Data and Modeling for Predicting Radionuclide Transport

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Presentation to the National Academy of Sciences
WIPP Review Panel

August 12-14, 1991
Idaho Falls, Idaho
Summary of Key Points

- $K_d$ model is of questionable utility for WIPP

- Successfully demonstrated adsorption model for uranium

- Adsorption model can predict retardation given technically-feasible data describing radionuclides

- Field-scale chemical/transport model will provide sensitivity of retardation to:
  - heterogeneity,
  - water compositions,
  - and source term,
  as validated by integrated experiments
Outline

- Summary of Recent Culebra Characterization Work
- Relationship of Big Picture to Little Picture
- $K_d$ Model and Available WIPP Culebra Data
- Adsorption Studies
- Solubility and Speciation Studies
- Integrated Chemical/Transport Model
- Conclusions
Major Characterization Work

Rustler formation (SAND87-7036, T Sowards, K Keil)  
- mineral composition vs location and depth

Culebra dolomite member (SAND90-7008, T Sowards, K Keil)  
- contains dolomite, gypsum, calcite, corrensite

Culebra fracture surfaces (SAND90-7019, T Sowards)  
- horizontal fractures along clay seams

Water compositions along “fast path”  
(SAND90-0418, 0419, Seigel)  
- Chemical interaction with other members necessary to describe water composition variation
Sample Locations for Characterization Reports

A: RUSTLER FORMATION
B: CULEBRA DOLOMITE
C: CULEBRA FRACKURES
D: WATER COMPOSITIONS ON "FAST PATH"

0 1 2 3 4 mi
0 2 4 6 km

H-8
H-9
- Engle Well

Fast Path
Five Culebra Groundwaters and Four Simulants Used for Batch Kd Experiments Show Wide Variation in Ionic Strength
Demonstrate Strength of Chemical Barrier in Important PA Scenarios

Culebra Dolomite

Fracture Castile Brine Reservoir

Tamarisk Member
Culebra Member (fractured)
Unnamed Member

Borehole into Repository

Flow
Radionuclide Plume
Mechanisms Causing Retardation in the Rock Matrix

Corrensite (clay) Fracture Lining

Diffusion

Soluble Species

Fracture

Flow

PuO$_2^{2+}$ UO$_2^{2+}$

Dolomite Matrix

Adsorption

PuO$_2^{2+}$ OH

O$^-$

Clay or Dolomite Particle

PuO$_2^{2+}$ Mg$^+$

Ion Exchange
Chemical Phenomena Responsible for Retardation

**Adsorption**

PuO$_2^{2+}$

OH

O$^-$

**Precipitation**

Na$^+$ + PuO$_2^{2+}$ + CO$_3^{2-}$ $\rightarrow$ NaPuO$_2$CO$_3$ (s)

**Coprecipitation**

0.99Ca$^{2+}$ + 0.01PuO$_2^{2+}$ + CO$_3^{2-}$

Coprecipitated Pu with CaCO$_3$ (s)

**Clay or Dolomite Particle**

PuO$_2^{2+}$

Mg$^+$

**Ion Exchange**
The $K_d$ Sorption Model

- Assumes retardation is a linear function of $K_d$
- Approximate relationship for the Culebra

$$R = 1 + 10 \, K_d$$

$K_d$ in $\frac{ml}{g}$
Current Assumptions in WIPP Application of the $K_d$ Sorption Model

- $K_d$ is independent of
  - liquid to solid ratio used in batch experiments
  - Culebra substrate composition and sample preparation
  - solution composition
Batch Kd Data for Uranium Sorption Depend on Solution Volume to Rock Mass Ratio, and Pretreatment of Rock

Data from SAND80-1595, R.G. Dosch; Figure from SAND91-1299, C.F. Novak

![Graph showing Batch Kd Data for Uranium Sorption Depend on Solution Volume to Rock Mass Ratio, and Pretreatment of Rock.](image)

- **Approximate in Situ Ratio**: Solution is Groundwater C
Batch Kd Data for Uranium Depend on Water Composition and Culebra Rock Sample

Data from SAND80-1595, R.G. Dosch; Figure from SAND91-1299, C.F. Novak

![Diagram showing Batch Kd Data for Uranium Depend on Water Composition and Culebra Rock Sample]

- Groundwater C
  - IS = 0.089 m
- "Culebra H2O"
  - IS = 0.23 m
- Brine B
  - IS = 5.6 m
- Brine A
  - IS = 7.8 m
Current Assumptions in WIPP Application of the $K_d$ Sorption Model

- $K_d$ is independent of
- liquid to solid ratio used in batch experiments \textit{CONTRADICTED BY DATA}
- Culebra substrate composition and sample preparation \textit{CONTRADICTED BY DATA}
- solution composition \textit{CONTRADICTED BY DATA}
<table>
<thead>
<tr>
<th></th>
<th>Brine A</th>
<th>Brine B</th>
<th>Groundwater C</th>
<th>&quot;Culebra H2O&quot;</th>
<th>Brine B + Organics</th>
</tr>
</thead>
<tbody>
<tr>
<td>U</td>
<td>8</td>
<td>8</td>
<td>28</td>
<td>8</td>
<td>~16</td>
</tr>
<tr>
<td>Am</td>
<td>0</td>
<td>3</td>
<td>3</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>Np</td>
<td>0</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Eu</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>Pu</td>
<td>0</td>
<td>10</td>
<td>2</td>
<td>4</td>
<td>~45</td>
</tr>
</tbody>
</table>
Model for Adsorption, General Framework

- Explicitly accounts for the chemical mechanism primarily responsible for retardation

- Predicts adsorption, and thus retardation, as a function of water and mineral chemistry

- Provides sensitivity to such parameters as:
  - liquid to solid ratio
  - substrate composition

- Ready for application, but data are needed
Model for $\text{UO}_2^{2+}$ Adsorption on Corrensite
SAND90-7084, J. Leckie

U(\text{VI}) = 10^{-6} \text{M}
I = 0.01 \text{M NaClO}_4
V/M = 10^4 \text{ ml/g}

CO_3 = 10^{-5}

CO_3 = 10^{-4}

\% Adsorbed

pH

U(\text{VI}) = 10^{-6} \text{M}
I = 0.01 \text{M NaClO}_4
\text{w/o CO}_2

V/M = 10^3 \text{ ml/g}

\% Adsorbed

pH
Adsorption Data Measurement and Modeling

1. Work in Progress

Measure $\text{UO}_2^{++}$ adsorption
- on corrensite as a function of concentrations of $\text{Na}^+$, $\text{Ca}^{++}$, $\text{K}^+$, $\text{Mg}^{++}$, $\text{Cl}^-$, $\text{SO}_4^{2-}$, $\text{B(OH)}_3^0$, and EDTA
- on corrensite for simulated WIPP Culebra waters

Validate $\text{UO}_2^{++}$ adsorption model against measurements in WIPP Culebra waters
Adsorption Data Measurement and Modeling

2. Proposed Work

- Measure $\text{UO}_2^{++}$ adsorption on dolomite as function of water compositions

- Measure adsorption of important radionuclides on corrensite and dolomite as function of water compositions

  - important radionuclide include:
    Am, Cm, Pb, Np, Pu, Ra, Th, U
Solubility and Speciation Studies

1. Solubility

- Empirical Studies
- Provide steady-state concentrations of radionuclides in Culebra waters
- Determine solubility-controlling minerals
- Provide steady-state redox states
  - a controlling factor for retardation
APPROACH TO EQUILIBRIUM OF ALSinR (SYNTHETIC) WATER SOLUTIONS OF PLUTONIUM IN DIFFERENT OXIDATION STATES at pH 7.5 and 25 °C
Solubility and Speciation Studies

2. Speciation

- Mechanistic Studies

- Provide species complexation in Culebra waters
  - a controlling factor for retardation

- Yields sensitivity of retardation to water composition

- Allows mechanistic extension of column/field retardation data to off-site transport path lengths
Integrated Chemical/Transport Model

- Incorporates submodels for chemistry responsible for retardation

- Validated against column experiments

- Aids in planning field-scale experiments and additional column experiments

- End result is retardation data for PA
Schematic Assembly of Fracture/Matrix Transport Model for Field Scale Simulation

