U.S. Department of Energy

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

Science and Modeling Update

Presented to:

Nuclear Waste Technical Review Board

Presented by:

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Las Vegas, NV

Caveats and Acknowledgments

The information presented here is preliminary and draft in nature in order to provide the NWTRB a current status of some areas of ongoing post-closure scientific work

Much of this work is expected to be included in updates to Analysis/Model Reports that support the Safety Analysis Report

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Outline

- Introduction/Purpose
- Technical areas with updated science and modeling activities to be presented
- Summary

Introduction – Purpose of Presentation

- The decision to not submit the SAR afforded DOE the opportunity to include additional science and modeling in an updated SAR
- The purpose of this presentation is to describe some of the ongoing testing and modeling
- These test and modeling results may be used to
  - support evaluations of features, events and processes (FEPs) screening decisions
  - support model and parameter confidence (or to revise models and/or parameters)
  - evaluate explicit conservatisms
  - address > 10,000 year dose projections

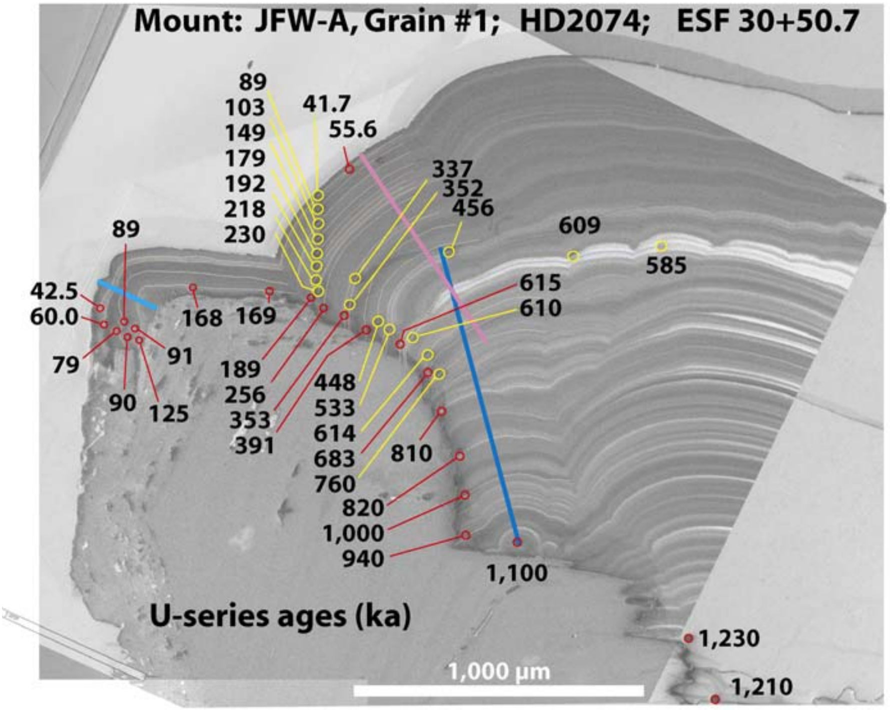
Technical Areas with Updated Science and Modeling to be Presented

- Effects of long term climate change on unsaturated zone flow
- Thermal-hydrologic-chemical-mechanical results from Drift Scale Test
- Time dependent rock strength tests
- Alcove 8 - Niche 3 seepage and transport test
- Dust deliquescence effects
- Corrosion studies
- Radionuclide solubility from laboratory testing
- Saturated zone flow and transport results from Nye County testing in Early Warning Drilling Program (EWDP) wells
- Dosimetry models based on International Commission on Radiological Protection (ICRP) 72
- Seismic mechanical damage effects
- Aeromagnetic data interpretation of potential buried volcanic centers

Unsaturated Zone Flow Effects of Long Term Climate

- Climate change has occurred in the past and is likely to occur in the future
  - Uncertainty exists in the timing and magnitude of future climate changes
- Over the past ~ 500,000 years:
  - ~ 20% of the time has been glacial,
  - ~ 20% of the time has been interglacial and
  - ~ 60% of the time has been glacial transition/monsoon
- Recent U-series age dating of opals by the USGS indicates that the repository level at Yucca Mountain is buffered from long term transient climate states

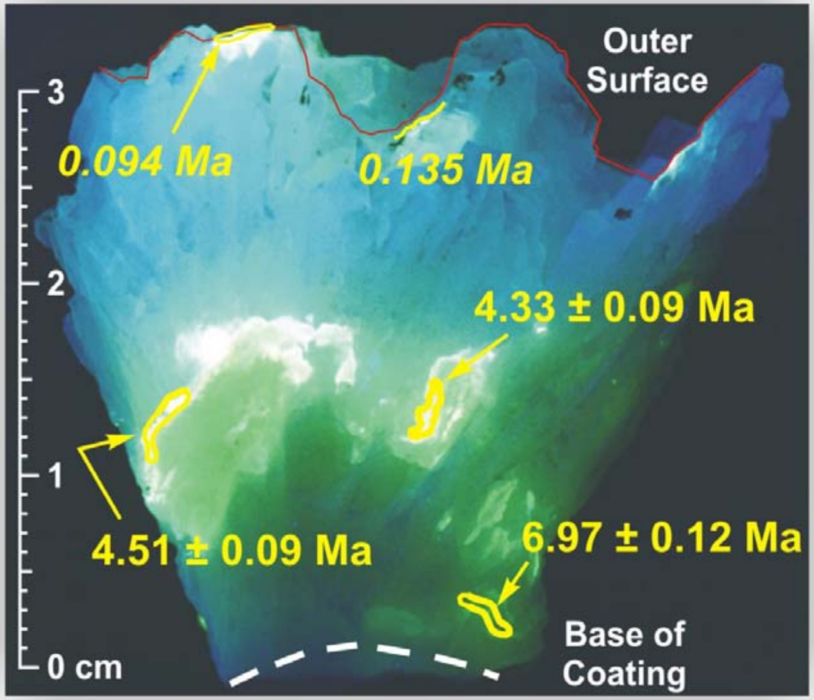
Examples of Long Term Opal Growth Rates



U-series dating results

Secondary Ionization Mass Spectrometry

(Jim Paces et al. 2004 (USGS))



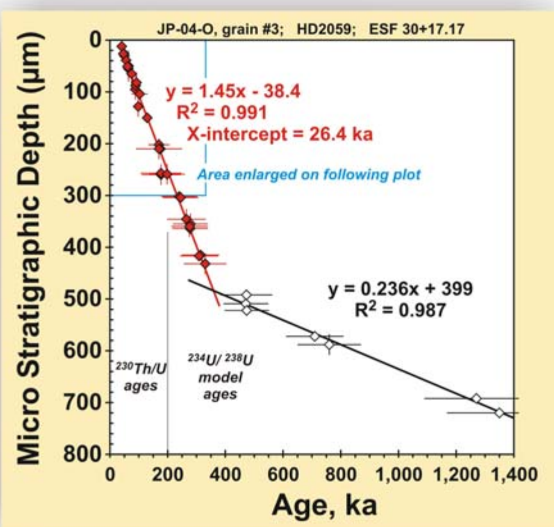
U-series and U-Pb dating results for a 3-cm-thick calcite-opal coating.

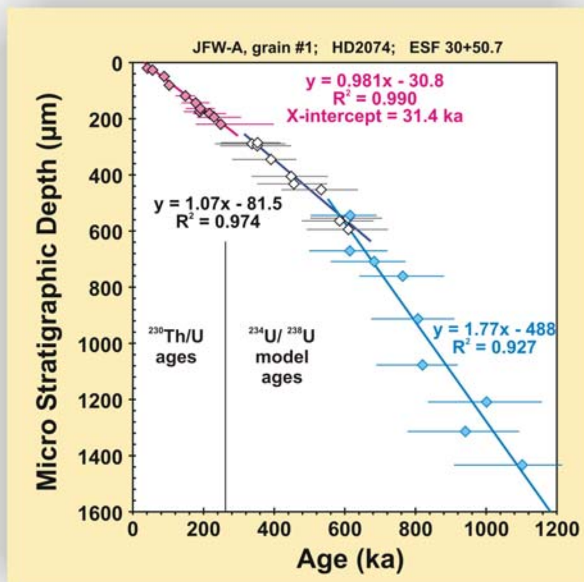
Thermal Ionization Mass Spectrometry (sample HD2019 from ESF 28+81) Photo taken in shortwave UV light.

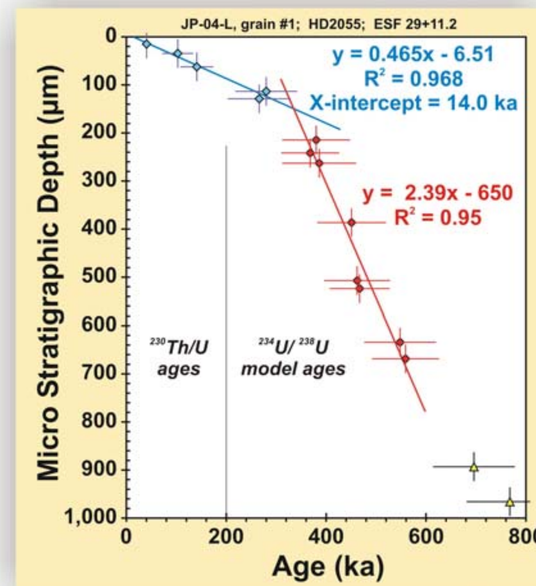
Examples of Long Term Opal Growth Rates

(Continued)

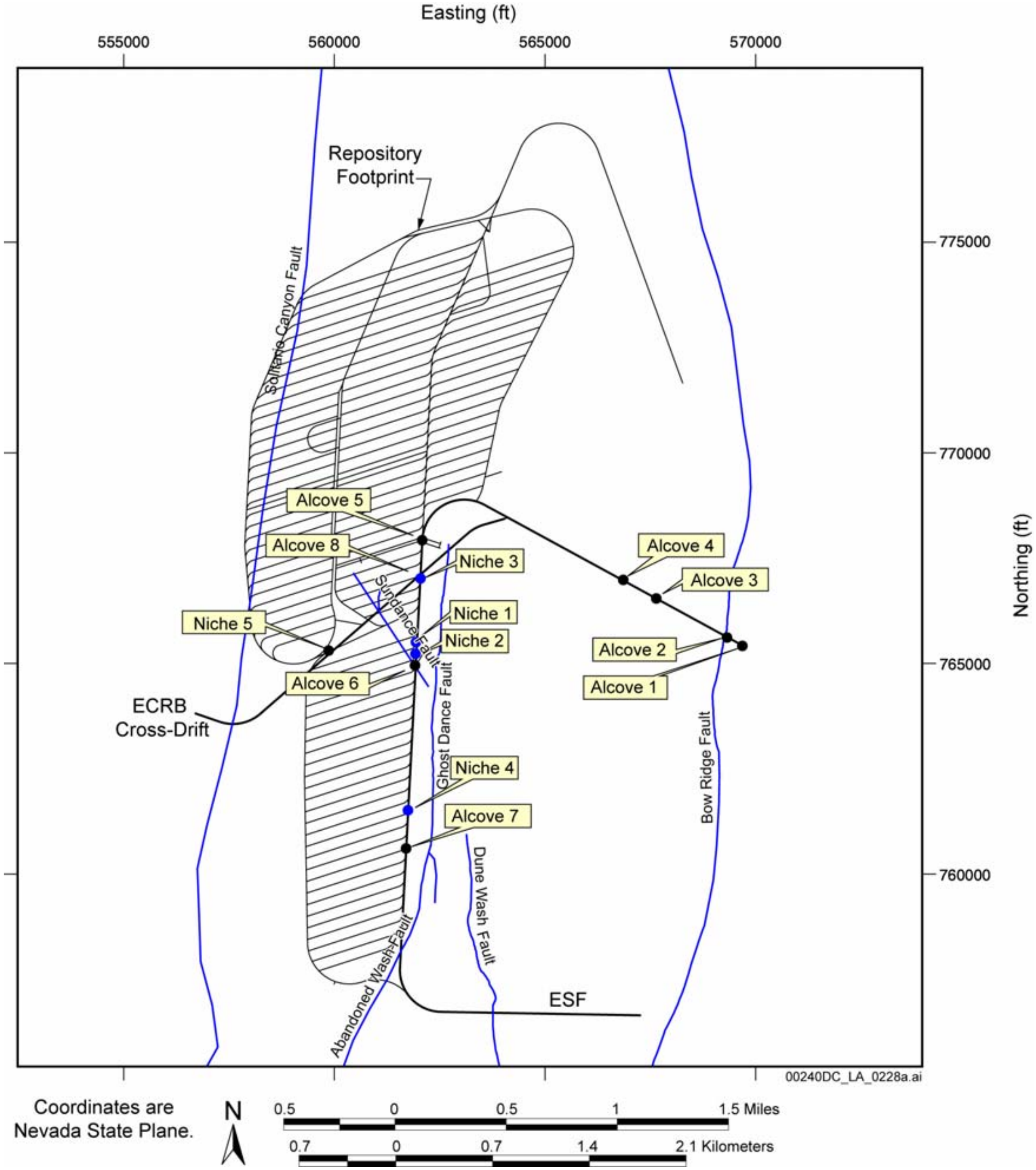
- **Rates vary spatially from about 0.24 to 2.4 microns per 1,000 years**
  - Over last ~ 300,000 years rates vary spatially from 0.47 to 1.5 microns per 1,000 years
  - Variations in growth rates may be due to (a) changes in mineral growth dynamics, (b) changes in $^{234}U/^{238}U$ in solution with time, (c) changes in cross-sectional geometry and dip of layers or (d) variability in percolation flux
- **Extremely uniform (with time) growth rates over the past**





