General Training On Methodologies For Geological Disposal in North America

IAEA Network of Centers of Excellence

The Yucca Mountain Project – Computer Modeling of Ambient and Thermal Processes

Presented by:

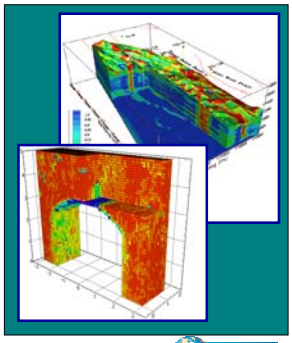
G.S. Bodvarsson, Lawrence Berkeley National Laboratory

OUTLINE

- Role of Numerical Models in YMP
- Forward and Inverse Modeling Capabilities
- Ambient Modeling Examples
  - Mountain-scale models
  - Drift-scale models
  - Design of laboratory experiment
- Thermal Test Models
  - TH models
  - THC models
  - THM models
- Concluding Remarks

Role of Process Modeling in Yucca Mountain Project

- Process understanding
- Test design
- Data analysis/ site characterization
- Predictive modeling
- Sensitivity analysis/ uncertainty analysis
- Basis for abstraction
- Basis for TSPA



TOUGH2 Family of Simulators

TOUGH: Transport Of Unsaturated Groundwater and Heat

multidimensional	1D, 2D, 3D
multiphase	liquid, gas, NAPL
multicomponent	water, air, VOC, radionuclides
nonisothermal	heat
flow and transport	multiphase Darcy law
fractured-porous media	dual-ϕ, dual-k, MINC, ECM

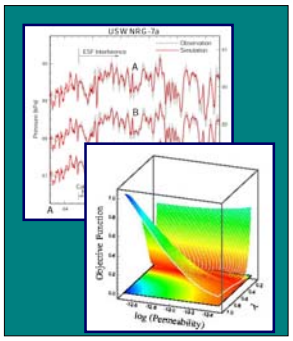
EOS: Accurate description of thermophysical properties

iTOUGH2 Summary Description

Provides inverse modeling capabilities for TOUGH2

Application Modes
- Sensitivity analysis
- Model calibration
- Uncertainty propagation

Features
- Multiple objective functions
- Multiple minimization algorithms
- Extensive error and uncertainty analysis

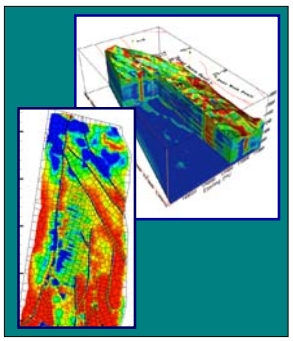


Mountain-Scale Model

Main Purpose
- Integrate all data collected for site characterization

Modeling Approach
- 3D dual-permeability model
- Variable infiltration
- Capillary-barrier effect
- Perched water
- Faults
- Based on laboratory data and calibrated against field data

Results
- ➢ Provides boundary conditions for drift-scale near-field models



Flow Focusing

Main Purpose

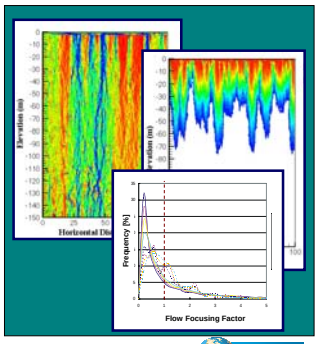
- Examine impact of heterogeneity on flow distribution

Modeling Approach

- Spatially correlated fracture permeability field
- High resolution (0.25 m, up to 2 million gridblocks)
- Flow and transport simulations: uniform at top → focused

Results

➢ Flow-focusing factors for drift-scale seepage models



Modeling of Ambient Geochemistry

Main Purpose

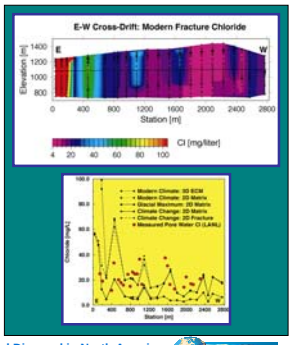
- Test predictive capabilities of mountain-scale model

Modeling Approach

- Infiltration model
- 3-D dual-permeability
- Coupled, nonisothermal flow and transport of aqueous and gaseous species
- Mineral-water-gas kinetic and equilibrium reactions