Vertical Communication

Tamarisk Member

Culebra Member (fractured)

Unnamed Member

Borehole into Repository

Radionuclide Plume

Flow
Example Results from Transport Model

![Graph](image-url)
Summary of Approach to Predicting Retardation

- **Integrated-Phenomena Experiments**
  - Batch
  - Column
  - Field

- **Sensitivity**

- **Strategy/Screening**

- **Validation**

- **Single-Phenomenon Experiments**
  - Adsorption
  - Solubility/Speciation

- **Plan/Screen**

- **Parameter Determination**

- **Models for Retardation**
  - Small Scale
  - Field Scale

**Retardation Determination Data to PA**
Conclusions

- $K_d$ model is of questionable utility for WIPP
- Successfully demonstrated adsorption model for uranium
- Complete uranium adsorption model can be applied with data currently being collected
- Data needed for modeling other radionuclides are unavailable but technically feasible
- Field-scale chemical/transport model will provide sensitivity of retardation to heterogeneity, water compositions, and source term, as validated by integrated experiments
Determining Retardation by Integrated-Phenomena Experiments

F. Gelbard

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Fluid Flow & Transport Division
Sandia National Laboratories

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Summary

- Objective: Take credit for retardation by existing chemical barriers in Culebra

- Three integrated-phenomena experiments to demonstrate radionuclide retardation
  - Batch
  - Column
  - Field

- Batch Tests
  - Use crushed rock
  - Provide data of limited use

- Column Tests
  - Use unaltered rock
  - Provide data on radionuclide retardation, scale, and analog retardation

- Field Tests
  - Potentially most informative
  - Definitely most expensive
Demonstrate Strength of Chemical Barrier in Important PA Scenarios

Culebra Dolomite

Fracture Castile Brine Reservoir

Borehole into Repository

Vertical Communication
Flow
Radionuclide Plume

Tamarisk Member
Culebra Member (fractured)
Unnamed Member
Fracture/Matrix Transport in the Rustler

- Vertical Communication
- Flow
- Radionuclide Plume

Borehole into Repository

Tamarisk Member

Culebra Member (fractured)

Unnamed Member
Fracture/Matrix Transport in the Rustler

Vertical Communication

Borehole Into Repository

Radionuclide Plume

Flow

Tamarisk Member

Culebra Member (fractured)

Unnamed Member

Corrensite (clay) Fracture Lining

Diffusion

Soluble Species

Fracture

Flow

PuO$_2^{2+}$ UO$_2^{2+}$

Dolomite Matrix
Mechanisms Causing Retardation in the Rock Matrix

Corrensite (clay) Fracture Lining

Diffusion

Soluble Species

Fracture

Flow

PuO$_2^{2+}$ UO$_2^{2+}$

Dolomite Matrix

Adsorption

PuO$_2^{2+}$

OH

O$^-$

Clay or Dolomite Particle

Mg$^+$

Ion Exchange
Retardation Processes That Influence Radionuclide Transport

\[
R_i = \frac{\text{Velocity of Water}}{\text{Velocity or Radionuclide i}}
\]

- Adsorption
- Ion exchange
- Physical retardation
- Precipitation/Coprecipitation
- Colloid formation
<table>
<thead>
<tr>
<th></th>
<th>Batch</th>
<th>Short Column</th>
<th>Long Column</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Length</strong></td>
<td>NA</td>
<td>3-4 Inches</td>
<td>2-4 feet</td>
</tr>
<tr>
<td><strong>Time</strong></td>
<td>Weeks</td>
<td>Months</td>
<td>~1 year</td>
</tr>
<tr>
<td><strong>Measurement</strong></td>
<td>Solution concentration</td>
<td>Effluent concentration</td>
<td>Effluent concentration</td>
</tr>
<tr>
<td><strong>Surfaces</strong></td>
<td>Artificial</td>
<td>Actual</td>
<td>Actual</td>
</tr>
<tr>
<td><strong>Fluid/Rock</strong></td>
<td>Mismatched</td>
<td>Matched</td>
<td>Matched</td>
</tr>
<tr>
<td><strong>Data</strong></td>
<td>Maximum sorption</td>
<td>Flow and sorption</td>
<td>Flow, sorption, scale effects and concentration profile</td>
</tr>
</tbody>
</table>
Sorbing Field Test Background

- Part of C & C Agreement

- Problems encountered (September 1986)
  - Scoping calculations needed first
  - Difficulty interpreting results
  - Tests at H-3 and/or H-11 begin late FY88 or FY89
  - Environment, cost, and time

- Preliminary design for a sorbing tracer test, SAND86-7177
# Retardation Determination by Flow Tests

<table>
<thead>
<tr>
<th></th>
<th>Short Columns</th>
<th>Long Columns</th>
<th>Field</th>
</tr>
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<tbody>
<tr>
<td><strong>Length</strong></td>
<td>3-4 inches</td>
<td>2-4 feet</td>
<td>100 feet</td>
</tr>
<tr>
<td><strong>Time</strong></td>
<td>Months</td>
<td>~1 year</td>
<td>2-5 years</td>
</tr>
<tr>
<td><strong>Measurement</strong></td>
<td>Radionuclide</td>
<td>Radionuclide</td>
<td>Analog effluent</td>
</tr>
<tr>
<td></td>
<td>&amp; analog effluent</td>
<td>&amp; analog effluent</td>
<td></td>
</tr>
<tr>
<td><strong>Flow Path</strong></td>
<td>Limited</td>
<td>Limited</td>
<td>Part of real world</td>
</tr>
<tr>
<td><strong>Data</strong></td>
<td>Flow and sorption</td>
<td>Flow, sorption, scale effects, concentration profile</td>
<td>Flow, sorption field scale &amp; effects</td>
</tr>
</tbody>
</table>
Integrated-Phenomena Experiments Schedule

<table>
<thead>
<tr>
<th>Year</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rock and Equipment Available</td>
<td>Setup</td>
<td>Batch</td>
<td>Short Columns</td>
<td>Long Columns</td>
<td>Field Test</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Setup</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

8345.991
Int-Phen
Conclusions

- Batch tests use crushed rock and provide limited information
- Column tests use unaltered rock and provide defensible retardation data on small scale
- Column tests on two scales can provide measure of scaling effects
- Column tests provide basis for analog field tests
- Field tests are potentially most informative but use analogs and are costly
WIPP Library

CRITICAL EXPERIMENTS

and

TIME LINES

August 12, 1991

Wendell D. Weart

SNL
Necessary Information Needs for 191 & RCRA PA

- Radionuclide Retardation Data in Culebra
- Validation of Dual Porosity Flow Model
- Salado Gas & Brine Flow Data
- Marker Bed Data (Gas & Fluid Transport)
- Climate Variability Modeling
- 3-D non-Salado Modeling
- Brine Reservoir Characteristics
- Brine Chemistry Data
- Culebra Geochemistry
- Existing Site Characterization Data

- Seal Effectiveness versus Time
- Disturbed Rock Zone Permeability
  - pre-sealing permeability
  - fracture healing in halite
  - grout effectiveness
- Shaft, Drift & Borehole Closure
- Seal/Formation Interface Permeability
- Shaft, Drift & Borehole Seal Designs
- Seal Emplacement Feasibility
- Seal Material Evaluations
  - (emplacement, longevity, compatibility)
- Small Scale Seal Performance Test Data
- Seal Design Concepts
- Preliminary Seal Material Data
  - (crushed salt, concrete formulations)

- Gas Dissipation Data/Model
- Backfill Permeability Data
- Human Intrusion Scenarios
- 3-phase Room Model
- Salt Fracture/Rehealing Data
- Waste & Backfill Compaction Data
- Room Closure Model
- Creep Model (including validation)
- Creep Parameter Data