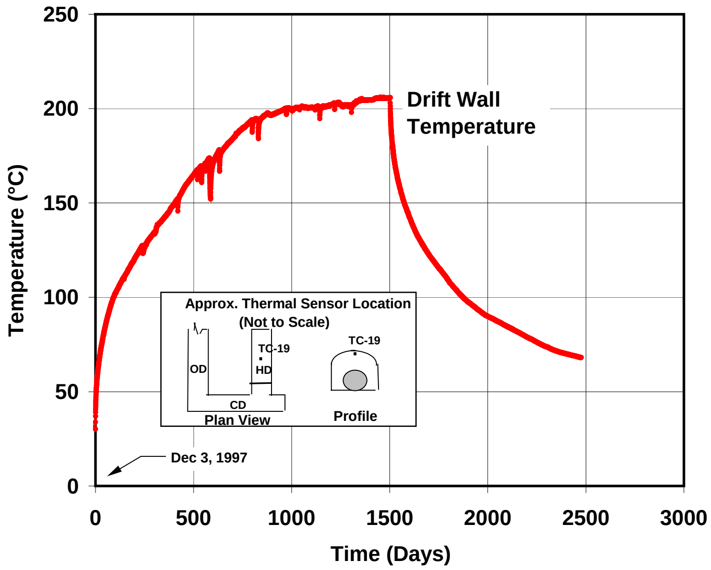


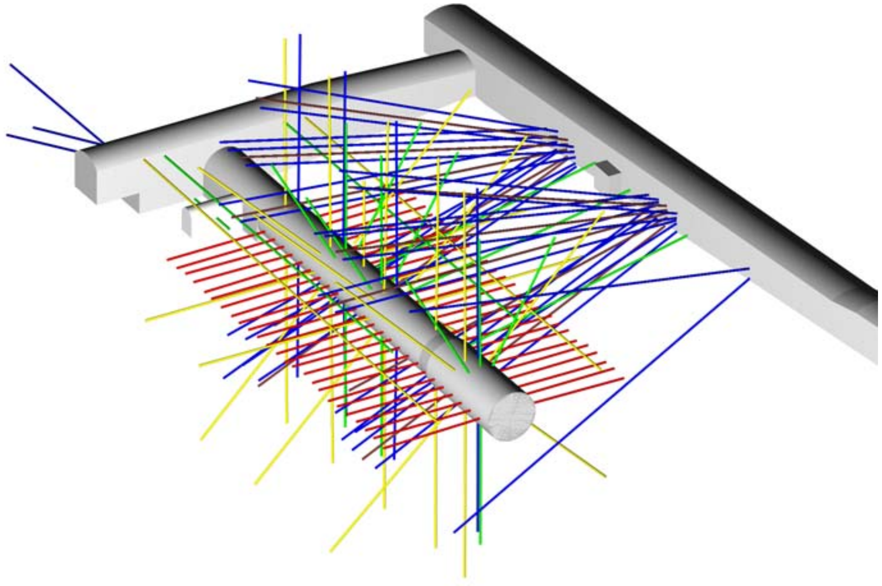
Location of Test Alcoves and Niches in the Exploratory Study Facility and Enhanced Characterization of the Repository Block (Cross Drift)

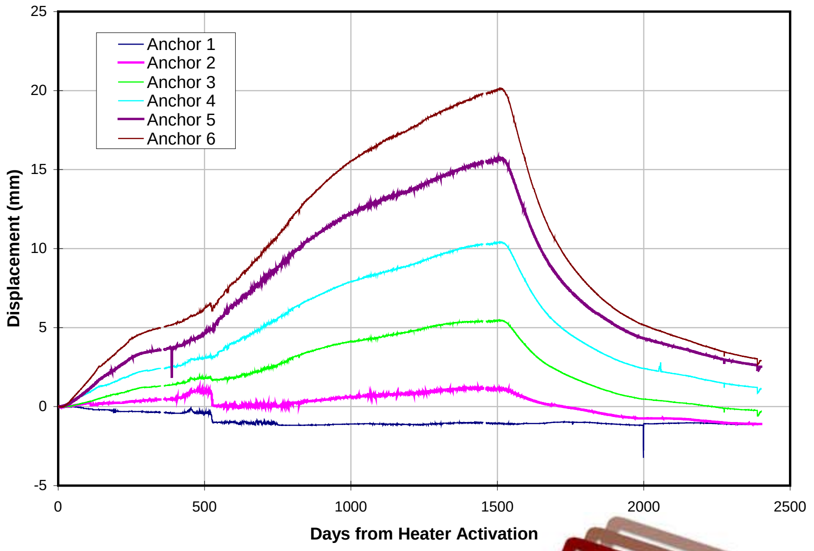


Thermal-Hydrologic-Chemical-Mechanical Results from Drift Scale Test

- Completed third year of cool down phase (after 4 years of heating)
- Continue monitoring of environment response
- Observations confirm drift scale coupled process models

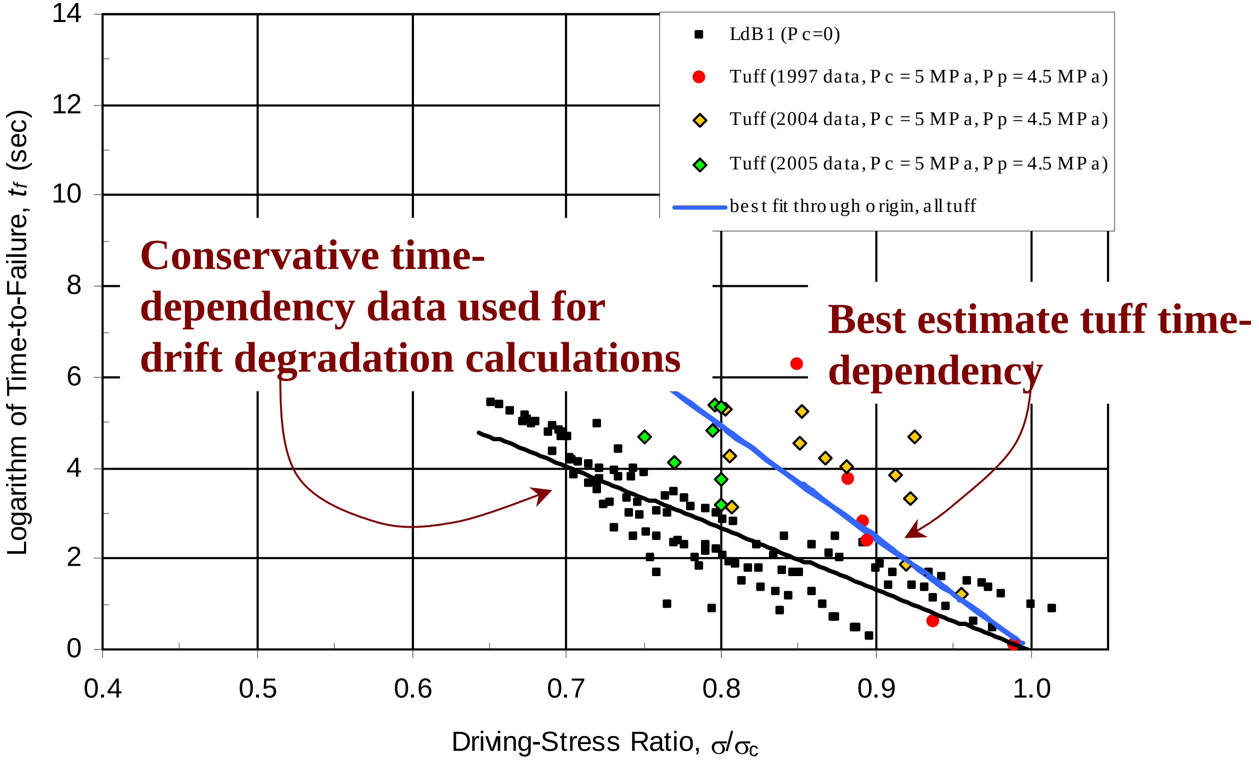




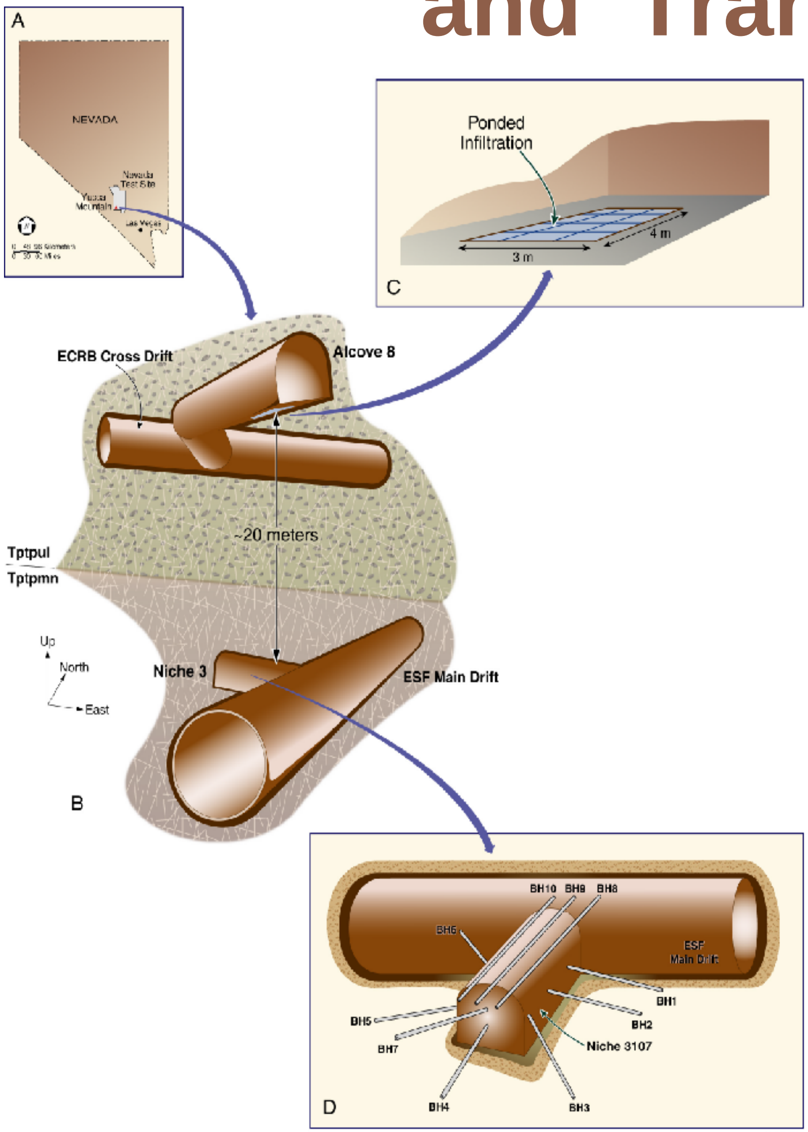


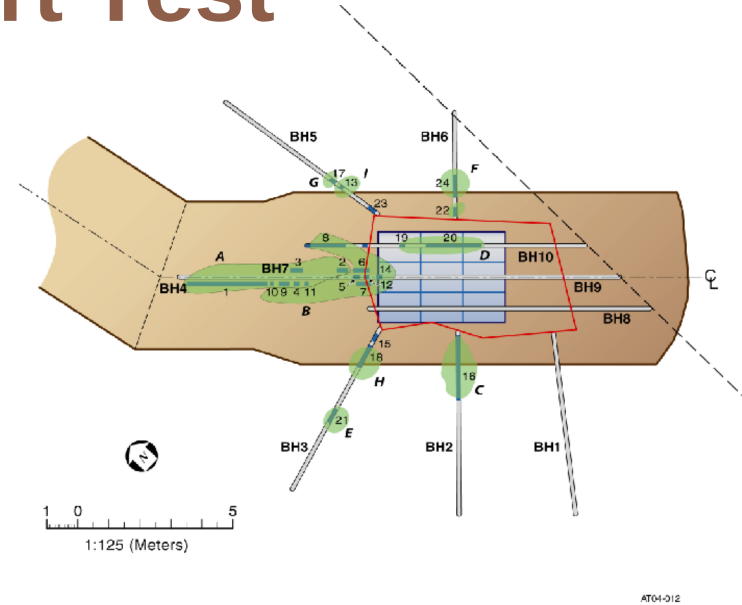
Time-Dependent Strength Data for Repository Rocks

