrowth



Conceptual Model Development

- Laboratory measurements of effective diffusion coefficient in tuff conducted with ^{3}H (as tritiated water), ^{99}Tc (as TcO_4^-), ^{14}C (as HCO_3^-), Br^-, and PFBA
- Effective diffusion coefficient varies as a function of:
  - Tuff matrix permeability
  - Tuff matrix porosity
  - Molecular weight and ionic radius
  - Temperature, viscosity of groundwater, and liquid saturation
- Field-scale (30 m distance), forced-gradient tracer testing conducted in fractured tuff at the C-holes complex using multiple tracers

Conceptual Model Development



Interface with Site Characterization

- Site characterization should be cautious about focusing attention on assumed dominant processes or pathways before performance assessment modeling is performed.
- For experimental guidance, performance assessment should use reasonable estimates of parameter and conceptual uncertainty and not conservative assumptions that may bias results towards preconceived ideas.
- Neither site characterization nor performance assessment should completely dominate iterative interactions.

Interface with Site Characterization

- Formalized integration between site characterization and performance assessment groups can be facilitated through workshops on major system components.
- Project management can enhance integration by encouraging collaboration between individual staff members from site characterization and performance assessment groups.
- Mutual technical review of project documentation by site characterization and performance assessment groups contributes to information exchange and consistency.

Assessment of Uncertainty and Variability

- The analysis of uncertainty includes consideration of alternative conceptual models and parameter uncertainty.
- The site characterization group plays a key role in the identification of alternative conceptual models for processes in the natural system.
- Alternative conceptual models must be considered when more than one valid interpretation of system behavior is possible from the existing data.

Assessment of Uncertainty and Variability

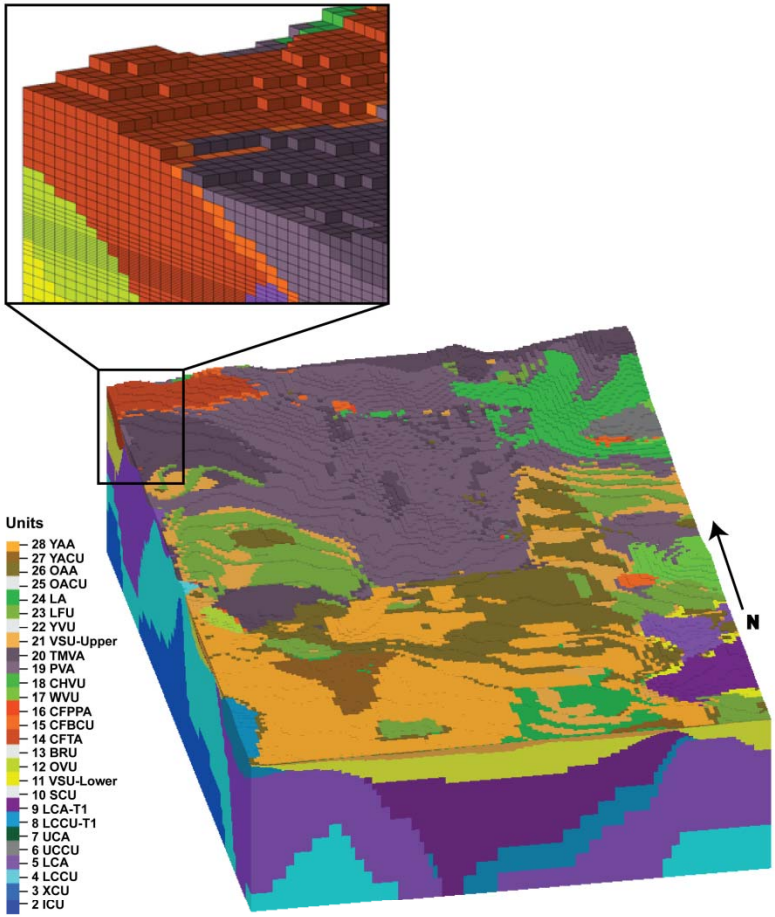
- Parameter uncertainty should be evaluated on a scale that is relevant to the model grid
- It is important to distinguish between parameter variability and parameter uncertainty
- Uncertainty and sensitivity analysis has been primarily based on TSPA model results; however, greater involvement of the site characterization groups can improve the analysis and “buy in” from these groups with regard to the analysis results
- Uncertainty and sensitivity analysis has the potential to be a unifying activity between site characterization and PA with regard to prioritization of work