- Radionuclide Solubility/Leaching Data
- Gas Generation Data
- RCRA VOC Inventory
  - RCRA Non-gas Inventory
  - Radionuclide Inventory
  - Waste Materials Inventory
  - critical need for performance assessment
  - information need mostly satisfied
<table>
<thead>
<tr>
<th>Information Need</th>
<th>Activities Producing Information</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radionuclide Retardation in Culebra</td>
<td>Expert Panel &amp; Laboratory Retardation Experiments</td>
</tr>
<tr>
<td>Waste Radionuclide Solubility</td>
<td>Lab Tests (surrogate &amp; radioactive nuclides)</td>
</tr>
<tr>
<td></td>
<td>Bench &amp; Field Scale Tests (TRU wastes)</td>
</tr>
<tr>
<td>Waste Panel Model</td>
<td>Laboratory/In-Situ Experiments/Analysis/Model Development</td>
</tr>
<tr>
<td>Validation of Dual Porosity Flow Model for Culebra</td>
<td>Analysis &amp; Evaluation of Existing Data</td>
</tr>
<tr>
<td>Salado Gas &amp; Brine Flow Data</td>
<td>Field Experiments/Analysis</td>
</tr>
<tr>
<td>Seal Effectiveness versus Time</td>
<td>Field &amp; Laboratory Experiments/Modeling</td>
</tr>
<tr>
<td>Human Intrusion Parameters</td>
<td>Expert Panel on Human Intrusion</td>
</tr>
</tbody>
</table>

Figure 5. Relationship of Information Needs to Data Gathering Activities for Categories Having High PA Sensitivity
Working-Level Plan Example: Retardation Tests

1.1.5 Non-Salado Flow and Transport

1.1.5.1 Laboratory Studies

1.1.5.1.1 Adsorption Studies

1.1.5.1.2 Radionuclide Solubility & Speciation

1.1.5.1.3 Brine Mixing and Radionuclide Coprecipitation

1.1.5.1.4 Empirical Sorption Studies

1.1.5.1.5 Column Experiments

1.1.5.1.6 Long Core Tracer Tests

1.1.5.1.7 Colloid Characterization & Transport

1.1.5.3 Field Studies

1.1.5.3.5 Sorbing/Retarding Tracer Tests

FY92 FY93

- transfer data to PA
- publish report on uranyl adsorption on corrensite
- research into neptunyl, uranyl & lead ion adsorption on corrensite & dolomite
- publish data report
- publish analysis report
- report on americium solubility
- report on plutonium solubility
- report on uranium solubility
- report on neptunium solubility
- initiate experiments
- complete experiments
- begin setup
- obtain Culebra core samples
- gather data
- complete apparatus construction
- obtain Culebra short core samples
- obtain initial retardation measurements
- setup
- obtain long cores
- apparatus construction complete
- complete experiments
- initiate experiments
- decision point
1.1.2 Transuranic Waste Experiments

1.1.2.2 Solubility Tests
   Site Selection & Prep

1.1.2.2.1 Test Design

1.1.2.2.2 Waste Characterization & Preparation

1.1.2.2.3 Test Operations
   Site Readiness
   Conduct Tests

1.1.2.2.4 Data Analysis

---

Working-Level Plan Example: Solubility Tests

- Site selected
- Issue test reqmts doc
- Test plan issued
- Revise QAPP
- Characterize & prepare waste
- Permitting & site preparation
- Start tests
- Record & validate solubility/leaching data from TRU wastes
- Transfer data to PA

FY92 FY93
1.1.2 Transuranic Waste Experiments

1.1.2.1, 1.1.2.3 Bin/Alcove Tests

NMVP

Issue bin test req'mts doc (Dec 90)

1.1.2.1.1, 1.1.2.3.1 Test Design

1.1.2.1.2, 1.1.2.3.3 Waste Characterization & Preparation

1.1.2.1.3, 1.1.2.3.4 Test Operations

Site Readiness

Conduct Tests

1.1.2.1.4, 1.1.2.3.5 Data Analysis

Wet bin design complete

FSAR addendum complete

Wet bin fabricated

Complete alcove gas barrier design

Revise QAPP

Characterize & prepare waste

Wet bin operational training, ISC & ORR

Record & validate dry & wet bin data

Conduct dry bin tests

Transfer data to PA

Decision on extent of alcove testing

Begin alcove gas barrier tests

Transfer data to PA

Begin preparation of NMVP

Submit NMVP
Performance Assessment Requirements for Bin Tests
40CFR191

- High gas generation rates lead to gas-dominated rooms
  - PA indicates less radioactive release for human intrusion scenarios
- Low gas generation may lead to brine saturated waste
  - PA indicates more release for human intrusion
- Neither case leads to releases in 10,000 years without human intrusion

Conclusion: Lower gas generation rates can lead to more severe waste room source term conditions
Performance Assessment Requirements for Bin Tests
40CFR268 (RCRA/ No Migration Determination)

• High gas generation rates will cause gases to migrate farther along interbeds
  - RCRA gases (VOCs) can be carried along with these gases toward RCRA boundary
• RCRA standard does not require consideration of human intrusion
• Conclusion: High gas generation rates can lead to a more severe waste room source term for VOC migration
Performance Assessment Requirements for Bin Tests

Conclusion

• Neither a high nor a low bounding assessment of gas generation rate is sufficient to assure the most severe long-term conditions for both WIPP standards since the bounds act in opposite directions.

• Conclusion: Realistic values of TRU waste gas generation must be determined to adequately represent the waste room source term for both standards.

• Bin tests are the most realistic simulation of repository/waste gas generation interactions and should be conducted to provide our best understanding of future waste room source term conditions.
Technical Concerns Often Raised Regarding Radioactive Tests at WIPP

Is gas generation really a major issue?

- Performance Assessment to date has not addressed RCRA, an area where high gas generation increases concern for compliance

- Evaluation of both 40CFR191 and RCRA requires best estimates of gas; bounds are not sufficient

- Lack of knowledge on the gas generation issue will not be acceptable to the public
Technical Concerns Often Raised Regarding Radioactive Tests at WIPP

Due to phasing of radioactive tests, experiments have been extended over a greater time interval

- Experience to date supports need to start with least complex test
- High organic waste to be tested in fourth bin
- Wet bins will be conducted as soon as new design bin is available
- All bins will yield data in time to support PA
Technical Concerns Often Raised Regarding Radioactive Tests at WIPP

Radioactive waste tests are commencing later than originally expected

• Wasteform complexity and regulatory & safety requirements do lengthen times

• Characterization will be required to ship waste to WIPP-- tests or not

• Bin tests will provide timely data to PA on present schedule

Test results will be difficult to interpret and extend to WIPP

• Test data will provide statistical knowledge of gas generation in WIPP

• Lab data will supplement bins for phenomenological interpretation

• Extensive test matrix will allow extrapolation to the WIPP repository
Technical Concerns Often Raised Regarding Radioactive Tests at WIPP

Solubility experiments have been removed from the WIPP bin tests

• DOE is committed to accelerating solubility experiments with TRU waste

• Other facilities are being actively considered to speed solubility tests

• New bin design to allow solubility testing at WIPP is being investigated
SUMMARY OF CRITICAL EXPERIMENTS

Retardation in the Culebra Aquifer
- Expert Panel Deliberations in Early 1992
- Laboratory Tests Accelerated

Solubility
- TRU Solubility Tests to Commence in Mid-'92

Bin Test
- Tests with Some High-Organic TRU Earlier in Program
- Redesign of Bins to Accelerate Wet Bin Testing into Mid-'92
- Decision on Alcoves in Early 1993 Based on Results of Bin Tests & Alcove Gas Barrier
Performance Assessment
Panel Modeling, Expert Elicitation, Status

D. R. Anderson and M. G. Marietta

Nuclear Waste Technology Department
Performance Assessment Division
Sandia National Laboratories

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Summary

Introduction - PA Schedules

PA Panel Modeling

- Assimilation of test program data and information into PA calculations
- Calculations still indicate zero release

(CONDITIONAL ON 91 MODELS AND DISTRIBUTIONS)

to the accessible environment (40 CFR 191, Subpart B) for undisturbed conditions
- Human intrusion calculations will be reported in December
Summary (Cont.)