Results

- Predicted Chloride in ECRB
- Confirmed percolation flux estimates



Calibration and Prediction of Radon Concentration in ESF

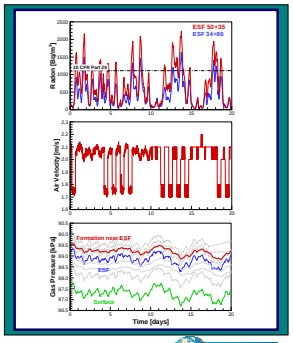
Objectives

- Estimate formation properties
- Examine probability of exceeding radon exposure limit along ESF

Mechanism

Radon accumulates along ESF as a function of:

- Ventilation regime
- Barometric pressure
- Formation properties



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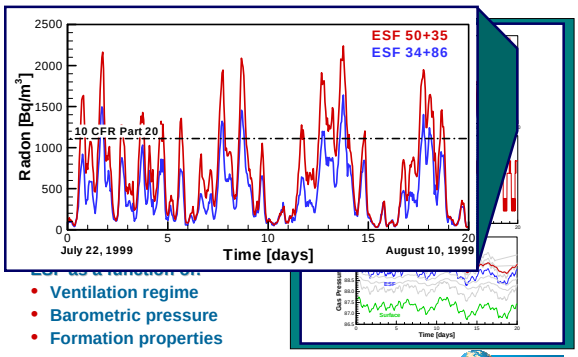

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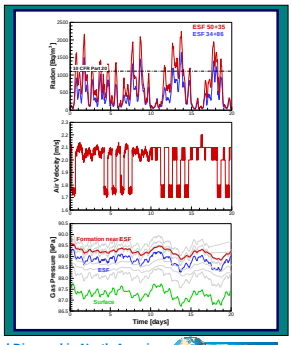

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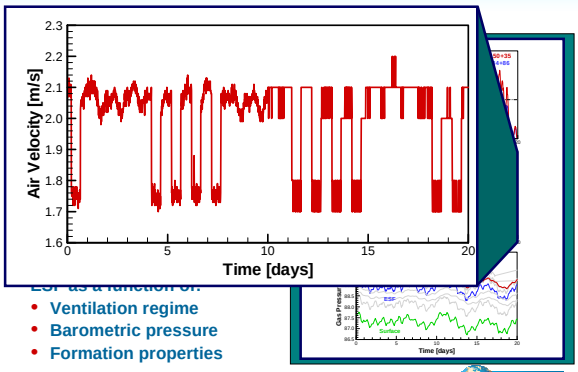

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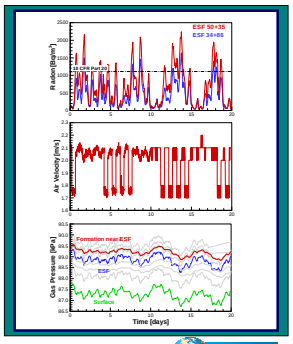

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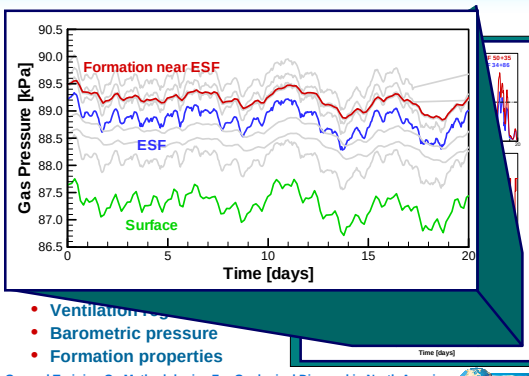

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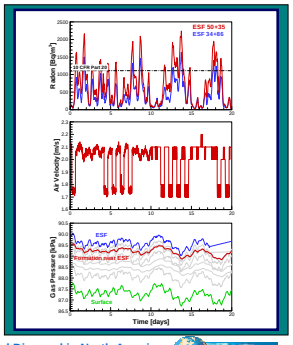


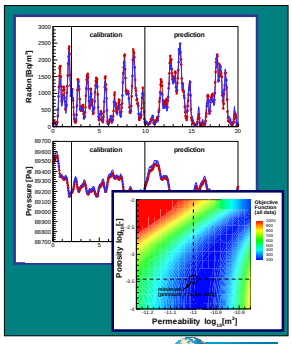
Calibration Against Radon and Pressure Data