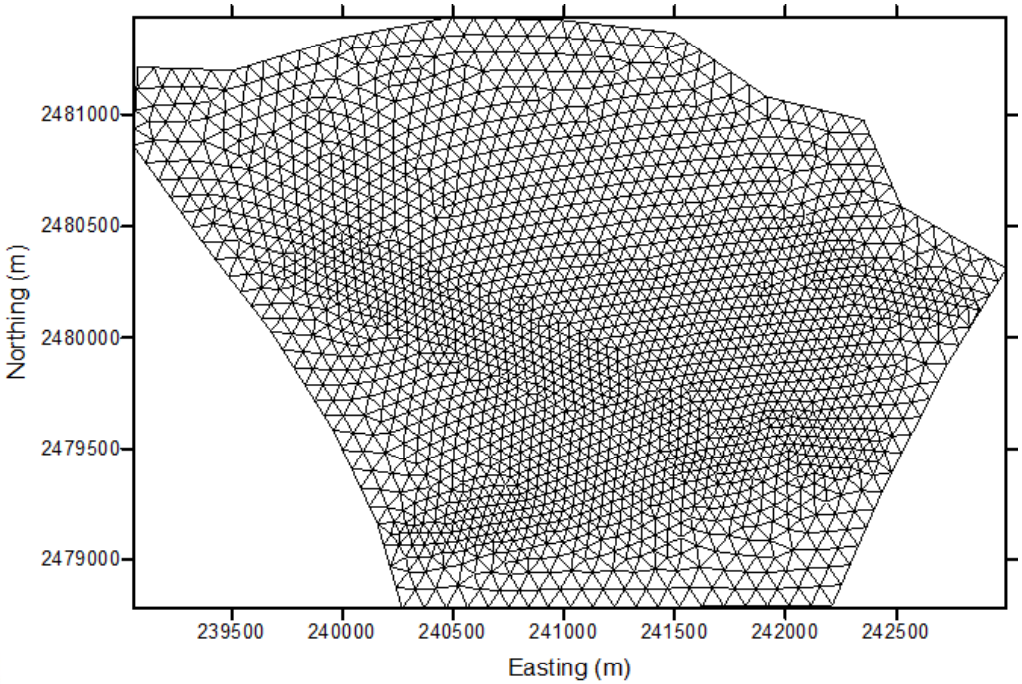
Numerical Model Implementation

- Choice of software code should be determined by the nature of the conceptual model:
  - Governing equations/ flow and transport processes
  - Numerical solution method (e.g., finite-difference versus finite-element methods)
  - Dimensionality
  - Flexibility in assigning boundary conditions, heterogeneous material properties, etc.
  - Confined versus unconfined groundwater flow system
  - Numerical accuracy (e.g., numerical dispersion in transport simulations in finite-difference versus particle-tracking methods)