PA expert panels

- Elicitation process, panel deliberations, and results for 1991 Preliminary Comparison

- Ranges and distributions for radionuclide concentrations (solubilities) in Salado brines

  - Ranges and distributions for radionuclide distribution coefficients in Culebra brines

Discussion -
Figure 2: Division 6342 Organization Chart

Division 6342 Program Plan numbers:
- Environmental Impact Statement Numbers by (x)(i) is 1, 1.5, 1.6 x.x
- Suppliers: Divisions 6341, 43, 44, 45, 46

- Compliance documentation, peer review, regulatory comparison & RCRA
- Literature review, waste acceptance criteria task group, RCRA
- Waste management, disposal, engineering & research
- Documentation support
- Compliance documentation, peer review, regulatory comparison & RCRA

- UNCERTAINTY/SENSITIVITY ANALYSIS
- GENIE calculation utility
- CAMCON maintenance & documentation, primary data base development & documentation, QA, execution of annual PA calculation, CAMCON comparisons
- Uncertainty/sensitivity analysis
- SECOXX development & documentation, CFO, MG, 2-phase, QA
- Room & transport modeling
- Repository, shaft, & transport, & cuttings modeling
- AEOSTAT: hydrology & transport modeling
- REACTOR design, hydrology & transport modeling
- Data base development & documentation, primary data base development & documentation, QA
- Data base development & documentation, QA
- Waste management, disposal, engineering & research
- Documentation support
- Compliance documentation, peer review, regulatory comparison & RCRA

- General technical documentation
- CDF construction, general data
- SEGCOX development & documentation
- Climate, technical documentation
- CDF construction, general data

Imbedded in Our Customer/Supplier Model
1.6 Performance Assurance Division Work Breakdown Structure

Customers:
- DOE
- NASA
- ORNL
- ELCID
- Research
Define 191B & RCRA Rec'nts

Develop Criteria for Disposal Phase Decision

Formulate Compliance Assessment Approach

Develop scenarios, probabilities and models for assessing performance

Certified Test Data & Phenomenological Models

Certify PA models & data (VQA)

Perform Calculations

 annual cycle

yes

compliance with as-received waste?

Perform sensitivity analysis

no

Systems Impact Studies

Select & characterize waste

Engineered Alternatives Evaluations

Test Guidance

Test Program

Describe Natural Barriers

Characterize repository environment

Determine waste interaction with repository

Test Guidance with as-received Waste and Baseline Design

Commit to an engineered alternative(s)

refine test plan

consider engineered alternatives

action required?

STOP

STOP

Abandon Project

Disposal Decision

Transformed with modified waste?

yes

no

Figure 4. Post-closure Performance Assessment
Fig. 5. Performance Assessment Time-Phased Activities
<table>
<thead>
<tr>
<th>1991 Preliminary Comparison Report</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOE Review and Workshop</td>
</tr>
<tr>
<td>WIPP Panel Review</td>
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<tr>
<td>Scope &amp; Format Fixed</td>
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<tr>
<td>Volumes I &amp; 2-Writing/Revising</td>
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<td>Vol. I-Methodology, Results, Analyses</td>
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<td>Chapter I, II</td>
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<tr>
<td>III</td>
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<td>VII</td>
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<td>VIII</td>
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<td>IX</td>
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<td>X, XI</td>
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<td>Appendix A-Standard</td>
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<td>Appendix B-Responses</td>
</tr>
<tr>
<td>Vol. II-Modeling Descriptions</td>
</tr>
<tr>
<td>Text</td>
</tr>
<tr>
<td>Appendix A-Computational Data Base</td>
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<tr>
<td>Appendix B-QA</td>
</tr>
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</table>

Draft of 2-AUG-91
1991 Preliminary Comparison Report (continued)

Volumes 1 & 2-Review/Revision/Production
- Deliver to PAPRP, DOE, SNL (9/13)
- DOE Comments Due (10/1)
- PAPRP Mtg. (10/7,8)
- DOE Mtg. (10/15,16)
- Respond to Comments, Revise Doc.
- SNL 6330 Review
- Prepare Pre-Publication Copy
- Deliver to WIPP Panel (11/27)
- Deliver to Print Shop (12/6)
- WIPP Panel Mtg. (12/?)

Volume 3- Reference Data Base
- Writing/Revising
- SNL Review
- Prepare Pre-Publication Copy
- Deliver Pre-Publication Copy to PAPRP (9/13)
- Deliver to Print Shop (9/13)
- PAPRP Mtg. (10/7,8)
- Deliver Pre-Publication Copy to WIPP Panel (11/27)
## 1991 Preliminary Comparison Report (continued)

**Volume 4 - Sensitivity Analyses**
- Writing/Revising
- Deliver to PAPRP, SNL (12/13)
- PAPRP Mtg. (1/7)
- Respond to Comments, Revise Document
- Deliver to Print Shop

## 1991 Comparative Analysis of EATF Options 2 & 6

- Complete Calculations for Options 2 & 6
- Review Calculations
- Continue Calculations if Needed

## 1991 Safety Analysis

- Writing and Revising
- Review
- Deliver to Print Shop

## 1991 Certification of PA Models and Data Report

- Writing and Revising
- Review
- Deliver to Print Shop

---

Draft of 2-AUG-91
System Model: Repository/Shaft

Sub-System Model: Panel

Component Model: Source Term

Process: Radionuclide Solubility
(Am, Np, Pb, Pu, Ra, Th, U)

Parameters: pH
Eh - solubility
Oxidation Potential
Carbonate Present
Chelating Agents
All Radionuclides

Dissolved Concentration (M)

SNL 90 Estimate of Radionuclide Solubility
Expert Panel Estimates of Radionuclide Solubilities

- Pu(IV)
- Np(IV)
- Th(IV)
- U(IV)
- SNL 90

Dissolved Concentration (M)
Measured Data For Radionuclide Solubilities
Expert Panel Estimates of Radionuclide Solubilities

Measured Data For Radionuclide Solubilities

SUMMARY
Summary

Introduction - PA Schedules

PA Panel Modeling

- Assimilation of test program data and information into PA calculations
- Calculations still indicate zero release

(CONDITIONAL ON 91 MODELS AND DISTRIBUTIONS)

to the accessible environment (40 CFR 191, Subpart B) for undisturbed conditions
- Human intrusion calculations will be reported in December
Cuttings

Release of cuttings to accessible environment

Culebra Dolomite

SECO 2D/STAFF2D (Flow/Transport)

Boast II (2-Phase Flow)

Repository

Anhydrite Layers A & B

Sutra (1-Phase Flow)

Panel (Brine Flow)

Panel (Radionuclide Concentrations)

Brine Reservoir

Subsurface boundary of accessible environment

WIPP PA Consequence Modeling
Panel Model

Run Parameters

BRAGFLO
BOAST II
SUTRA

Flow into Panel from Salado

PANEL

Nuclide Transport from Panel into Borehole

STAFF2D

Nuclide Transport in Culebra

SECO2D

Regional & Local Flow Field in Culebra

CUTTINGS

Cuttings Removal from Borehole

CCDFCALC
CCDFPLOT

Uncertainty Analysis Results

STEPWISE
PCCSRC

Sensitivity Analysis Results

Diagrammatic Representation of Example Analysis
Data Flow for 91 PA Panel Model

Components: Salado Geology/Hydrology and DRZ

Gorham (6/91), Beauheim and Howarth (6/91), Beauheim (3/90), Finley (6/91)
Fluid Flow and Transport Division

Intact and DRZ Halite and Anhydrite
Pore Pressure
Permeability
Diffusivity

Wawersik (8/91, 12/89)
Geomechanics Division

Fracturing
Pore Pressure

BEAUHEIM AND HOWARTH

(6/91)

QPP01 (MB 138) 13.9 MPa
QPP02 (Map Unit 13) 1.1 MPa
QPP03 (Anhydrite b) 12.8 MPa
QPP04 (Map Unit 7) 10.3 MPa
QPP05 (Map Unit 6)

QPP15 (Map Unit 0)
QPP14 (Polyhalite halite)
QPP13 (MB 139) 12.8 MPa
QPP12 (Halite below clay c) 8.6 MPa
QPP11 (Halite below anh. c)

Map Unit 3

QPP21
QPP22 9.1 MPa
QPP23 9.4 MPa
QPP24 9.1 MPa
QPP25 9.1 MPa
Permeability
Stiff-matrix Model
No damage zone
\[ C_{test-zone} = C_{brine} \]
Pre-excitation
No borehole closure

Beauheim and Howarth
(6/91)

QPP15 (Map Unit 0) TLTM
QPP14 (Polyhalitic halite) TLTM
QPP13 (MB 139) 3 E-22 m²
QPP12 (Halite below clay d) 2 E-23 m²
QPP11 (Halite below anh. c) TLTM

QPP01 (MB 138) 1.5 E-21 m²
QPP02 (Map Unit 13) TLTM
QPP03 (Anhydrite b) 2.4 E-22 m²
QPP04 (Map Unit 7) 5 E-23 m²
QPP05 (Map Unit 6) TLTM

QPP21 TLTM
QPP22 1 E-22 m²
QPP23 1 E-21 m²
QPP24 1 E-21 m²
QPP25 1 E-22 m²
Beauheim and Howarth (6/91)

Summary Of Permeability Testing Results

1. Halite permeability is typically < $10^{-20}$ m$^2$. Anhydrite permeability is typically between $10^{-19}$ and $10^{-18}$ m$^2$.