- **32 additional laboratory static fatigue tests (creep tests) have been conducted on repository host rocks (colored diamonds below)**
- **New data confirm conservative nature of time-dependent strength response of repository host rocks**



Alcove 8 - Niche 3 – Seepage and Transport Test

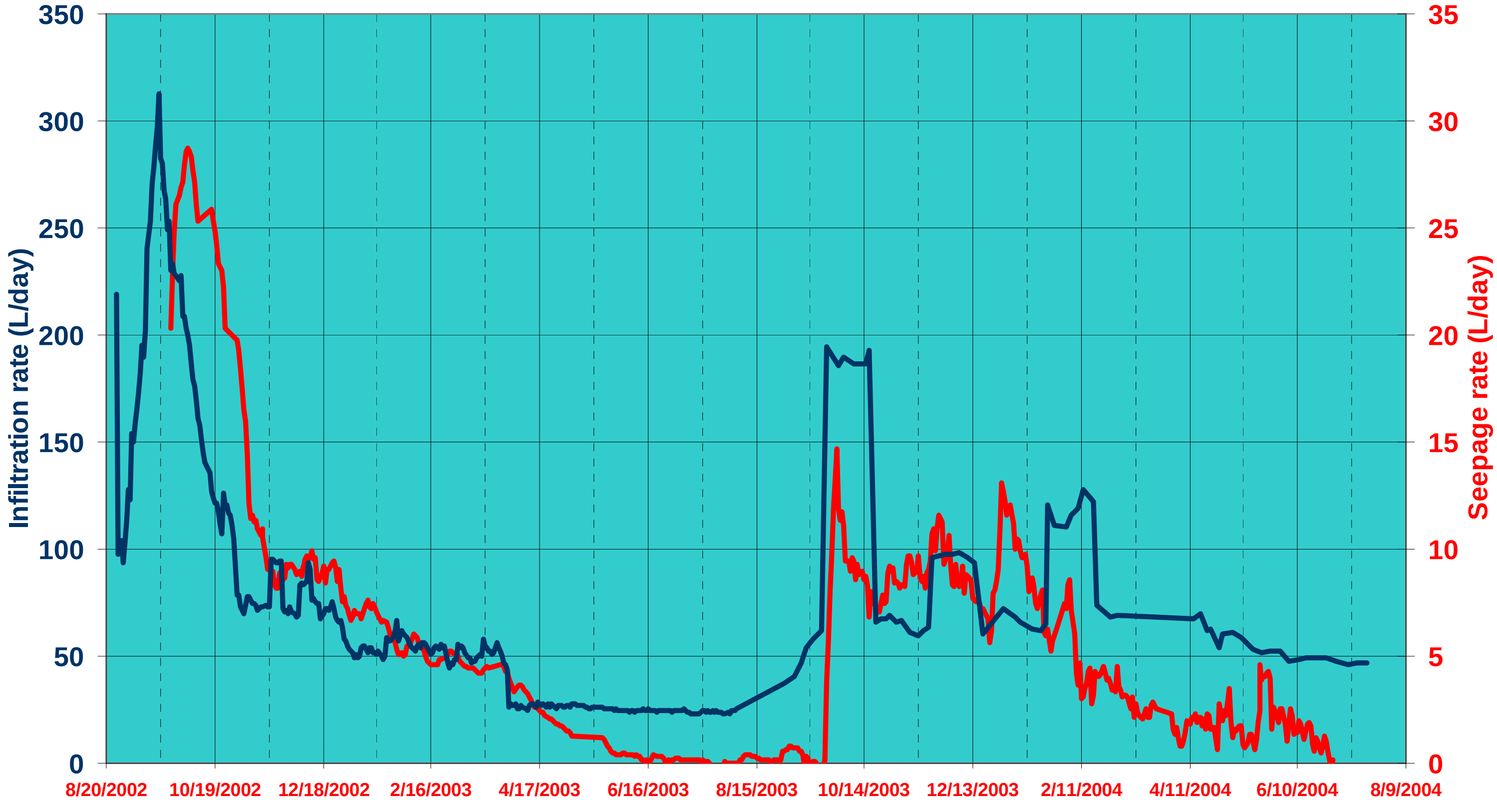




- **Alcove 8 - Niche 3 fault test conducted first**
- **Alcove 8 - Niche 3 large plot test then conducted**
- **Both tests evaluate seepage and transport**

Alcove 8 – Niche 3 Large Plot Seepage Test

- Monitoring of seepage and infiltration has continued in large plot test
- Observed and predicted seepage confirm seepage model

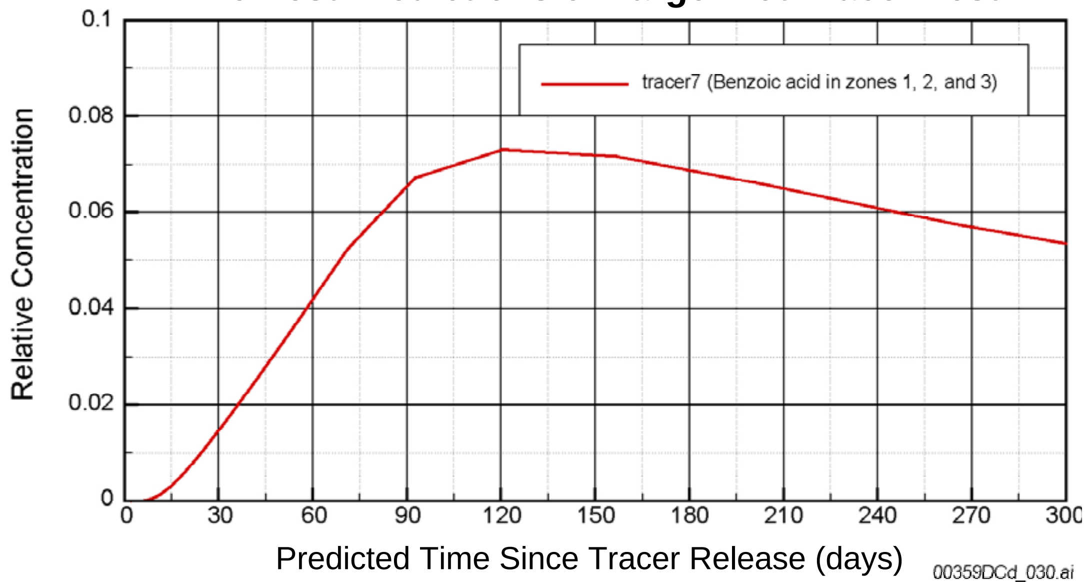


Alcove 8 – Niche 3 Large Plot Tracer Test

- **Pre test predictions (using transport model) predicted breakthrough would be observed in tens of days**
- **To date (about ten months), no breakthrough observed**
- **Believe lack of observed breakthrough is a result of more significant matrix diffusion than is represented in transport model**
- **Transport model is conservative (leads to more rapid transport) then this test area would indicate**
- **Transport model does reasonably reproduce Alcove 1 data and Alcove 8 - Niche 3 fault test data**

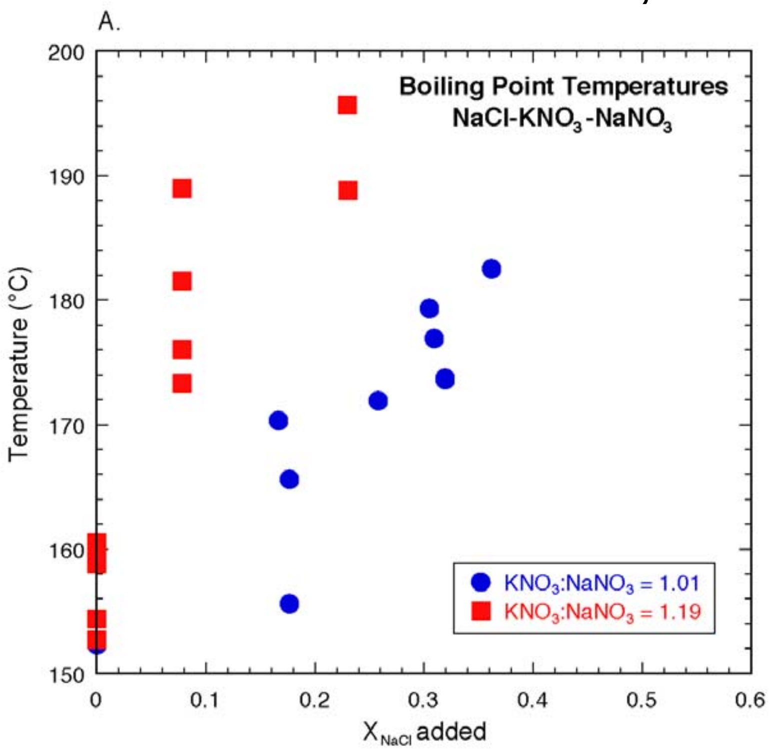
Zone	Tracer	Conc. (ppm)	Application Period Start	Application Period End
1	2,6-Difluorobenzoic Acid	50	3/1/04	4/13/04
	Potassium Iodide	10		
2	2,5-Difluorobenzoic Acid	50	3/1/04	3/17/04
	Calcium Bromide	500		
3	2,4,5-Trifluorobenzoic Acid	50	3/1/04	4/13/04
	Potassium Fluoride	50		

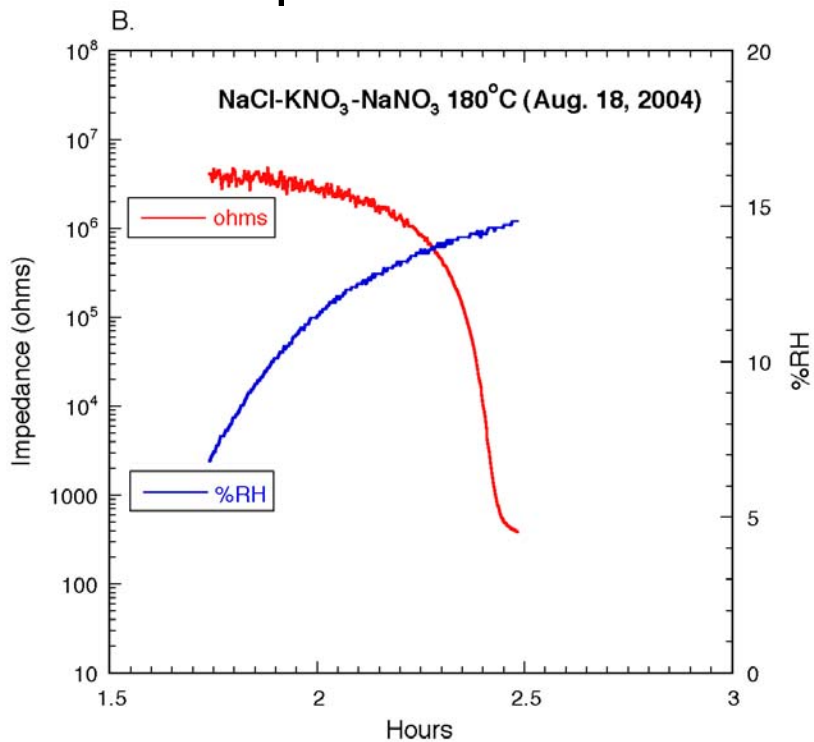
Pre-Test Predictions of Large Plot Tracer Test



Dust Deliquescence Test Information

- Likely dusts include small fraction of salts
  - less than 1 % of observed dusts in ESF (during construction)
  - about 10% of atmospheric dust in arid southwest
- Soluble salts are inferred to be varying salt contents of NaCl, KNO_3, $CaSO_4$, $NaNO_3$, $Ca(NO_3)_2$ and NH_4 (Cl, NO_3, SO_4 or HSO_4)
  - None of these salts alone deliquesce above 160°C – however if certain combinations of these salts were in contact, the mixture could deliquesce above 160°C