Numerical Model Implementation

- Structured Versus Unstructured Grid

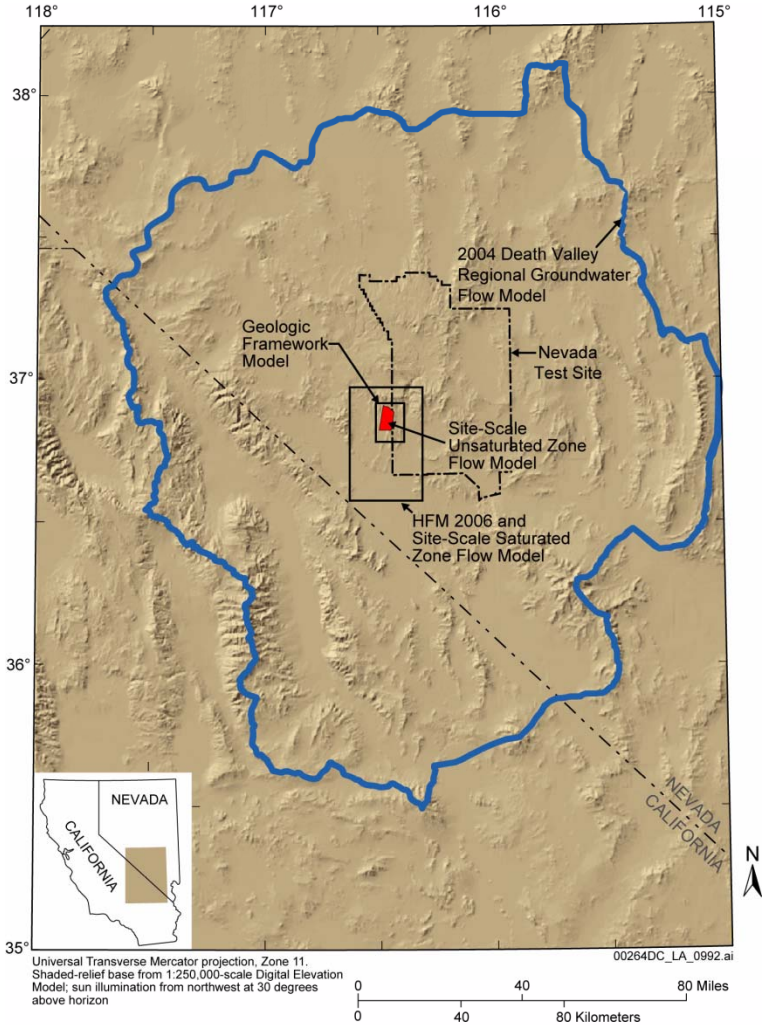




Finite-Element Grid

Numerical Model Implementation

- Regional-Scale and Site-Scale Flow Modeling

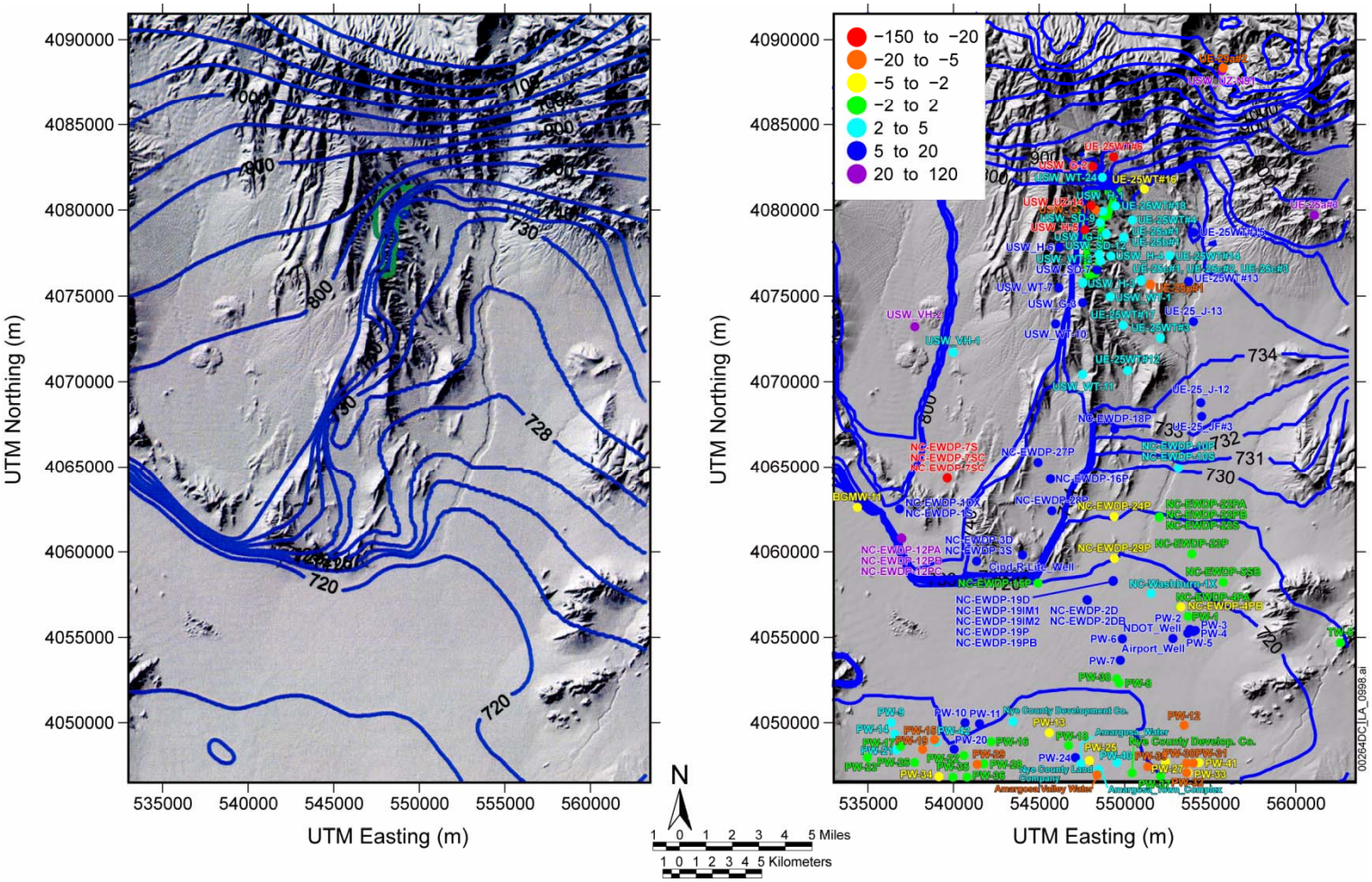


Numerical Model Implementation

- Model parameters are adjusted to match water-level and flow-rate observations during the model calibration process.
- Model calibration can be conducted using a trial-and-error process or using automated methods.
- Automated model calibration (inverse modeling) results in an optimal calibration and also provides valuable information on model sensitivities, correlations among input parameters, and uncertainty in calibrated parameters.