2. Halites containing no clay show no permeability (limit of resolution is approximately $10^{-23}$ m$^2$) or apparent pore pressure.

3. Pore pressures approaching lithostatic pressure are observed in anhydrites far from excavations.

4. Pore pressures decrease with increasing proximity to excavations.

5. Uncertainty in the specific storage of halite results in significant uncertainty in permeability, potential flow volumes, and the radius of influence of the tests.

6. Constant-pressure flow tests can help resolve uncertainty in specific storage.
Conclusions
Beauheim and Howarth (6/91)

1. A simple Darcy flow model is adequate to explain all anhydrite tests and about half of the halite tests. The remainder of the halite tests show no apparent permeability.

2. Hydraulic properties are different between strata, and also exhibit lateral heterogeneity within individual strata.

3. Within the DRZ around the excavations, pore pressures are lower and permeabilities are higher than in the far field. Specific storage is probably also higher within the DRZ. We cannot as yet define the boundaries of the DRZ, or the exact nature or mechanics of the changes that occur within the DRZ.

4. No evidence has been observed to date of two-phase flow under undisturbed (far-field) pressures. Two-phase flow does appear to occur in anhydrite interbeds close to excavations where significant depressurization has occurred.
Data Flow for 91 PA Panel Model, Cont.

Component: Creep Closure/Expansion

Munson (12/88)
Repository Isolation Division

Elastic Constants
Creep Constituitive Model Constants
Data Flow for 91 PA Panel Model, Cont.

Component: Waste-Form and Backfill Compaction

Mendenhall (6/91) and Butcher (9/89)
Disposal Room Systems Division

Waste-Form (as received for 91 PA)
Porosity and Permeability

Peterson (IDB 90, IT)
Performance Assessment Division

Material Inventory (volumes and masses of metals, cellulosics, organics, and sludges)
Approaches for Capturing the Disposal Room Model into Performance Assessment

- Three phase flow models
- Simplified closure descriptions (IT type EATF models)
- Path dependent porosity surfaces

Mendenhall (6/91)
Summary
Mendenhall (6/91)

- A Disposal Room Model has been developed that takes into account:
  - Salt creep
  - Backfill
  - Waste
  - Gas generation
  - Preexisting cracks
  - Preliminary study of geomechanical and saturated fluid flow

- The Model has been exercised with various test problems and the results of these test problems presented.

- Work is progressing to develop approaches that incorporate the results of the Disposal Room Model into the Performance Appraisal process.

- Work that still needs to be done includes:
  - Panel scale modeling
  - Human intrusion
  - Complete coupled geomechanical-fluid flow models
  - Crack opening in an isolated or edge room
Data Flow for 91 PA Panel Model, Cont.

Component: Gas Generation

Brush (3/91, 12/90, 12/89, 12/88)
Disposal Room Systems Division
Gas Generation Rates

Peterson (IDB 90, IT)
Performance Assessment Division
Material Inventory (volumes and masses of metals, cellulosics, organics, and sludges)
Data Flow for 91 PA Panel Model, Cont.

Component: Brine/Gas Flow

Davies (12/89)
Fluid Flow and Transport Division

Threshold Pressure
Residual Saturation
Brooks and Corey Exponent
Capillary Pressure
Relative Permeability
Data Flow for 91 PA Panel Model, Cont.

Component: Source Term

Phillips and Butcher (8/91)
Brush (3/91 ...)
Disposal Room Systems Division

Radionuclide Solubility (expert panel)

Peterson (IDB 90, IT)
Performance Assessment Division
Radionuclide and RCRA Inventory
Modeling Guidance for 91 PA Panel Model

Davies (12/89, 9/90)
Fluid Flow and Transport Division
Code: ECLIPSE

Webb
Fluid Flow and Transport Division
Code: TOUGH

Mendenhall and Butcher (6/91, 9/89)
Disposal Room Systems Division
Weatherby (12/89)
Engineering and Structural Mechanics Division
Code: SANCHO
Davies (9/90)
Summary Observations - Fixed "Inundated"
Gas Generation Rates

- Gas release through interbeds causes significant reduction in peak room pressure and in gas energy stored in disposal room.

- Peak room pressure is sensitive to degree of room closure and to interbed intrinsic permeability; peak room pressures range from approximately 12 1/2 to 24 1/2 MPa.

- Stored gas energy is also sensitive to room-closure state, however, the impact is opposite in character to that of peak room pressure.
• Once gas penetrates an interbed, lateral migration occurs relatively efficiently.

Within the first several tens of meters, gas pressure within the interbed tracks gas pressure in the room quite closely.

• If gas pressures exceed lithostatic, a likely response will be dilatation and/or extension of preexisting, near-horizontal fractures within the interbeds.

The magnitude of interbed permeability (fracture aperture) increase required to maintain room pressure \(\leq 15\) MPa is small.
Davies (9/90)
Summary Observations - Variable Gas Generation Rates

- All simulations (fixed and variable rate) suggest that much of the room remains highly unsaturated due to limited brine inflow.

- Simulations in which gas generation rates vary as a function of local saturation conditions produce significant differences in system response than are produced by fixed rate simulations.

- Peak room pressures are lower than in comparable fixed rate simulations by as much as 10 MPa; peak pressures range from approximately 13 1/2 to 15 1/2 MPa.
Davies (9/90)
Summary Observations - Variable Gas Generation Rates (cont.)

- Peak room pressure is much less sensitive to interbed permeability and room-closure state than in comparable fixed rate simulations.

- Unlike the fixed rate simulations, the variable rate simulations produce lower peak pressures in the fully consolidated room-closure state than are produced in the intermediate room-closure state simulations. This occurs because gas generation in the variable rate simulations is closely tied to brine availability, and less brine enters the fully consolidated room due to more rapid pressurization.
Intrusion Borehole

Anhydrite Layers A and B

With Open Fractures Due to Excavation
Within Intact Salado

Disturbed Rock Zone

Waste Room

Salt

Disturbed Rock Zone

With Open Fractures Due to Excavation
Within Intact Salado

Salt

MB139

SUTRA Geologic/Waste Panel Model.
91 Panel Model (BRAGFLO)

Two dimensional cylindrical geometry

Materials - Culebra, Salado (halite, anhydrite, MB139, DRZ), Waste, HI borehole fill, Castile

No-flow boundaries

Two-phase (brine and gas) Darcy flow

Brooks-Corey relative permeabilities and capillary pressure

Dissolved gas
91 Panel Model (BRAGFLO), Cont.

- Saturation dependent corrosion and biodegradation rates
- Brine and iron consumption during corrosion
- Cellulose consumption during biodegradation
- Fully implicit and coupled (handles HI)
- Time invariant room porosity for 91 only
- Rock and fluid compressibilities
91 Panel Model (BRAGFLO), Cont.