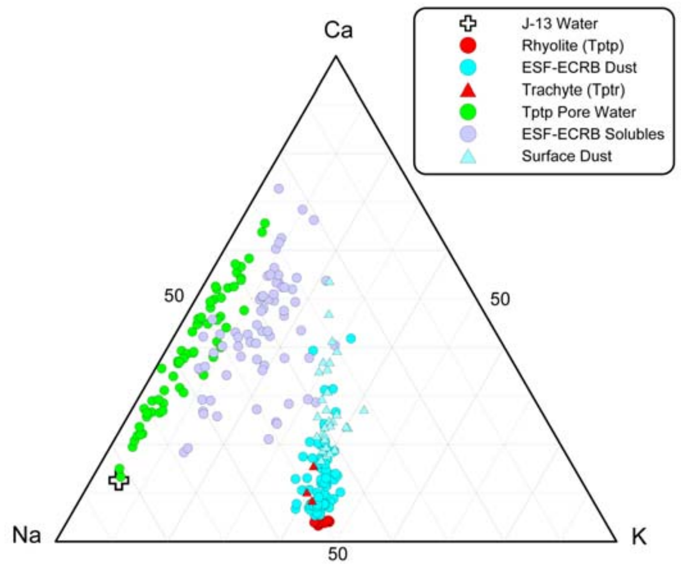


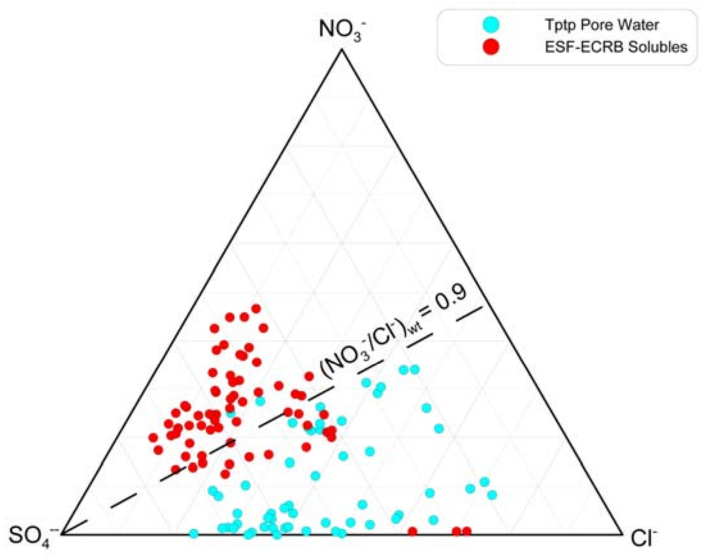
Analyses of Potential High Temperature Salt Deliquescence and Effects

- Some combinations of salts might deliquesce above 160°C
  - Given low percentage of soluble salts (1 to 10%), likelihood of such combinations occurring is low
- Even if such combinations existed, the resulting brine has a high NO_3/Cl ratio (slide 17)
- Even if brine formed, the ammonium salts sublimate (slide 18)
  - Ammonium chloride sublimates more, leading to higher NO_3/Cl ratio
- Even if brine formed it would (slide 19)
  - React with other dust solids to increase deliquescent relative humidity
  - React with atmosphere to degas HCl and HNO_3
- Even if brine persisted, it would be too thin to allow process to initiate or sustain localized corrosion (slide 20)

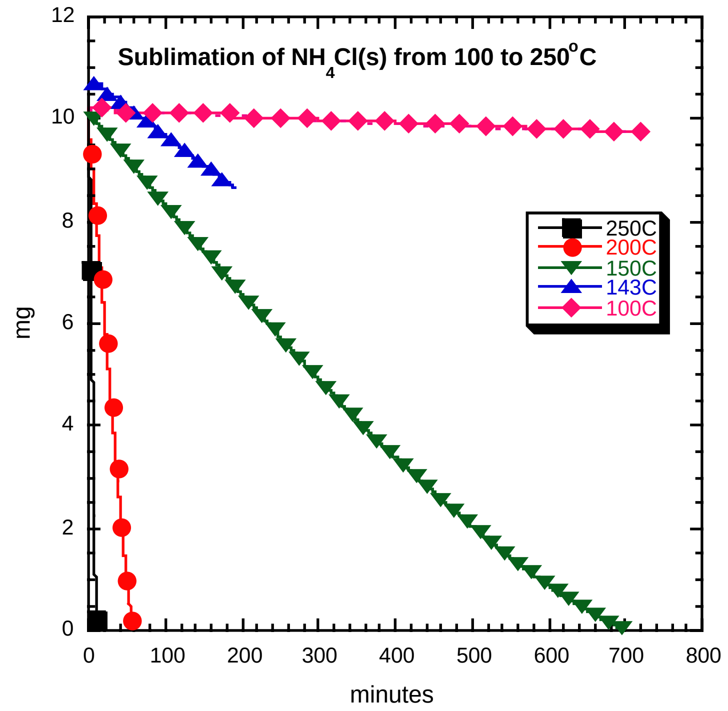
Dust Chemical Composition

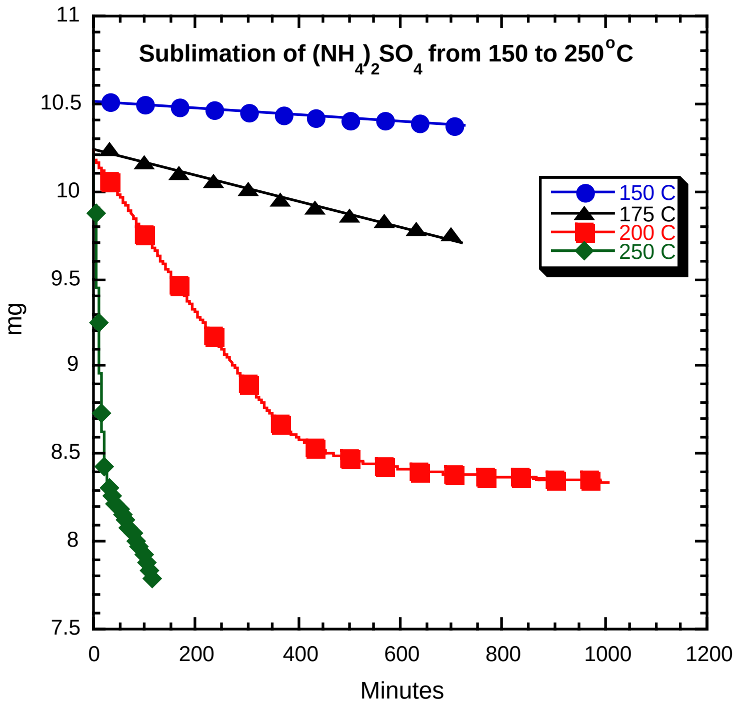
- **Recent USGS dust analyses indicate:**
  - **Dust solubles are between dust and pure water compositions**
  - **Most dust solubles are greater than NO_3/Cl molal ratio of 0.5 (weight ratio of 0.9)**
  - **Three outlier samples are from ESF conveyor belt (neoprene)**
- **Ongoing study of ammonia and ammonium**





Sublimation of Ammonium Salts

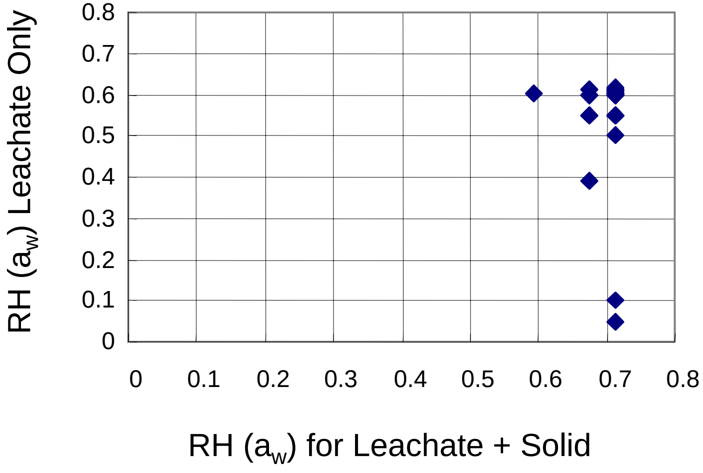


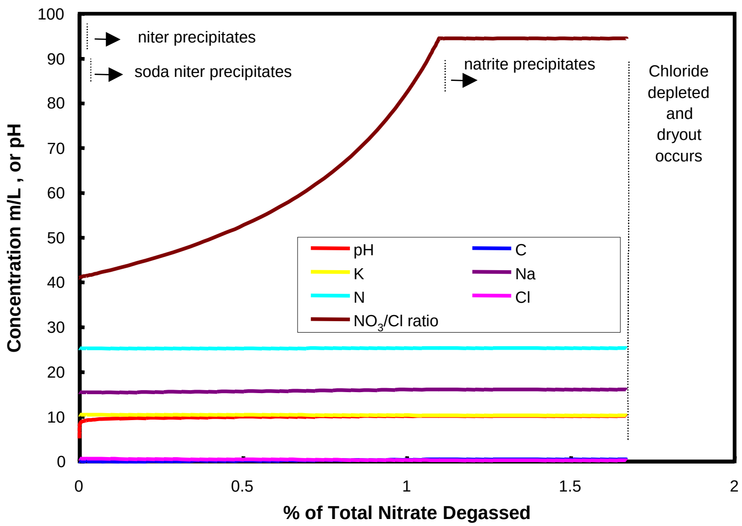


- **Ammonium salts decompose to the gas phase**
- **NH_4Cl is favored over NH_4NO_3 as a constituent of atmospheric dust**
  - **Therefore a greater proportion of chloride will be sublimated at elevated temperature**
  - **Sublimation and degassing increases NO_3/Cl ratio**

Dust Deliquescence and Brine Degassing Calculations

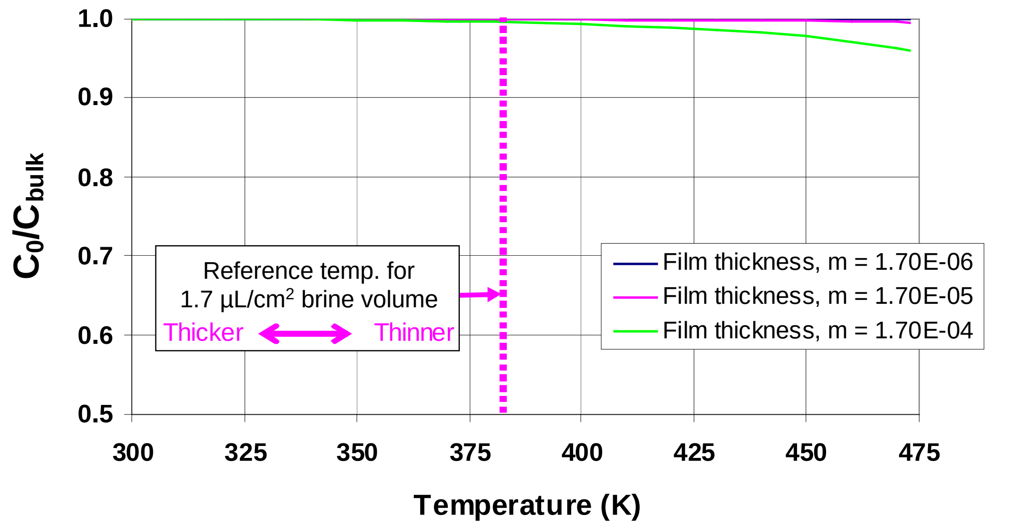
- Numerically evaporate all 53 observed dust leachate compositions, with and without rock-forming solid mineral phases
  - Use water-rock interaction and atmospheric CO_2 to establish pH
  - pH with solids present is buffered in the range neutral to mildly basic
  - Higher dryout RH and simpler behavior is predicted with solids present
- Numerically remove acid-gas species (HCl, HNO_3) in relation to abundance
  - Chloride depleted earlier than nitrate
  - Increase NO_3/Cl ratio prior to chloride depletion





Analysis of Dissolved Oxygen Variation with Potential Film Thickness

- **Although uncertainty exists in dust deposition, dust composition, dust particle size and deliquescent salt particle size, a conservative estimate of brine volume is about 1.7 micro liters per square centimeter at 70% RH (~110 C)**
- **Equivalent film thickness is about 17 microns**



- **Film thickness is so small that molecular diffusion will inhibit the formation of anodic and cathodic regions within a corrosion cell**
  - **Oxygen supply is significantly greater than oxygen depletion**
- **Therefore, passive film is expected to be stable and localized corrosion is not expected to initiate or propagate**

Ongoing Alloy 22 Corrosion Studies

- **Polarization resistance measurements**
- **Long-term corrosion potential**
- **Cyclic (potentiodynamic) polarization – Repassivation potential**
- **Passive film studies**
- **Potentiostatic tests**

Alloy 22 General Corrosion

- **Corrosion rates from long-term corrosion potential studies at 100°C exposed > 100 days**