Modeling Approach

- Developed gas flow and radon transport model
- Performed joint inversion of radon concentration and pressure data

Results

- Model accurately reproduces and predicts radon concentrations along ESF
- Estimated formation parameters and initial and boundary conditions



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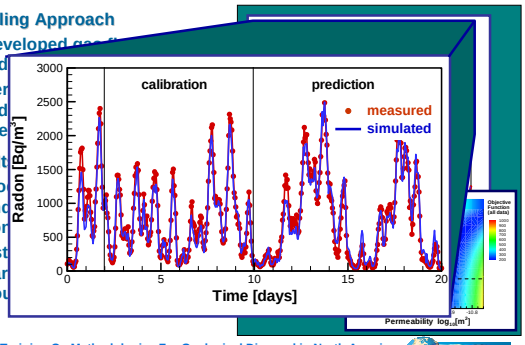

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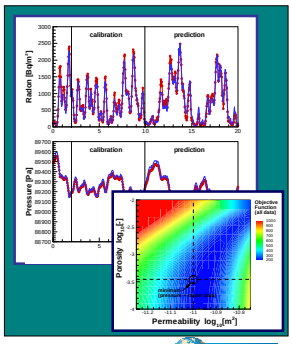

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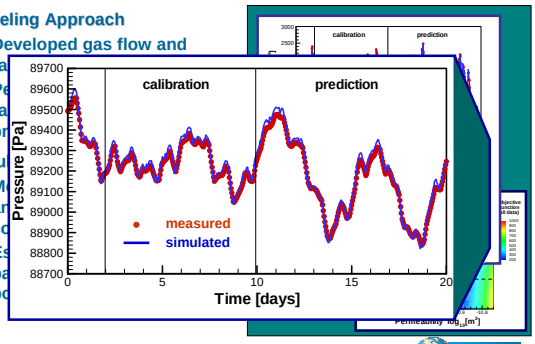

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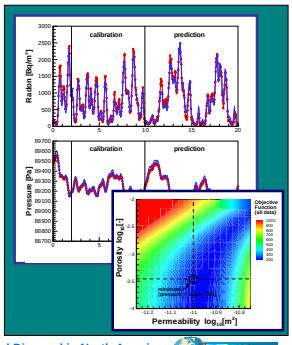

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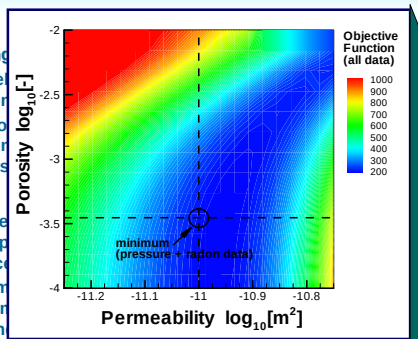

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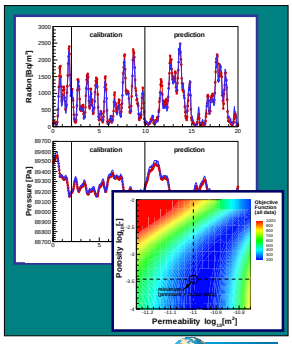


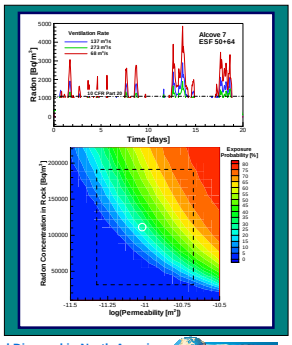
Prediction of Radon Exposure Risk

Predictions

- Predicted radon concentrations in ESF for different ventilation scenarios
- Examined probability of exceeding radon exposure limit

➢ Radon data suitable for estimation of large-scale formation parameters

➢ Numerical model used to:
  - Design ventilation system
  - Address health and safety issue



Construction Water Migration

Main Purpose

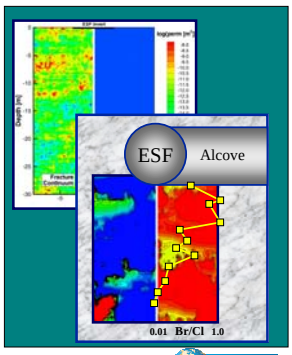
- Fracture/Matrix interaction
- Interpretation of geochemical data