Anisotropic permeabilities

Gravity effects

Benchmarked against BOAST, TOUGH, and ECLIPSE

Based on three-phase compositional petroleum model (TSRS) used for enhanced oil recovery and tar sands

PANEL/calculates radionuclide concentration up to solubility limit or inventory limit and radionuclide flux into HI borehole
BENCHMARK #2

Conditions:

<table>
<thead>
<tr>
<th>Room</th>
<th>Salado</th>
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<tbody>
<tr>
<td>P = 0.1 MPa</td>
<td>11 MPa</td>
</tr>
<tr>
<td>ϕ = 1.0</td>
<td>0.01</td>
</tr>
<tr>
<td>k = 10^{-11} m^2</td>
<td>10^{-18} m^2</td>
</tr>
</tbody>
</table>

Gas Generation: 2 x 10^{-7} kg/sec/m^3

Simulate 700 yr

Fluids: Air, Water

Fluid Compressibility
Dissolved Gas
Brooks-Corey Relative Permeability
Benchmark #2

BRAGFLO

Time (x 10^6)

BOAST

Time (x 10^6)

TOUGH

Time (years)

Reporification Pressure (Pa x 10^6)

- - - Gas Sand

- - - All Brine

Time (sec x 10^6)
**BENCHMARK #3**

<table>
<thead>
<tr>
<th>Material</th>
<th>Index</th>
<th>$\chi$</th>
<th>$P_{Threshold}$</th>
<th>$S_{or}$</th>
<th>$S_{gr}$</th>
<th>$k_x$</th>
<th>$k_y$</th>
<th>$\phi$</th>
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<tr>
<td>Salado</td>
<td>1</td>
<td>0.7</td>
<td>23.0</td>
<td>0.2</td>
<td>0.2</td>
<td>$1.0 \times 10^{-21}$</td>
<td>$1.0 \times 10^{-21}$</td>
<td>0.01</td>
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<tr>
<td>Salado-DRZ</td>
<td>2</td>
<td>0.7</td>
<td>$2.0 \times 10^{-3}$</td>
<td>0.2</td>
<td>0.2</td>
<td>$1.0 \times 10^{-21}$</td>
<td>$1.0 \times 10^{-17}$</td>
<td>0.01</td>
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<td>MB30-DRZ</td>
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<td>0.7</td>
<td>$2.0 \times 10^{-3}$</td>
<td>0.2</td>
<td>0.2</td>
<td>$1.0 \times 10^{-18}$</td>
<td>$1.0 \times 10^{-17}$</td>
<td>0.10</td>
</tr>
<tr>
<td>MB30</td>
<td>4</td>
<td>0.7</td>
<td>$2.0 \times 10^{-3}$</td>
<td>0.2</td>
<td>0.2</td>
<td>$1.0 \times 10^{-18}$</td>
<td>$1.0 \times 10^{-18}$</td>
<td>0.01</td>
</tr>
<tr>
<td>Anhydrite-DRZ</td>
<td>5</td>
<td>0.7</td>
<td>$2.0 \times 10^{-3}$</td>
<td>0.2</td>
<td>0.2</td>
<td>$1.0 \times 10^{-18}$</td>
<td>$1.0 \times 10^{-17}$</td>
<td>0.10</td>
</tr>
<tr>
<td>Anhydrite</td>
<td>6</td>
<td>0.7</td>
<td>0.3</td>
<td>0.2</td>
<td>0.2</td>
<td>$1.0 \times 10^{-18}$</td>
<td>$1.0 \times 10^{-18}$</td>
<td>0.01</td>
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<tr>
<td>Waste</td>
<td>7</td>
<td>2.89</td>
<td>$2.0 \times 10^{-3}$</td>
<td>0.276</td>
<td>0.02</td>
<td>$1.0 \times 10^{-15}$</td>
<td>$1.0 \times 10^{-15}$</td>
<td>0.08</td>
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</table>

* Brooks-Corey Equation for Relative Permeability*
Benchmark #3

4.1 km
31 Blocks

Intrusion Borehole

Anhydrite Layers A and B
With Open Fractures Due to Excavation
Within Intact Salado

Disturbed Rock Zone

Waste Room

Disturbed Rock Zone

Salt

Simulate 10000 yrs
0 - 527 yrs Gas Generation 1.823 lb/day
527 - 712 yrs Gas Generation 0.603 lb/day
1200 yrs Intrusion
Modeling Guidance for 91 PA Panel Model

Performance Assessment Division

Codes: NORIA, SUTRA, STAFF2D, BOAST, BRAGFLO
Performance Assessment

Undisturbed Scenario Calculations
- Brine Transport
- Radionuclide Transport

Human Intrusion Scenario Calculations

--- To Be Reported in December ---
Undisturbed Conditions: Solute Mass Fraction at 10,000 Years in MB139 Below Panels
Undisturbed Conditions: Solute Concentrations at 10,000 Years

CONPU239

0.0020E-3
0.0520E-3
0.1020E-3
0.1520E-3
0.2020E-3
Undisturbed Conditions

Including Waste-Generated Gas Effects

Assuming No Fracturing Occurs

(CONDITIONAL on 91 MODELS and DISTRIBUTIONS)

Zero Releases in 10,000 Years

Compliance with Individual Protection

For 91 Calculations, Only HI Scenarios Contribute to CCDF for Containment

(Same as 89 and 90 Calculations)
Expert Panels for Parameter Elicitation

Expert Panel on Radionuclide Source Term

Composition

- All external experts

Results

- Ranges and distributions of the concentrations of radionuclides in brines in the rooms and drifts
  - Am, Cm, Np, Pu, Th, U, Ra, Pb
Expert Panel on Radionuclide Source Term (cont.)

Selection of panelists

- Nominations
  - Initial nominees from several outside sources
  - Additional nominations from all those contacted

- Selection criteria

- Selection committee
  - Dr. Ross Heath, University of Washington (oceanography)
  - Dr. Detlof von Winterfeldt, University of Southern California (decision analysis)
<table>
<thead>
<tr>
<th>Name</th>
<th>Organization</th>
<th>Discipline</th>
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<tbody>
<tr>
<td>Carol Bruton</td>
<td>Lawrence Livermore National Laboratory</td>
<td>Geochemistry</td>
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<tr>
<td>I-Ming Chou</td>
<td>U.S. Geological Survey</td>
<td>Geochemistry</td>
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<tr>
<td>David Hobart</td>
<td>Los Alamos National Laboratory</td>
<td>Actinide Chemistry</td>
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<tr>
<td>Frank Millero</td>
<td>University of Miami, Rosenstiel School</td>
<td>Physical Chemistry</td>
</tr>
<tr>
<td></td>
<td>School of Marine &amp; Atmospheric Science</td>
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</tbody>
</table>
Expert Panel on Radionuclide Source Term (cont.)

Results

- Organized themselves into a team to utilize different areas of expertise.

- Established a strategy for developing probability distributions for radionuclide concentrations due to dissolved material.

  - With little data, the strategy was based on
    - basic solubility principles
    - experimental data where available
    - considering the effect of variable conditions
    - judgement based on experience
  
  - The concentrations are theoretical values which may be higher than what could exist at the WIPP given the inventory.
Expert Panel on Radionuclide Source Term (cont.)

Results

- Were not able to develop probability distributions for radionuclide concentrations due to suspended material.