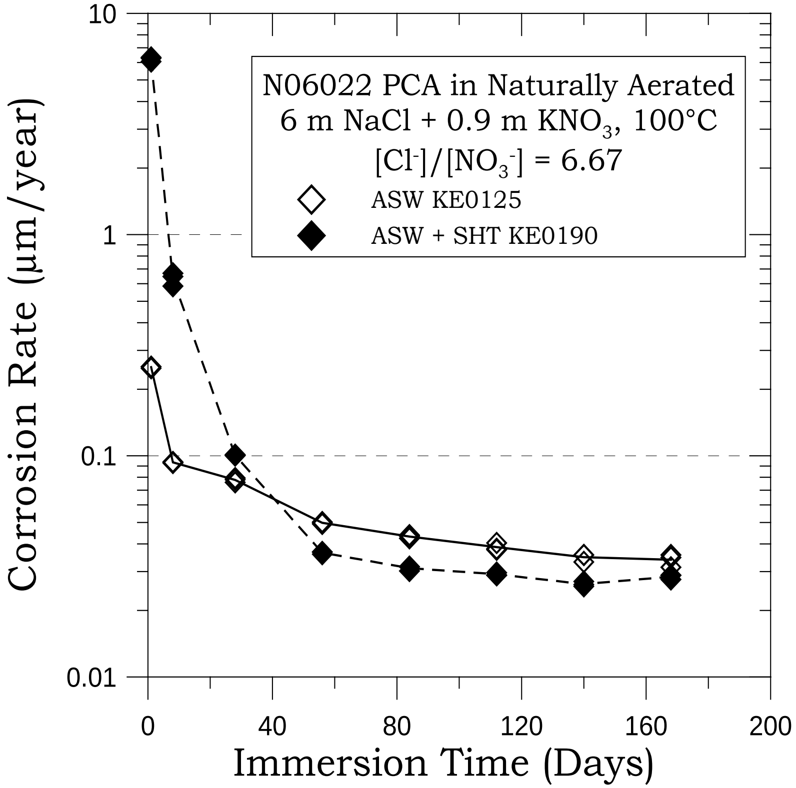
Solution			Corrosion Rate (µm/yr)	
$[Cl^-]$ (m)	$[NO_3^-]$ (m)	$[NO_3^-]/[Cl^-]$	ASW	ASW + SHT
1	0.05	0.05	0.05	0.07
1	0.15	0.15	0.04	0.04
3.5	0.175	0.05	0.04	0.03
3.5	0.525	0.15	0.04	0.09
6	0.3	0.05	0.04	0.05
6	0.9	0.15	0.04	0.03

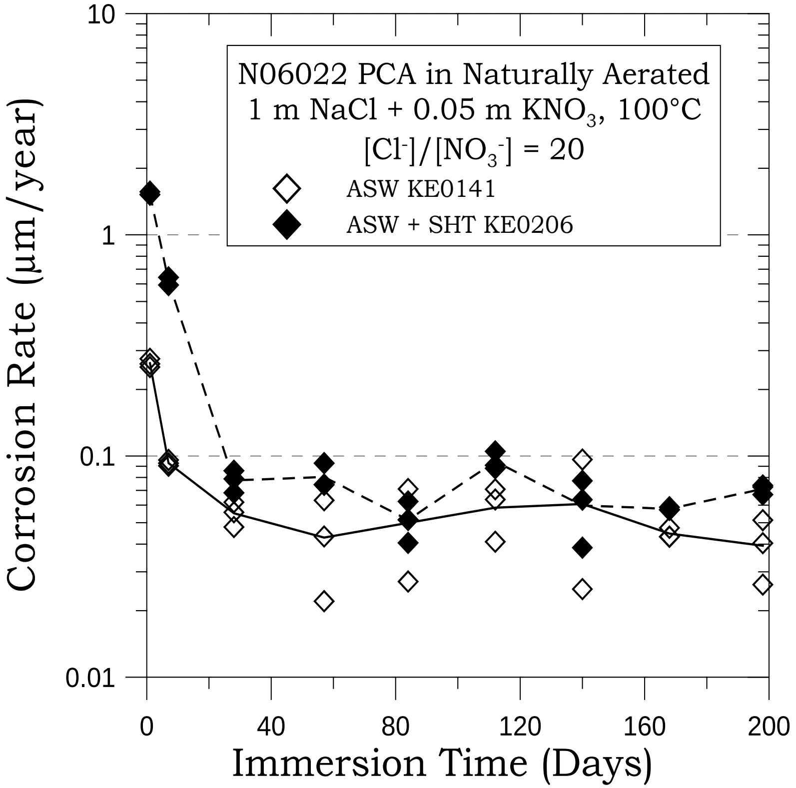
ASW = As Welded
SHT = Solution Heat Treated (1120°C + Water Quench – Oxide Film Left on Surface)

- **Measured corrosion rates are within variation of Alloy 22 general corrosion model**
- **No significant difference in general corrosion rates due to solution heat treatment**

Alloy 22 General Corrosion

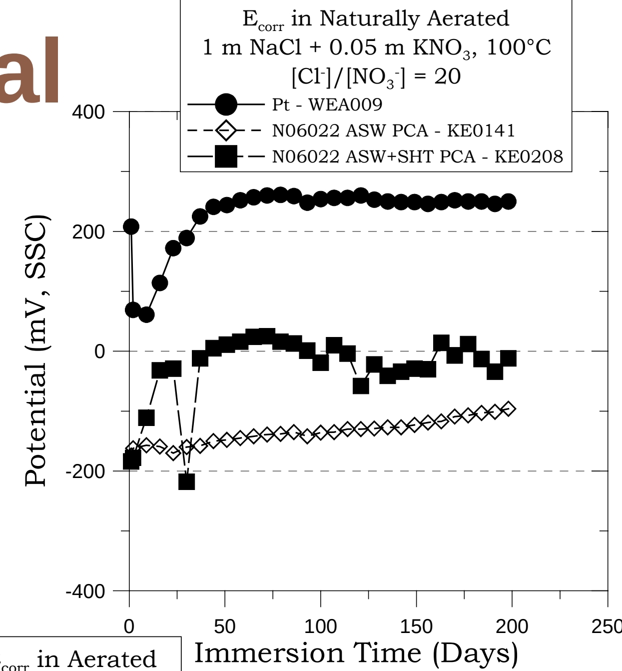
- **Alloy 22 corrosion rates decrease with time and nitrate concentration (based on data from polarization resistance measurements)**

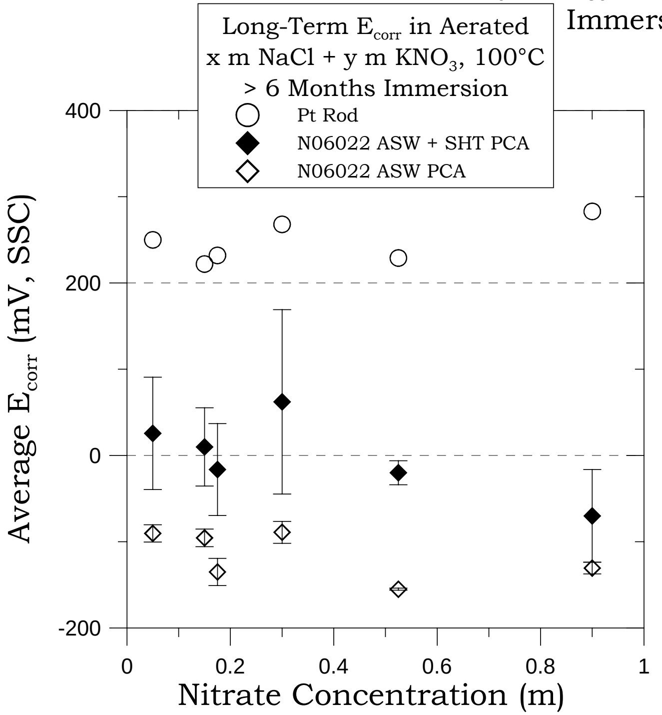




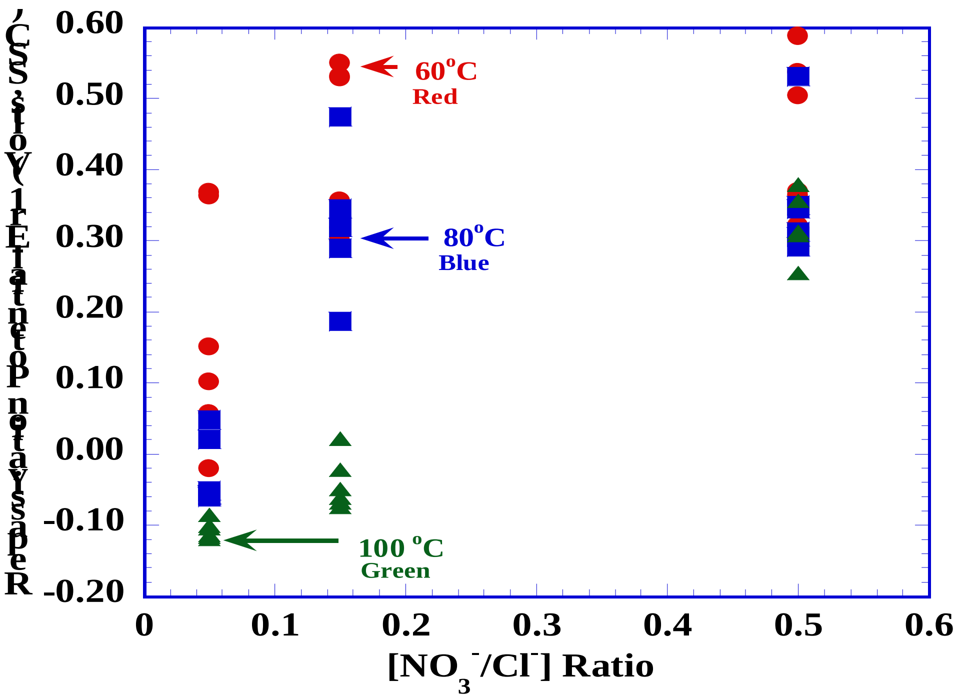
Long-Term Corrosion Potential

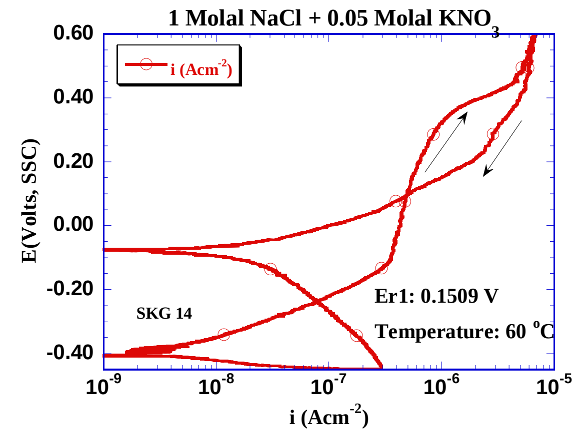
- Additional environments
  - 1, 3, and 6 m NaCl at 100°C and KNO_3:NaCl of 0.05 and 0.15
  - 22.5 m $Ca(NO_3)_2$ + 0.225m $MgCl_2$ at 145°C
  - 18 m $CaCl_2$ + (9 or 0.9) m $Ca(NO_3)_2$ at 155°C
- Mill annealed, as-welded (ASW), welded + aged (700°C for 173 h), solution heat treated (SHT)
- Prism Crevice Assembly (PCA) specimen geometry
- Corrosion potential is not a strong function of either chloride or nitrate ion concentration over range tested