Modeling Approach

- Heterogeneous fracture-matrix system (MINC)
- Ponded release of construction water
- Variability and uncertainty

Results

- Fast flow through fractures
- Consistent with Br/Cl data



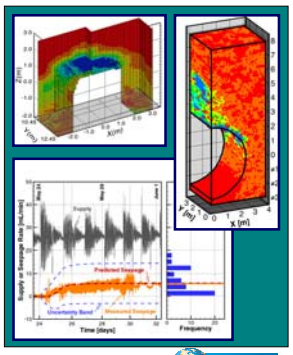
Drift Seepage

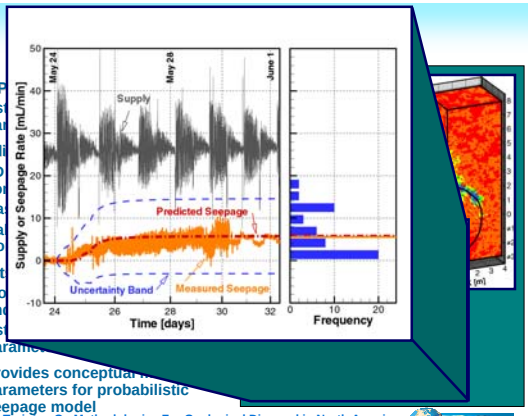
Main Purpose
- Estimate seepage-relevant parameters

Modeling Approach
- 3D heterogeneous fracture-continuum model
- Based on air-k data
- Calibrated against seepage data from liquid-release tests

Results
- Model accurately reproduces and predicts seepage data
- Estimated seepage-relevant parameters

➢ Provides conceptual model and parameters for probabilistic seepage model





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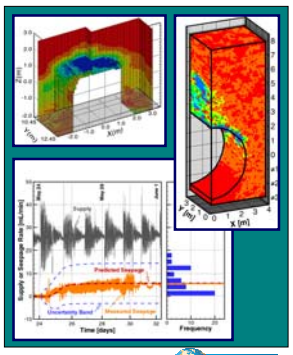


Design of Laboratory Experiment on Fractured Tuff Block

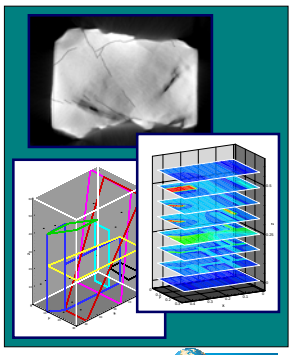
Main Purpose

- Preparation for validation experiments on 1-m^3 block (flow, transport, thermal)

Modeling Approach

- CT scans of 1-ft^3 block → fracture network
- Discrete fracture network model embedded in matrix
- Simulate proposed experiments
- Perform synthetic inversions to optimize test design

➢ Pretest modeling improves experimental design



Thermal Issues

The United States Civilian Waste Program does not call for reprocessing of spent fuel

Forced ventilation for 50 to 300 years following waste emplacement can remove ~ 70% of heat generated from the radioactive decay of the high-level nuclear waste

- Following cessation of ventilation and closure of repository, temperature in the repository can rise above boiling

Heat gives rise to coupling between thermal (T), hydrological (H), chemical (C) and mechanical (M) processes within the unsaturated rock mass

THCM processes affect the performance of the repository

- Potential seepage of water into waste emplacement drifts
- Chemistry of fluids that potentially enter the drift
- Transport of radionuclides, were they to escape the engineered barrier

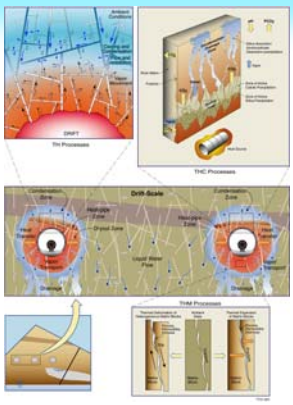
Thermal Tests at Yucca Mountain

Test Objective

- To acquire a more in-depth understanding of the coupled processes: THCM in the rock mass surrounding the proposed repository