- Correlations between radionuclides
  - Possibly between Am (III) and Cm (III)
  - Np (IV) and Pu (IV)
<table>
<thead>
<tr>
<th>Element</th>
<th>Solution Species</th>
<th>Solid Species Maximum and Minimum</th>
<th>Condition</th>
<th>Cumulative Probabilities of Concentrations (M)</th>
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</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.0</td>
</tr>
<tr>
<td>Pb(II)</td>
<td>PbCl$_4^{2-}$</td>
<td>PbCO$_3$ Carbonate Present</td>
<td></td>
<td>1.0 x 10$^{-9}$</td>
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<tr>
<td></td>
<td></td>
<td>PbCl$_2$ Carbonate Absent</td>
<td></td>
<td>0.01</td>
</tr>
<tr>
<td>Ra(II)</td>
<td>Ra$^{2+}$</td>
<td>RaSO$_4$ Sulfate Present</td>
<td></td>
<td>1.0 x 10$^{-11}$</td>
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<td></td>
<td></td>
<td>RaCO$_3$ Carbonate Present</td>
<td></td>
<td>1.6 x 10$^{-9}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>RaCl$_2$·2H$_2$O Carbonate and Sulfate Absent</td>
<td></td>
<td>2.0</td>
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<tr>
<td>Th(IV)</td>
<td>Th(OH)$_4$</td>
<td>Th(OH)$_4$</td>
<td></td>
<td>5.5 x 10$^{-6}$</td>
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<tr>
<td>U(VI)</td>
<td>UO$_2$(CO$_3$)$_2$</td>
<td>UO$_3$·2H$_2$O</td>
<td></td>
<td>1.0 x 10$^{-7}$</td>
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<td></td>
<td></td>
<td>UO$_2$ (amorphous) U$_3$O$_8$</td>
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</tr>
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<td>Element</td>
<td>Solution Species</td>
<td>Solid Species Maximum and Minimum</td>
<td>Condition</td>
<td>Cumulative Probabilities of Concentrations (M)</td>
</tr>
<tr>
<td>---------</td>
<td>-----------------</td>
<td>----------------------------------</td>
<td>-----------</td>
<td>-----------------------------------------------</td>
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<tr>
<td>Np(V)</td>
<td>(NpO₂CO₃⁻)</td>
<td>NpO₂(OH)₃⁻⁻⁻ Np₂O₇(0H)</td>
<td>0.0</td>
<td>3.0 x 10⁻¹¹ 3.0 x 10⁻¹⁰ 3.0 x 10⁻⁸ 6.0 x 10⁻⁷ 1.0 x 10⁻⁵ 1.2 x 10⁻³ 1.2 x 10⁻²</td>
</tr>
<tr>
<td></td>
<td>(amorphous)</td>
<td>N₂Np₂O₂CO₃⁻ -3.5H₂O</td>
<td>0.10</td>
<td></td>
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<tr>
<td></td>
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</tr>
<tr>
<td>Np(IV)</td>
<td>(Np(OH)₅⁻⁻⁻⁻⁻⁻⁻)</td>
<td>Np(OH)₄⁻⁻⁻⁻⁻⁻⁻ Np₂O₂⁻⁻⁻⁻⁻⁻⁻</td>
<td>0.0</td>
<td>3.0 x 10⁻¹⁶ 3.0 x 10⁻¹⁵ 6.0 x 10⁻¹¹ 6.0 x 10⁻⁹ 6.0 x 10⁻⁷ 2.0 x 10⁻⁶ 2.0 x 10⁻⁵</td>
</tr>
<tr>
<td>Pu(V)</td>
<td>(PuO₂)⁺</td>
<td>Pu(OH)₄⁻⁻⁻⁻⁻⁻⁻ Pu₂O₂⁻⁻⁻⁻⁻⁻⁻</td>
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<td>2.5 x 10⁻¹⁷ 2.5 x 10⁻¹⁶ 4.0 x 10⁻¹³ 6.0 x 10⁻¹⁰ 2.0 x 10⁻⁷ 5.5 x 10⁻⁵ 5.5 x 10⁻⁴</td>
</tr>
<tr>
<td>Pu(IV)</td>
<td>(Pu(OH)₅⁻⁻⁻⁻⁻⁻⁻)</td>
<td>Pu(OH)₄⁻⁻⁻⁻⁻⁻⁻ Pu₂O₂⁻⁻⁻⁻⁻⁻⁻</td>
<td>0.0</td>
<td>2.0 x 10⁻¹⁶ 2.0 x 10⁻¹⁵ 6.0 x 10⁻¹² 6.0 x 10⁻¹⁰ 6.0 x 10⁻⁸ 4.0 x 10⁻⁷ 4.0 x 10⁻⁶</td>
</tr>
<tr>
<td>Am(III)</td>
<td>(AmCl₂)⁺</td>
<td>Am(OH)₃⁻⁻⁻⁻⁻⁻⁻ AmOH₃⁻⁻⁻⁻⁻⁻⁻</td>
<td>0.0</td>
<td>5.0 x 10⁻¹⁴ 5.0 x 10⁻¹¹ 2.0 x 10⁻¹⁰ 1.0 x 10⁻⁹ 1.2 x 10⁻⁶ 1.4 x 10⁻³ 1.4</td>
</tr>
<tr>
<td>Cm(III)</td>
<td>Cm³⁺</td>
<td>Cm(OH)₃⁻⁻⁻⁻⁻⁻⁻ CmO₂⁻⁻⁻⁻⁻⁻⁻</td>
<td>0.0</td>
<td>5.0 x 10⁻¹⁴ 5.0 x 10⁻¹¹ 2.0 x 10⁻¹⁰ 1.0 x 10⁻⁹ 1.2 x 10⁻⁶ 1.4 x 10⁻³ 1.4</td>
</tr>
</tbody>
</table>
Radionuclide Source Term Expert Panel

The blocks represent, from left to right, the 0.00, 0.10, 0.25, 0.50, 0.75, 0.90 and 1.00 fractiles
Radionuclide Source Term Expert Panel

The blocks represent, from left to right, the 0.00, 0.10, 0.25, 0.50, 0.75, 0.90 and 1.00 fractiles from B.M. Butcher.

- Pb(II) and PbCl$_4^{2-}$: Carbonate Present
- Pb(II) and PbCl$_4^{2-}$: Carbonate Absent
- Ra(II) and Ra$_2^+$: Sulfate Present
- Ra(II) and Ra$_2^+$: Carbonate Present
- Ra(II) and Ra$_2^+$: Carbonate & Sulfate Absent

Concentration (M)

from B.M. Butcher
Radionuclide Source Term Expert Panel

Cumulative Probability

Concentration (M)

10^{-17} 10^{-15} 10^{-13} 10^{-11} 10^{-9} 10^{-7} 10^{-5} 10^{-3} 10^{-1} 10^1

Am (III)
Radionuclide Source Term Expert Panel

Cumulative Probability

Concentration (M)

Cm (III)
Radionuclide Source Term Expert Panel

Cumulative Probability

Concentration (M)

- O - Np (V)
- + - Np (IV)
Radionuclide Source Term Expert Panel

Cumulative Probability

Concentration (M)

- • Pb (II) Carbonate Present
- ■ Pb (II) Carbonate Absent

1.0
0.8
0.6
0.4
0.2
0.0
10^{-17} 10^{-15} 10^{-13} 10^{-11} 10^{-9} 10^{-7} 10^{-5} 10^{-3} 10^{-1} 10^1
Radionuclide Source Term Expert Panel

- **Ra (II) Sulfate Present**
- **Ra (II) Carbonate Present**
- **Ra (II) Carbonate and Sulfate Absent**

Cumulative Probability vs. Concentration (M)
Expert Panel on Radionuclide Source Term (cont.)

Strategy for Developing Probability Distributions

• Given the room conditions, what oxidation states are possible?

• For each oxidation state of each element, what compounds will have the highest and lowest solubility?

• Estimate the mode of the concentrations for both the highest and lowest solubilities. These numbers were often used as the 0.10 and 0.90 fractiles.

• Establish the lower and upper endpoints (0.00 and 1.00 fractiles) by considering how changes in the room chemistry (e.g., pH) could impact the concentrations.
Expert Panel on Radionuclide Source Term (cont.)

Strategy for Developing Probability Distributions

- Where possible, concentration data from a well (J-13) at the Nevada Yucca Mountain site, corrected for ionic strength, was used as the 0.50 fractile.

- The 0.25 and 0.75 fractiles were established based on which speciation was believed to be more likely.

- For lead and radium, the above procedure was repeated, not for different oxidation states but for the presence of compounds that change the controlling species, and therefore the solubility.
Expert Panel on Radionuclide Retardation in the Culebra

Composition

- All Sandia experts

Results

- Ranges and distributions of distribution coefficients, $K_d$
  - Dolomite matrix
  - Clay in fractures
  - Transport fluid dominated by Castile brine
  - Transport fluid dominated by Culebra water
  - Am, Cm, Np, Pu, Th, U, Ra, Pb
Expert Panel on Radionuclide Retardation in the Culebra (cont.)

Sandia Personnel

Robert Dosch

Craig Novak

Malcom Siegel
Expert Panel on Radionuclide Retardation in the Culebra (cont.)

1st meeting (April 12, 1991)
- Issue statement

2nd meeting (April 23, 1991)
- Issue statement

3rd meeting (May 29-30, 1991)
- Expert judgement training
- Discussion of approaches/cases
- Elicitation sessions
Expert Panel on Radionuclide Retardation in the Culebra (cont.)