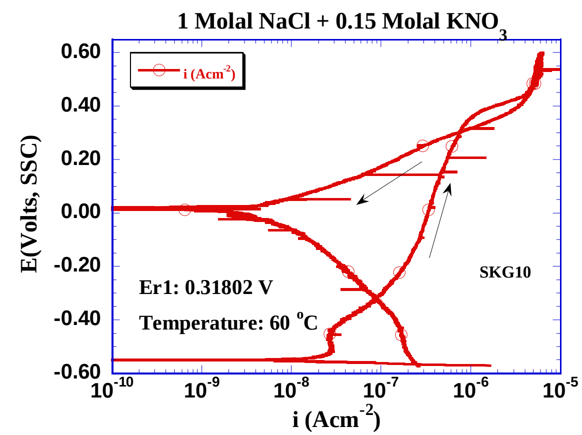


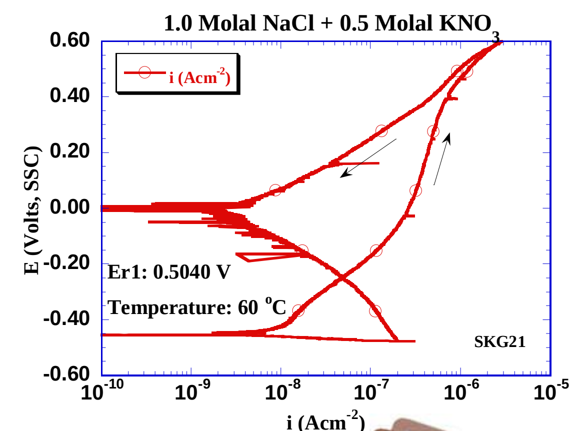


Repassivation Potential for Range of Environments



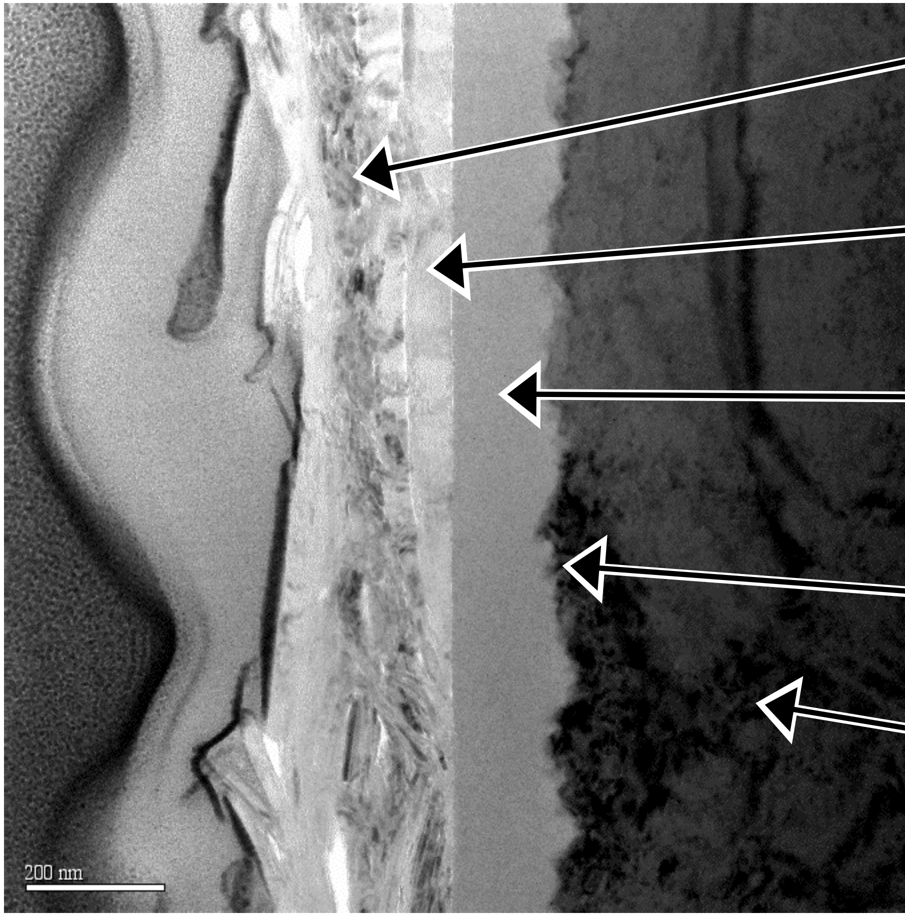






- **Repassivation potentials used as basis for localized corrosion initiation likelihood**
- **Er1 rises with [NO_3]/[Cl] ratio, falls with temperature**

Passive Film Studies of Alloy 22

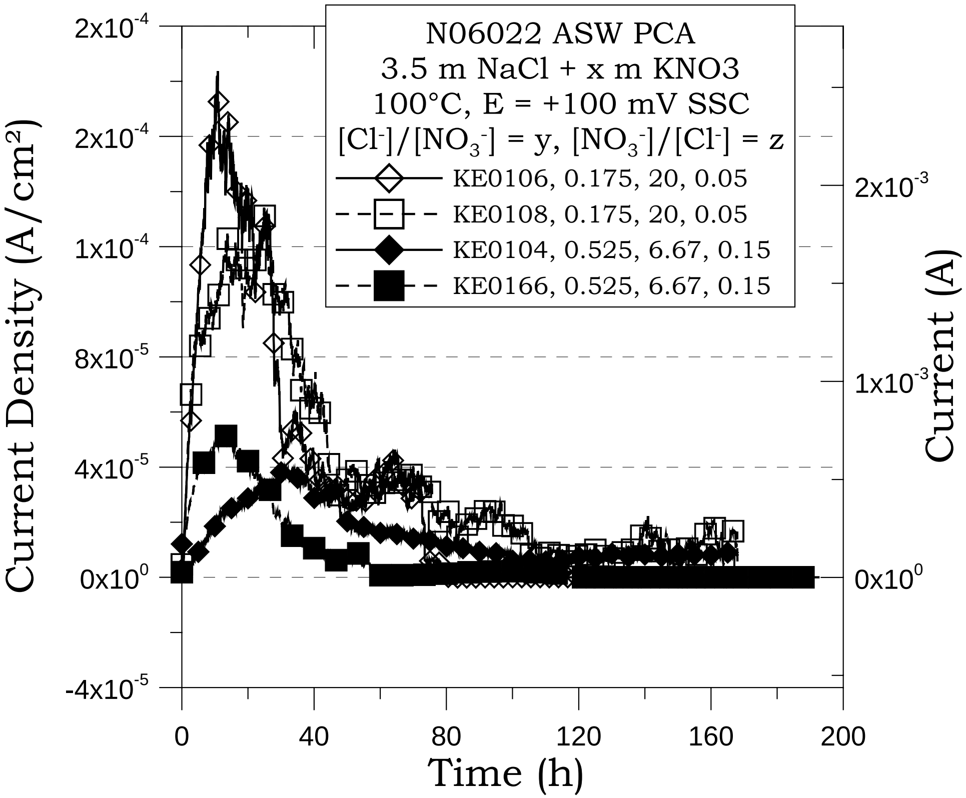


Example cross-section TEM image of autoclaved sample held ~ 9 months at 220 C with NO_3/Cl ratio of 0.3; corrosion rate ~ 0.15 µm/yr

- **Oxide has four distinct layers**
- **Chromium oxide layer forms similar to that found in passive film studies over a range of solution conditions**

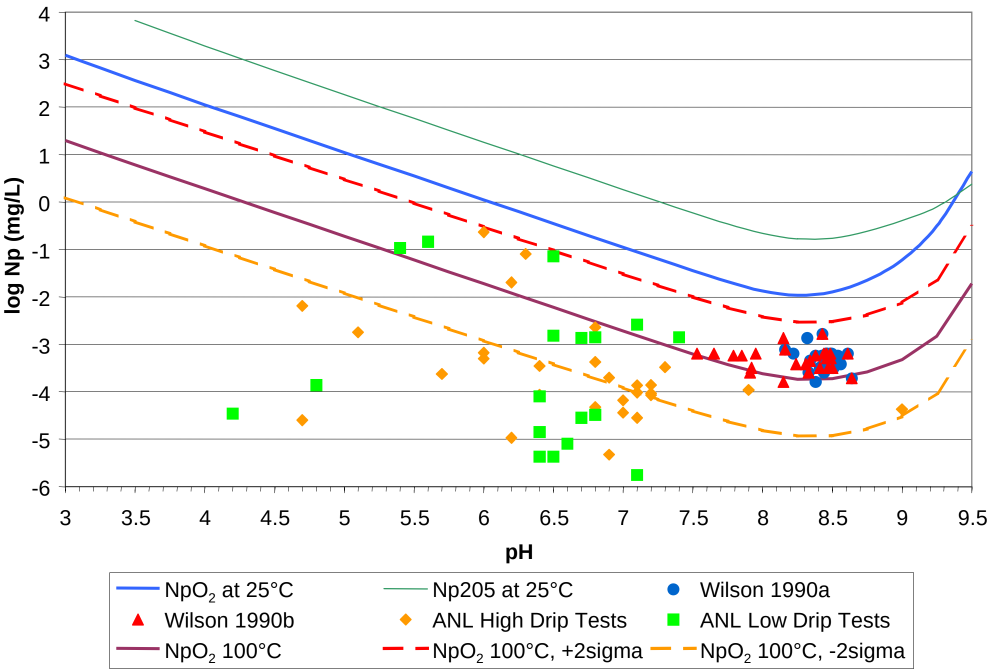
Potentiostatic Tests to Evaluate Localized Corrosion Stifling Mechanisms

- **Reduction in current density implies stifling of initiated pit**
- **Stifling mechanism has been conservatively excluded from models to date**



Radionuclide Solubility from Laboratory Testing and Thermodynamic Modeling – Neptunium example

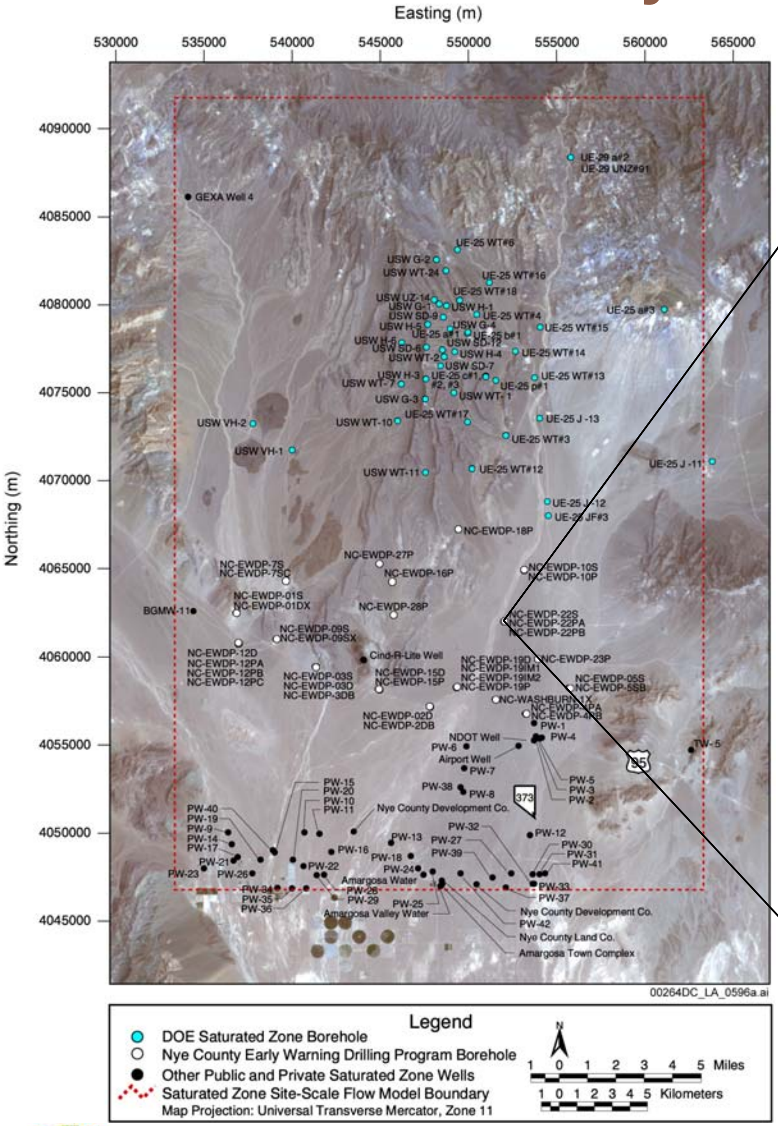
- NpO_2 is the most stable pure phase Np solid over most of Eh/pH range
- Pure phase NpO_2 model (at 25°C) conservatively overpredicts observations from spent fuel laboratory tests (at 80-90°C)
  - Most recent Argonne National Laboratory (ANL) data (Fall 2004) represent 9 years of drip tests

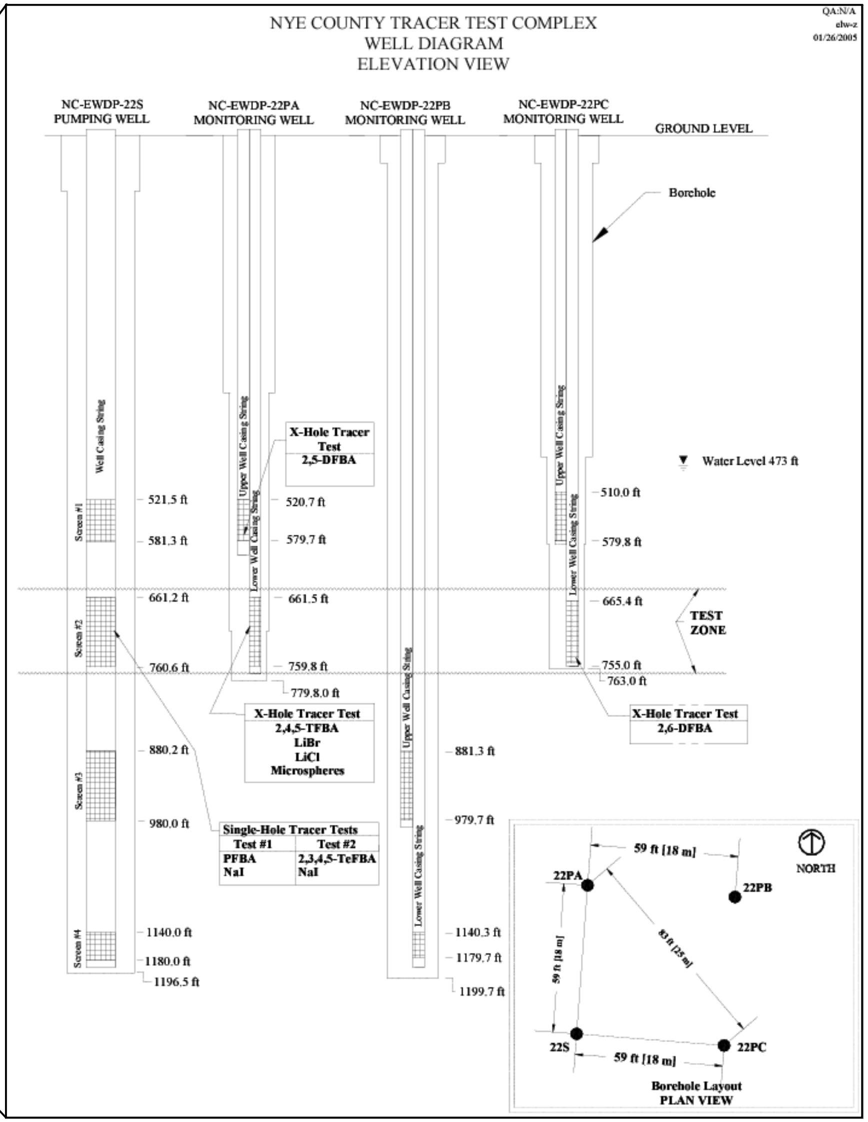


- Secondary phase uranium minerals may be incorporating or sorbing Np during these tests
- Several recent studies indicate Np retention in uranyl solids – although mechanism is uncertain
  - Burk et al (2004), Burns et al (2004), Douglas et al (2004), Friese et al (2004), Cunnane et al (2004)