Approach

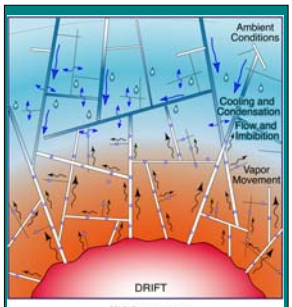
- Close integration of modeling and measurements
  - Pre-heat characterization to measure site-specific properties important for coupled processes
  - Model predictions prior to commencement of test
  - Use of early test results to discriminate alternative conceptual models applied in pre-test simulations
  - Continue interpretative analysis of measurements, refining the numerical model as needed



TH Coupled Processes

Heat Transfer
- Conduction, convection
- Counterflow of liquid and vapor – heat pipe

Moisture Redistribution
- Fast transport of vapor in fractures
- Condensation
- Imbibition into matrix
- Gravity drainage in fractures
- Drying front moves out from heat source with time
- As heat output declines, dryout zone contracts



TH Processes

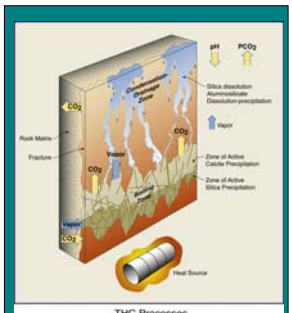
THC Coupled Processes

Reaction rates
- Generally increase with elevated temperatures

pH affected by
- CO_2 degassing and transport

Chemical evolution of waters, gases and minerals intimately coupled to TH processes
- Drying concentrates aqueous species in remaining liquid phase
- Pure water in condensation zones promotes dissolution of minerals

Mineral dissolution and precipitation
- Changes porosity and permeability
- Affects seepage into drifts
- Alters chemistry of water that could contact waste package



THC Processes

THC Coupled Processes

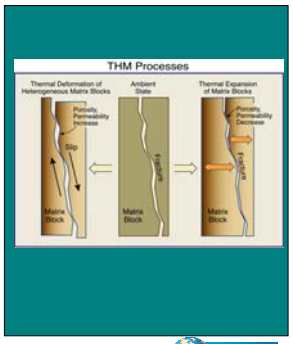
Thermal expansion and thermally induced stresses

Mechanical stresses and displacement

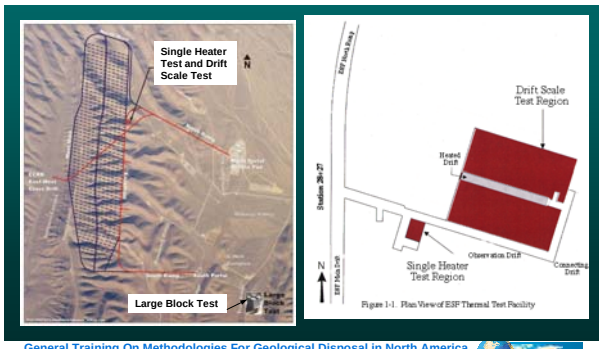
- Open or close fractures
- Change porosity
- Change permeability
- Affect flow and transport

Stress field surrounding emplacement drifts

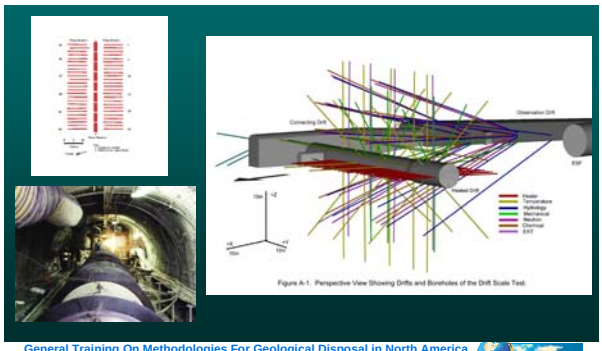
- Altered by heating and cooling cycles associated with the emplacement of waste



Yucca Mountain Heater Tests Sites



DST Test Block and Borehole Layout



Probing THMC Processes-Drift Scale Test

Pre-Test Characterization

Laboratory	Field
T-Properties	Rock Classification
H-Properties	Fracture Mapping
M-Properties	Borehole Videos
MIN/PET	Air Permeability
Pore water	

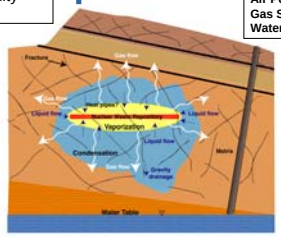
Periodic Active Testing during Heating and Cooling