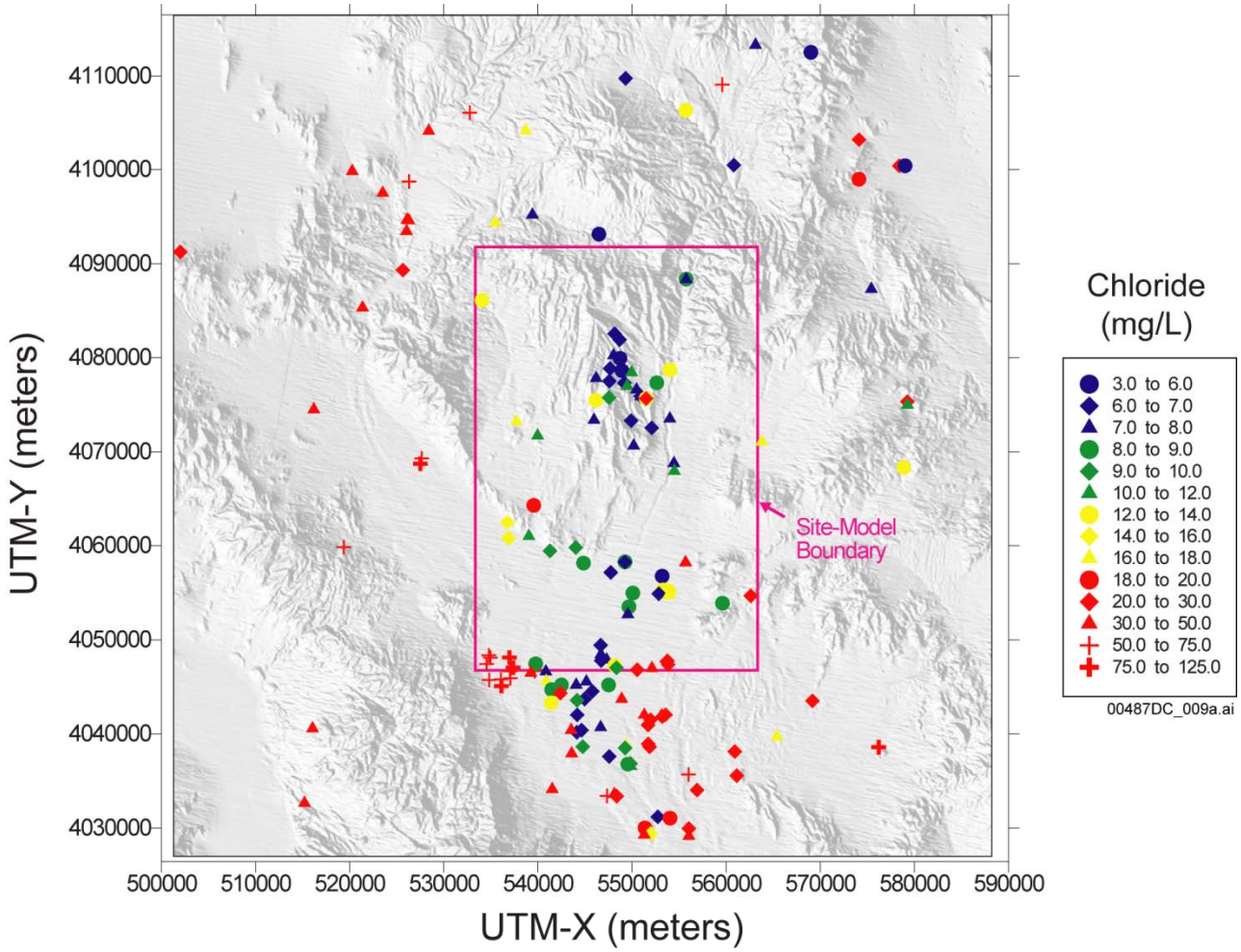
Numerical Model Implementation

- Model calibration



Numerical Model Implementation

- Model validation using hydrochemistry data



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