Saturated Zone Alluvial Investigations

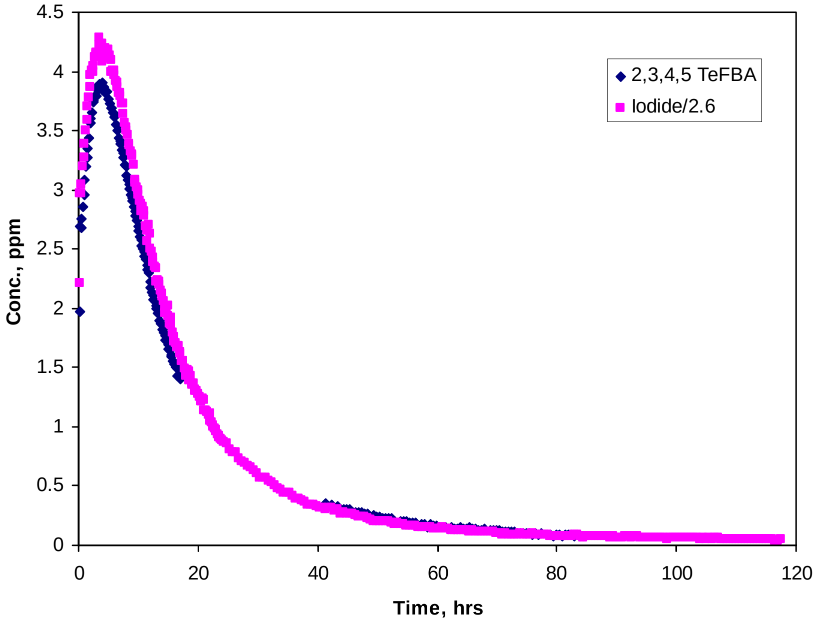
Nye County EWDP-22S

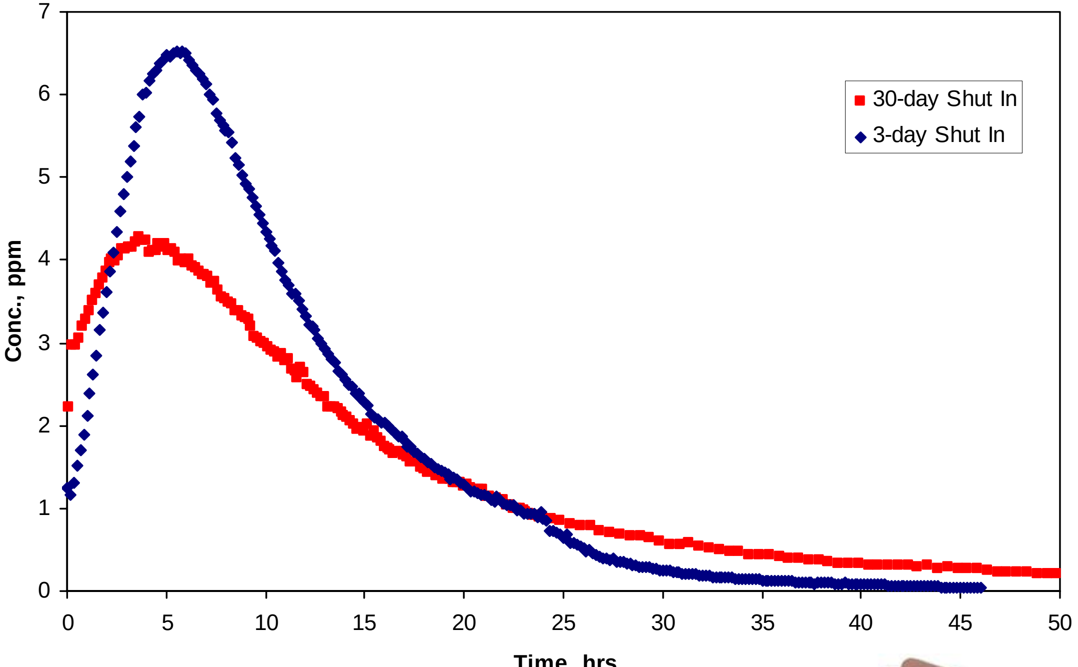




Recent Nye County Tracer Test Results

- Single-well test with ~3-day shut-in period using iodide and fluorobenzoic acid (FBA)
- Single-well test with ~30-day shut-in period using iodide and a 2nd fluorobenzoic acid (FBA)
- Test analyses ongoing

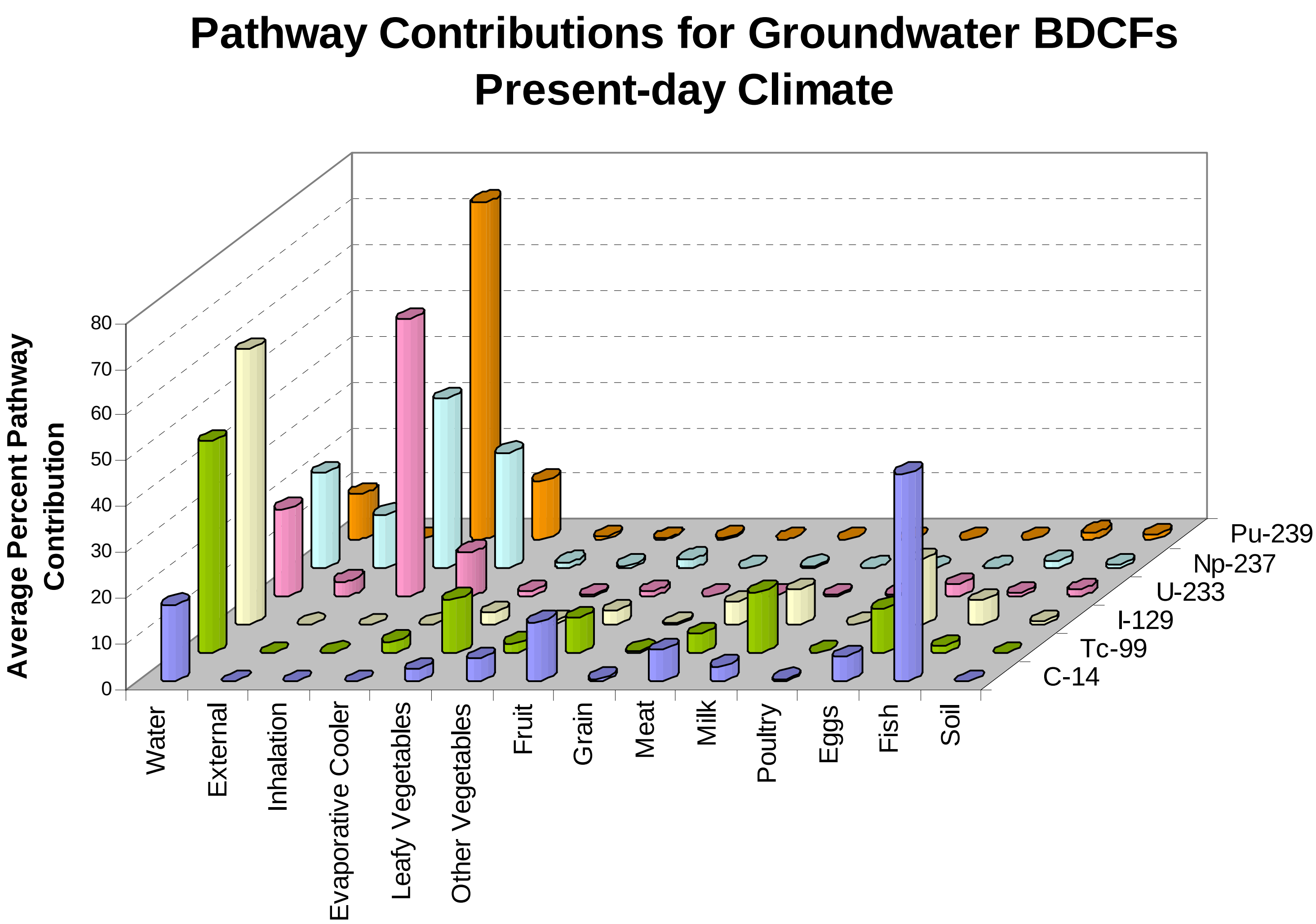




ICRP 72 Dosimetry Models

- Peer Review of DOE Biosphere Model by International Atomic Energy Agency (IAEA), recommended use of more modern dosimetric data
  - International Commission on Radiological Protection 72 provides updated models and related parameters for calculation of exposure from radioactive materials
- NRC has granted licensee requests to use revised ICRP internal dosimetry models on a case-by-case basis (SECY-01-0148). NRC staff noted:
  - it is generally agreed among the national and international scientific community that the newer models provide more accurate dose estimates than the models used in Part 20
- EPA has used these updated models in its activities addressing the Comprehensive Environmental Response, Compensation and Liability Act (CERCLA) activities

Biosphere Pathway Contribution Using ICRP 72 Dosimetry Models

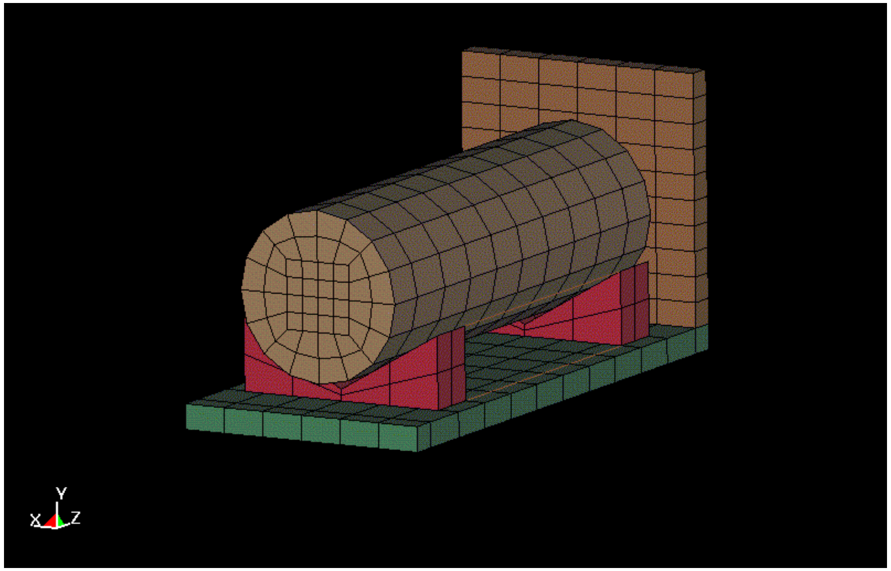


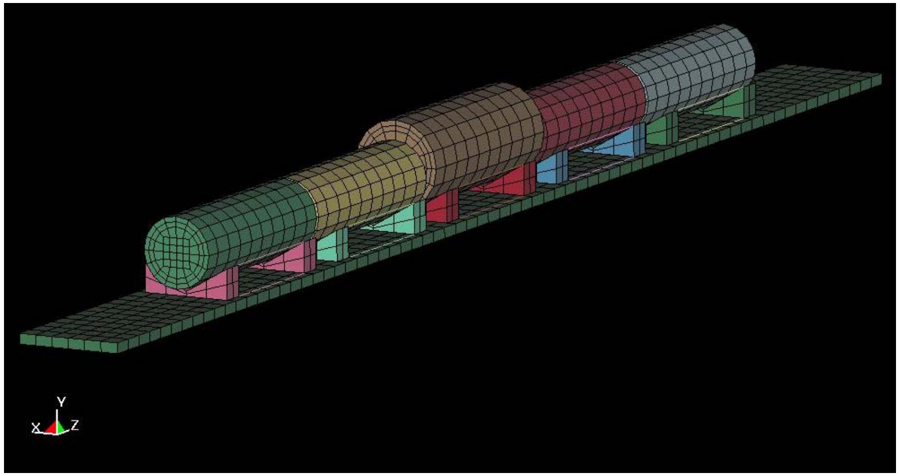
Seismic-Induced Mechanical Damage Effects