GPR, Neutron log, ERT } Matrix Liquid Saturation

Air Permeability
Gas Sampling
Water sampling

Passive Monitoring during Heating and Cooling

- Temperature
- Displacement
- Strain
- Humidity
- Pressure
- Acoustic Emission (microfracturing)



Multiple Laboratory Test Team
(LBNL, LLNL, SNL, LANL)

Data shared among multi-lab Thermal Test Team
Berkeley team

- TH: Yvonne Tsang, Jens Birkholzer, Barry Freifeld, Sumit Mukhopadhyay
- THC: Eric Sonnenthal, John Apps, Mark Conrad, Nic Spycher
- Geophysics: John Peterson, Ken Williams
- Data: Melani Menendez-Barreto
- Preheat field and laboratory characterization: Paul Cook and Max Hu
- THM modeling: Johnny Rutqvist

Close Integration Between Modeling and Measurements

Numerical Tools

- **TH: TOUGH2**
- **THC: TOUGHREACT**
- **THM:TOUGHFLAC**

Model predictions compared to data: selected examples

- **Temperature**
- **Moisture redistribution**
- **Water and gas chemistry**
- **Dissolution and precipitation**

Modeling of TH and THC Processes for the DST

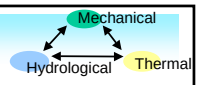
TH Processes modeled by TOUGH2

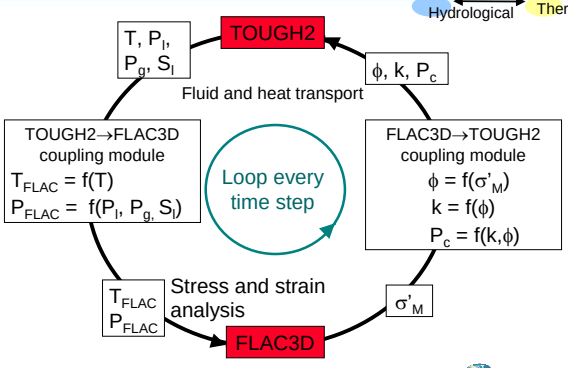
- Transport of heat by conduction, convection, vaporization and condensation
- Water-air-heat-vapor flow
- Dual permeability (fractures and matrix treated as separate continua)

THC processes modeled by TOUGHREACT

- Kinetic and equilibrium gas-water-mineral reactions
- Aqueous and gaseous species transport
- Permeability, porosity, and capillary pressure coupling

TOUGH FLAC to model THM Processes





TH Modeling - Base for THC and THM Modeling

Geometric Representation

- 3D honoring realistic test geometry: alcoves, drifts

Input Parameters

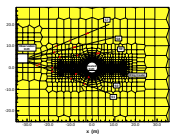
- Site specific if available

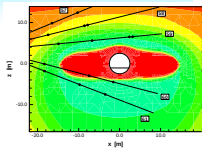
Boundary Conditions

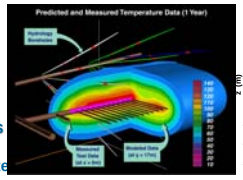
- Open alcoves and drifts

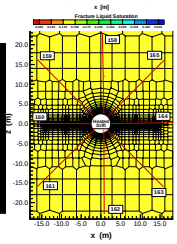
Alternative conceptual models and uncertain hydrological properties