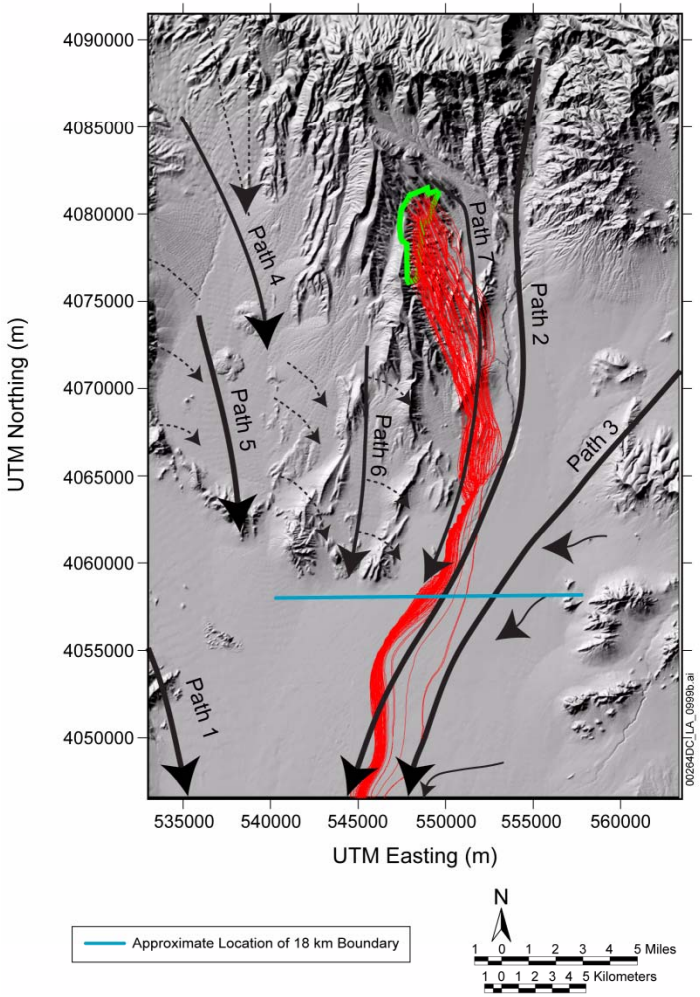
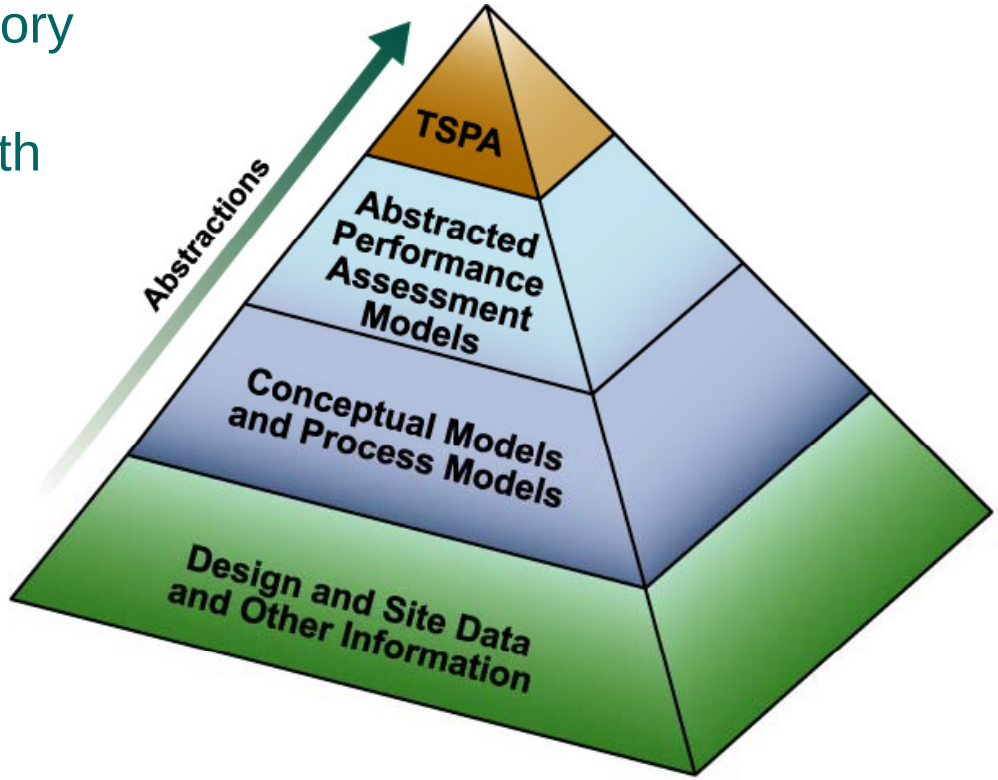


Interface with Performance Assessment

Representation of repository system becomes more focused and simplified with increasing abstraction.