- **Seismic-induced mechanical damage is a function of**
  - **magnitude of event which is a function of recurrence probability**
  - **peak ground velocity (PGV)**
  - **model of mechanical damage**
- **Recurrence probability and PGV were discussed with NWTRB by John Ake in May and September 2004**
- **Mechanical damage representation is a function of end constraints on model**

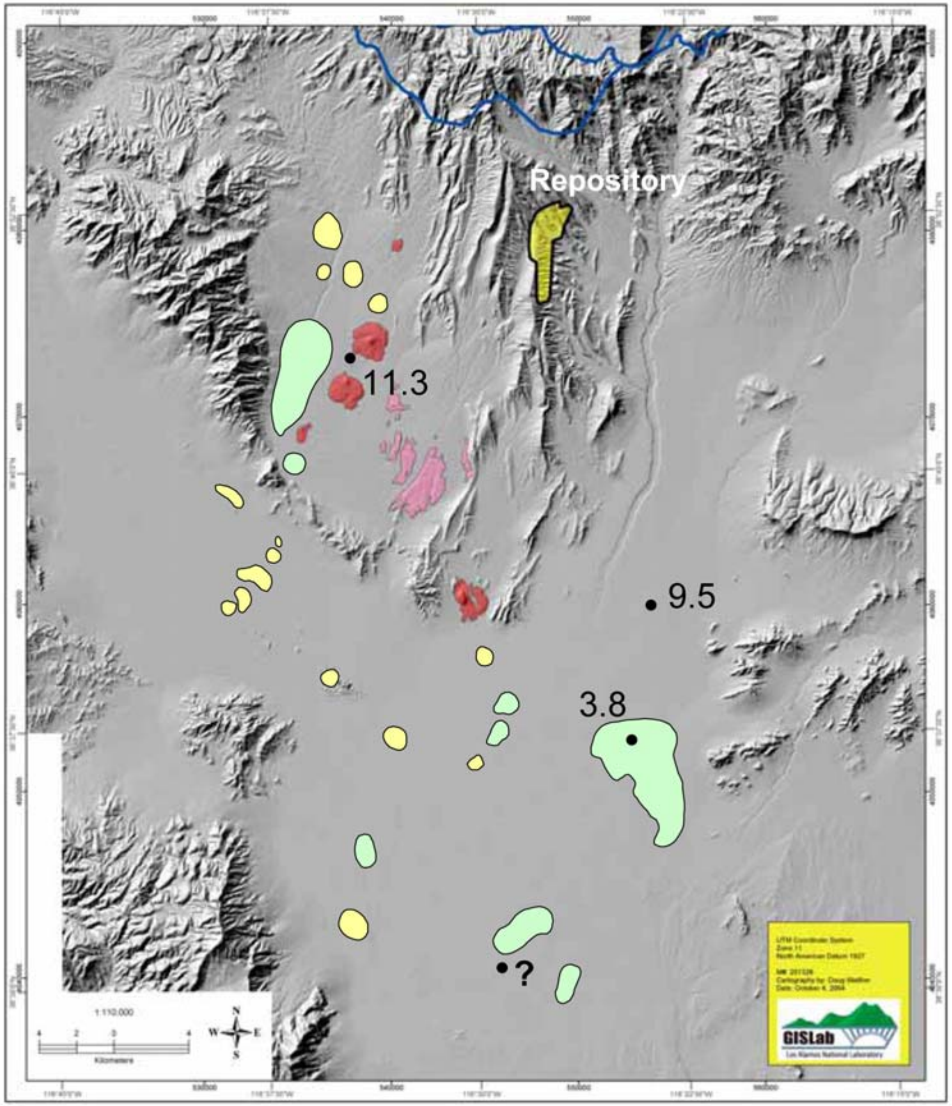
Revised Seismic Mechanical Damage Models

- Constrained model (upper right) conservatively assumed a waste package confined within closed surfaces representing the adjacent waste packages, drift walls and roof
- More reasonable representation (lower right) assumes a string of waste packages capable of synchronous motion
- Analyses underway for open and collapsed emplacement drifts
- Parametric analysis of waste packages response to 17 potential ground motions at postclosure annual probability levels of 10^{-5}, 10^{-6} and 10^{-7}
- Results to date indicate a difference of about a factor of 5 in waste package end-to-end impacts and impact relative velocity



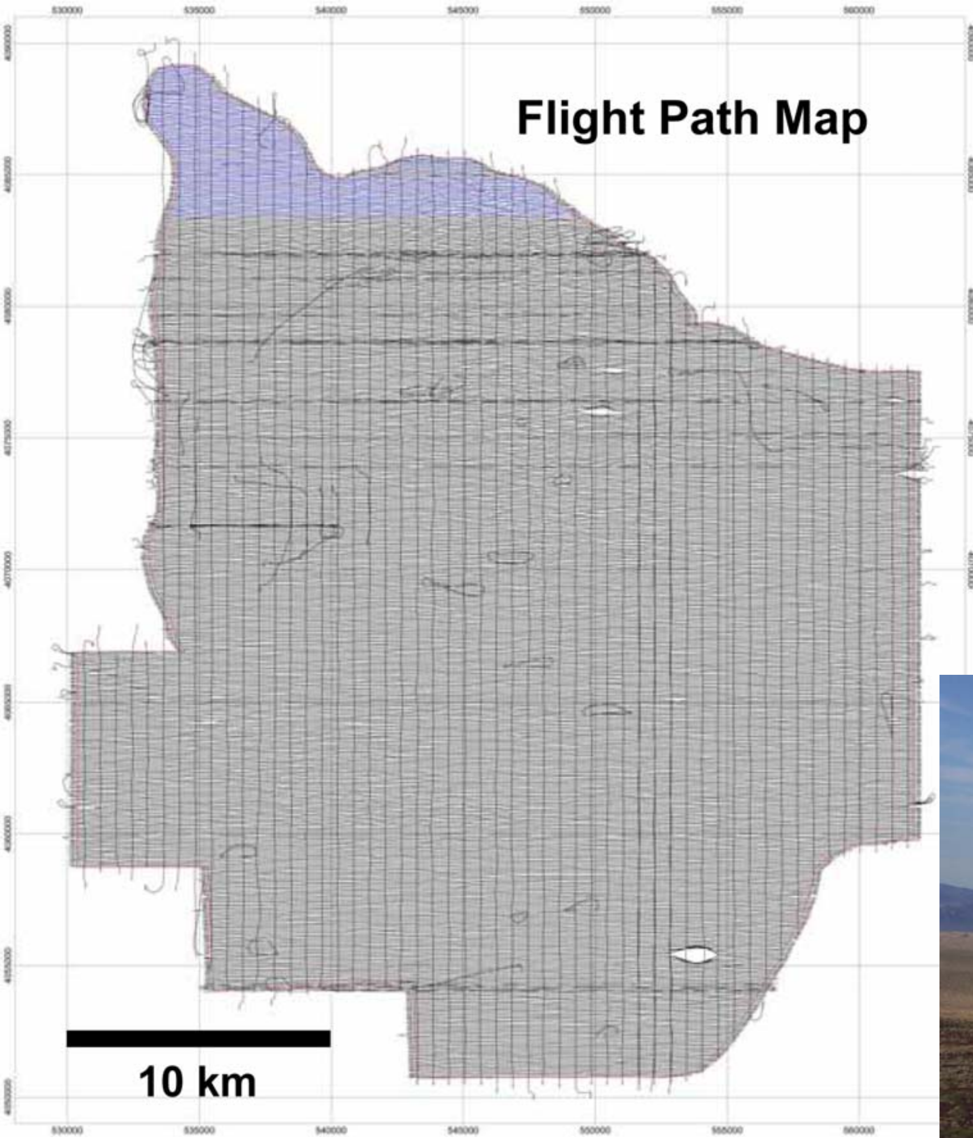


Aeromagnetic Data Interpretation of Potential Buried Volcanic Centers – History



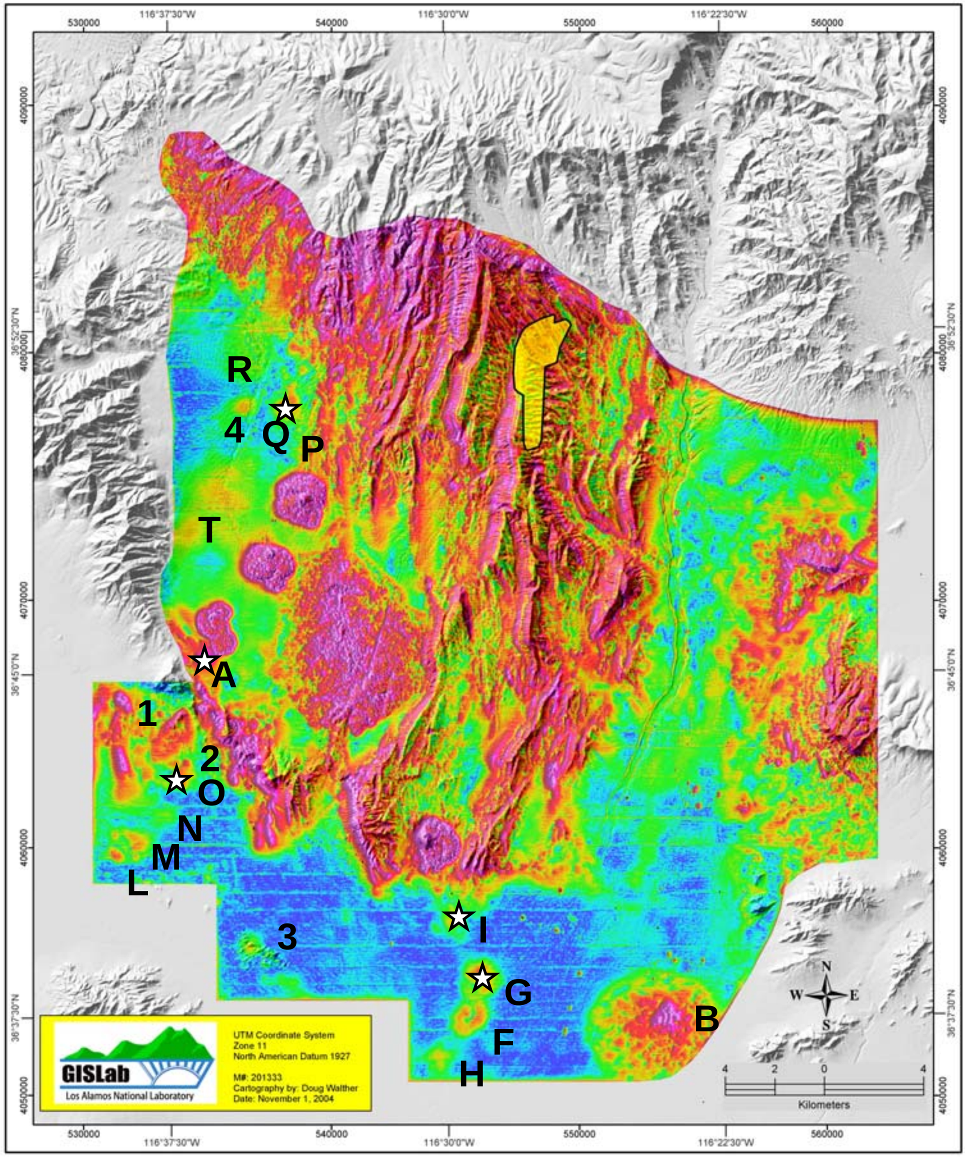
- Eight aeromagnetic anomalies (possible buried basalt) known at time of 1996 Probabilistic Volcanic Hazard Assessment (PVHA) expert elicitation (in green)
- Fifteen additional anomalies identified since 1996 in ground and aeromagnetic surveys (O'Leary et al, 2002) (in yellow)
- Buried basalt identified in four boreholes (ages in millions of years)

2004 Yucca Mountain Aeromagnetic Survey



- High-resolution, low altitude helicopter survey designed to optimize detection of subsurface basaltic features
- East-west flight lines spaced 60 m apart
- North-south tie lines spaced 600 m apart
- Total of 16,000 km of flight line data acquired, covering an area of approximately 870 km²

2004 Aeromagnetic Results and Interpretation



- Map emphasizes shallow, high-amplitude magnetic features
- Analytic signal in Crater Flats (Q and P) likely represent faulted tuff
- Drilling (stars) will evaluate presence of basalt and, if present, the age
- Provide input to PVHA update (ongoing)

Summary

- Collection of scientific data continues
- These data are being used to
  - support the evaluation of the relevance of particular FEPs
  - support (or revise) the models and parameters used in support of the TSPA and SAR
- Scientific testing will continue through the Performance Confirmation period