- Rely on early time data to discriminate



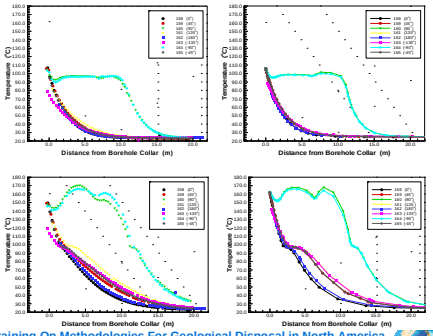






Temperature Profiles at 3 and 12 months

Measured | Simulated

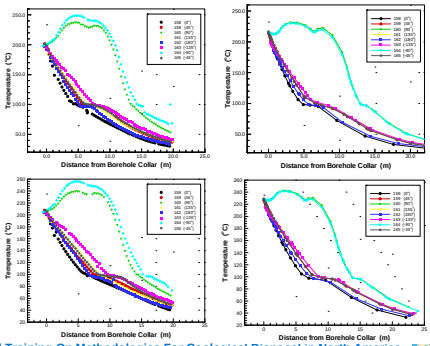


3 months

12 months

Temperature Profiles at 30 and 45 months

Measured | Simulated



30 months

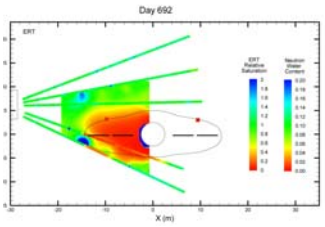
45 months

Time Evolution of Moisture Distribution in Rock Matrix

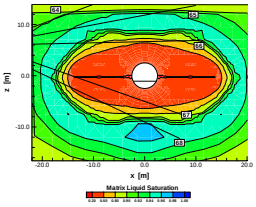
Periodic geophysical surveys to track moisture changes

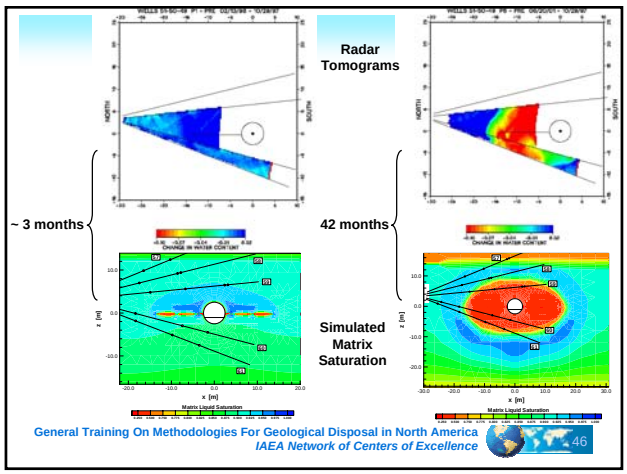
Locations of drying and wetting as function of time in general correlate well with simulated liquid saturation in rock matrix

Electric Resistance Tomography, Neutron Log

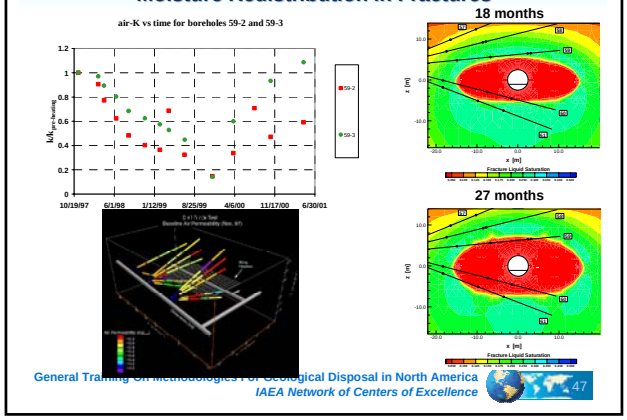


Simulated Saturation



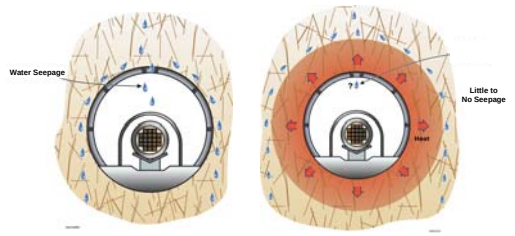


Periodic Air-K Tests to Track Moisture Redistribution in Fractures

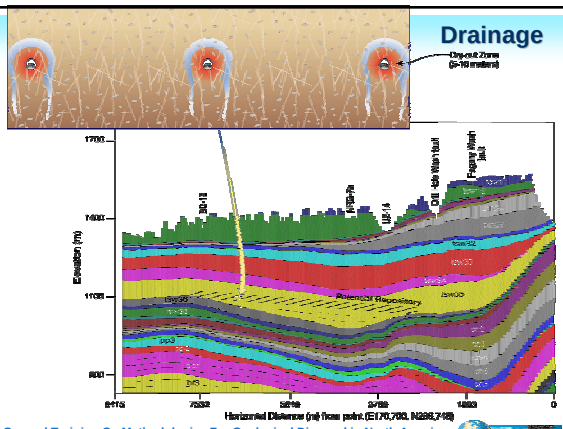


Coupled Process Models Applied to Assess Repository Performance: Seepage

- Water cannot penetrate through the vaporization barrier as long as the local temperature at the drift wall is above boiling
- Temperature drops below boiling typically after 1000 years of waste emplacement
- Seepage percentage is always smaller than the respective ambient reference values