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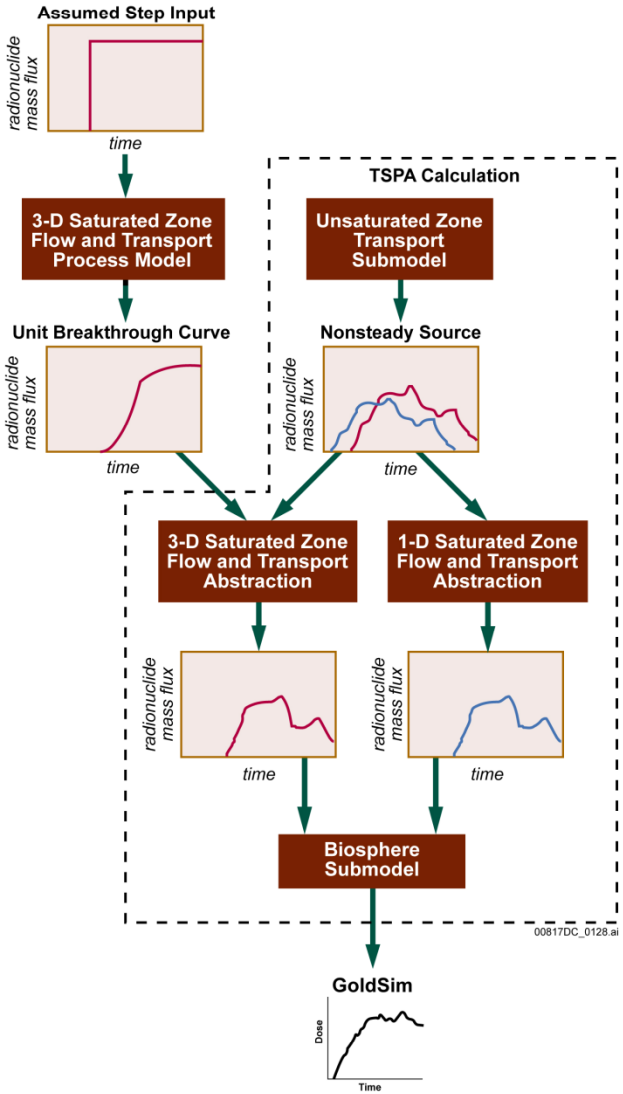
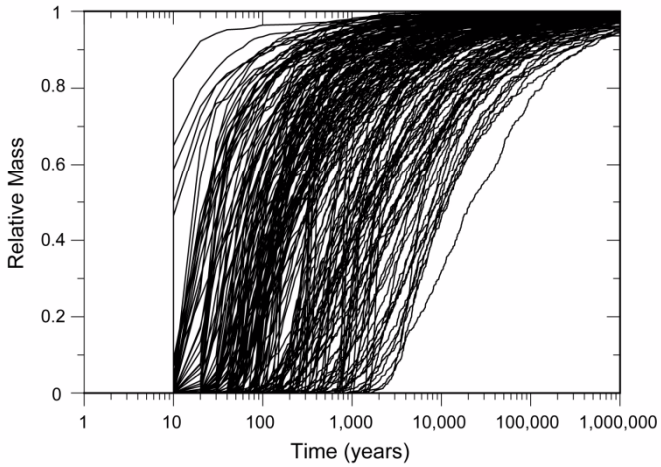
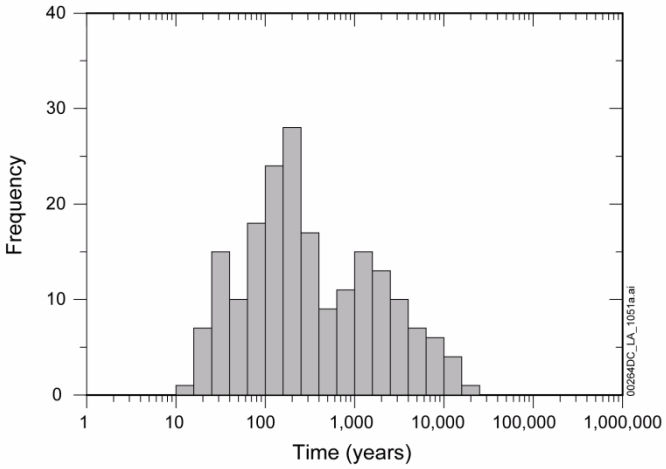
Interface with Performance Assessment

- Development of numerical models may occur at different levels:
  - Testing interpretation models (site characterization)
  - Sub-system models (site characterization and/or PA)
  - Total system performance assessment models (PA)
- Abstraction of sub-system models may be necessary for incorporation into the TSPA model.
- Abstractions may include reduction in dimensionality, simplified processes, look-up tables, etc.

Interface with Performance Assessment