Drainage



Model Geochemical System

Primary aqueous Species

- H^+, Na^+, Ca^{+2}, Mg^{+2}, K^+, Al^{+3}, SiO_2, Fe^{+3}, Cl^-, F^-, SO_4^{2-}, HCO_3^-

Minerals

- Calcite, cristobalite, tridymite, quartz, amorphous silica, feldspars, clays (smectite, illite, kaolinite, sepiolite), zeolites (clinoptilolite, stellerite, heulandite, mordenite), volcanic glass, hematite, goethite, gypsum, fluorite

Gas

- H_2O, Air, CO_2

Measured and Modeled CO_2 over time

Gas Sampling

Degassing of CO_2 from pore water with elevated temperature

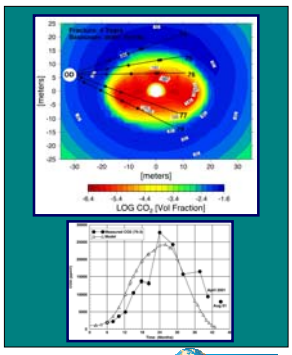
CO_2 concentration in gas samples initially increases with temperature

As temperature exceeds boiling, rock mass dries out and CO_2 concentration drops

Model Predictions

Successfully captured trend of CO_2 field data without calibration

Changes in CO_2 partial pressure play important role in pH and water chemistry and subsequent mineral alteration



Water Chemistry (pH and Cl) over time

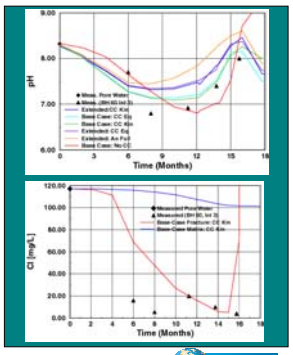
Water Sampling

Water draining into boreholes follow a path of initially decreasing pH (due to increasing PCO_2) followed by increasing pH as temperature increases and the zone dries out

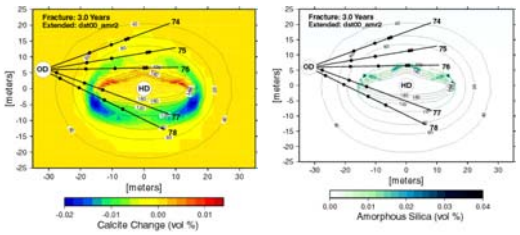
Model Predictions

Modeled fracture water pH matches the trend in measured pH

Cl concentrations indicate very limited fracture-matrix interaction



Precipitation and Dissolution in Fractures



Calcite precipitation above heaters owing to boiling of water draining in fractures

Calcite dissolution occurs in drainage and condensation zones

Amorphous silica precipitation in narrow zone above heaters (evaporative concentration from boiling exceeds its solubility)

Samples taken by *in-situ* sidewall coring have shown amorphous silica, and calcite in fractures in the now above-boiling intervals above the heaters

Chemistry of Potential Seepage Water

Chemistry of seepage water impacts corrosion of waste packages

Fracture water above the drifts is more concentrated during the boiling period when no seepage is anticipated

Chemistry of the seepage water is at all times similar to that of the initial, dilute pore waters (total dissolved solids<1000 ppm)

Concluding Remarks

- Numerical modeling is a key element in support of the Yucca Mountain Project:
  - Process understanding
  - Test design
  - Data analysis
  - Performance assessment
- Development of models is driven by field data – data collection activity is supported by modeling
- Development of new modeling capabilities is driven by application needs

Challenges and Future Work

Challenges

- Spatial and temporal variability
- Coupled process modeling (THCMB)
- Site-specific properties on different scales
- Assessing validity of assumptions and modeling approach

Future Work

- Develop alternatives to volume-averaged, macroscale continuum models
- Develop computational techniques to simulate coupled processes with different time constants
- Joint inversion techniques
- Design and conduct laboratory and field experiments for model testing