Results

- Experts elicited separately
- Interpretation of existing data
- One set of results not used in 1991 calculations
  - Different information provided
- Some estimates incomplete
  - Insufficient data
- Minimum estimates
  - Expert #1: ranged from 0, to 0.1, 10, and 1000
  - Expert #2: always zero
Expert Panel on Radionuclide Retardation in the Culebra

Results (cont.)

- Impact of dolomite matrix vs. clay in fractures on $K_d$
  - Expert #1: $K_d$ (fractures) > $K_d$ (matrix)
    - 2 or 4 orders of magnitude for the 0.00 fractile and 1 order of magnitude for the 1.00 fractile
    - Am, Cm, Np, Pu
  - Expert #1: $K_d$ (fractures) < $K_d$ (matrix)
    - No difference for the 0.00 fractiles and 3 orders of magnitude for the 1.00 fractile
    - Ra
Expert Panel on Radionuclide Retardation in the Culebra

Results (cont.)

- Expert #1: Th and Pb not reported, U incomplete
- Expert #2: \( K_d \) (fractures) > \( K_d \) (matrix)
  -- 1 order of magnitude
  -- Am, Cm, Np, Pb, Pu, Ra, Th, U

- Impact of Culebra brine vs. Salado brine as dominant transport fluid on \( K_d \)
  - Expert #1: \( K_d \) (Culebra) = \( K_d \) (Salado)
    -- Within the same type of rock
    -- Am, Cm, Np, Pu, Ra
  - Expert #1: \( K_d \) (Culebra) > \( K_d \) (Salado)
    -- Dolomite matrix
    -- More than 1 order of magnitude
    -- U
Expert Panel on Radionuclide Retardation in the Culebra

Results (cont.)

- Expert #1: Th and Pb not reported

- Expert #2: \( K_d \) (Culebra) = \( K_d \) (Salado)
  -- Within the same type of rock
  -- Pb, Ra, Th

- Expert #2: \( K_d \) (Culebra) > \( K_d \) (Salado)
  -- 1 order of magnitude for the 0.25 fractile to no difference for the 1.00 fractile
  -- Am, Cm, Pu,

- Expert #2: \( K_d \) (Culebra) < \( K_d \) (Salado)
  -- Factor of 4
  -- Np, U
Radionuclide Retardation Expert Panel
M.D. Siegel: Plutonium

A $K_d$ of 0 represented by $1 \times 10^{-14}$

- Open circle: Dolomite Matrix; Culebra Brine
- Solid square: Dolomite Matrix; Salado Brine
- Triangle: Clay in Fractures; Culebra Brine
- Open square: Clay in Fractures; Salado Brine

Cumulative Probability

Distribution Coefficient, $K_d$

Included fitted probability zone is value without variability in value.

Data from field test.
Radionuclide Retardation Expert Panel
R. G. Dosch: Plutonium

A $K_d$ of 0 represented by $1 \times 10^{-14}$

- Dolomite Matrix; Culebra Brine
- Dolomite Matrix; Salado Brine
- Clay In Fractures; Culebra Brine
- Clay In Fractures; Salado Brine

Cumulative Probability

Distribution Coefficient, $K_d$
Radionuclide Retardation Expert Panel
C. F. Novak: Plutonium

A $K_d$ of 0 represented by $1 \times 10^{-14}$

- ∙ Dolomite Matrix; Culebra Brine
- † Dolomite Matrix; Salado Brine
- △ Clay In Fractures; Culebra Brine
- □ Clay In Fractures; Salado Brine

Cumulative Probability

Distribution Coefficient, $K_d$
Uranium - M.D. Siegel

A $K_d$ of 0 represented as $1 \times 10^{-14}$

- O Dolomite Matrix; Culebra Brine
- - Dolomite Matrix; Salado Brine
- A Clay in Fractures; Culebra Brine
- C Clay in Fractures; Salado Brine

Cumulative Probability

Distribution Coefficient, $K_d$
A $K_d$ of 0 represented as $1 \times 10^{-14}$

- O Dolomite Matrix; Culebra Brine
- + Dolomite Matrix; Salado Brine
A $K_d$ of 0 represented as $1 \times 10^{-14}$

- O Dolomite Matrix; Culebra Brine
- Dolomite Matrix; Salado Brine
- Δ Clay in Fractures; Culebra Brine
- ■ Clay in Fractures; Salado Brine

Cumulative Probability

Distribution Coefficient, $K_d$

10$^{-15}$ 10$^{-13}$ 10$^{-11}$ 10$^{-9}$ 10$^{-7}$ 10$^{-5}$ 10$^{-3}$ 10$^{-1}$ 10$^1$ 10$^3$ 10$^5$ 10$^7$
Radionuclide Retardation Expert Panel
C. F. Novak: Americium and Curium

A $K_d$ of 0 represented by $1 \times 10^{-14}$

- ○ Dolomite Matrix; Culebra Brine
- • Dolomite Matrix; Salado Brine
- △ Clay In Fractures; Culebra Brine
- □ Clay In Fractures; Salado Brine
Radionuclide Retardation Expert Panel
C. F. Novak: Radium and Lead

A $K_d$ of 0 represented by $1 \times 10^{-14}$

- Dolomite Matrix; Culebra Brine
- Clay in Fractures; Culebra Brine
- Clay in Fractures; Salado Brine

Distribution Coefficient, $K_d$
Radionuclide Retardation Expert Panel
C. F. Novak: Thorium

A $K_d$ of 0 represented by $1 \times 10^{-14}$

- Dolomite Matrix; Culebra Brine
- Dolomite Matrix; Salado Brine
- Clay in Fractures; Culebra Brine
- Clay in Fractures; Salado Brine

Cumulative Probability

Distribution Coefficient, $K_d$
A K_d of 0 represented as $1 \times 10^{-14}$

- O Dolomite Matrix; Culebra Brine
- Dolomite Matrix; Salado Brine
- ▲ Clay in Fractures; Culebra Brine
- □ Clay in Fractures; Salado Brine
A $K_d$ of 0 represented by $1 \times 10^{-14}$

- O Dolomite Matrix; Culebra Brine
- + Dolomite Matrix; Salado Brine
- ▲ Clay in Fractures; Culebra Brine
- □ Clay in Fractures; Salado Brine
Radionuclide Retardation Expert Panel
M.D. Siegel: Americium

A $K_d$ of 0 represented by $1 \times 10^{-14}$

- Dolomite Matrix; Culebra Brine
- Dolomite Matrix; Salado Brine
- Clay In Fractures; Culebra Brine
- Clay In Fractures; Salado Brine

Cumulative Probability

Distribution Coefficient, $K_d$
A $K_d$ of 0 represented by $1 \times 10^{-14}$

- $K_d$ of Dolomite Matrix; Culebra Brine
- $K_d$ of Dolomite Matrix; Salado Brine
- $K_d$ of Clay in Fractures; Culebra Brine
- $K_d$ of Clay in Fractures; Salado Brine
Neptunium - M.D. Siegel

A $K_d$ of 0 represented as $1 \times 10^{-14}$

- Dolomite Matrix; Culebra Brine
- Dolomite Matrix; Salado Brine
- Clay in Fractures; Culebra Brine
- Clay in Fractures; Salado Brine

Cumulative Probability

Distribution Coefficient, $K_d$
Radionuclide Retardation Expert Panel
M.D. Siegel: Lead and Radium

A $K_d$ of 0 represented by $1 \times 10^{-14}$

- ○ Dolomite Matrix; Culebra Brine
- □ Dolomite Matrix; Salado Brine
- △ Clay In Fractures; Culebra Brine
- ■ Clay In Fractures; Salado Brine

Cumulative Probability

Distribution Coefficient, $K_d$
Radionuclide Retardation Expert Panel
M.D. Siegel: Thorium

A $K_d$ of 0 represented by $1 \times 10^{-14}$

- Dolomite Matrix; Culebra Brine
- Clay in Fractures; Culebra Brine

Cumulative Probability

Distribution Coefficient, $K_d$
Expert Panels for Parameter Elicitation

Expert Panel on Radionuclide Retardation in the Culebra, Proposed for FY 1992

Composition

- All external experts

Results

- Evaluate existing data base
  - Can it justify minimum estimates of distribution coefficients
- Provide minimum estimates, if possible
  - Am, Cm, Np, Pu, Th, U, Ra, Pb
- Review proposed research plan
  - Can the plan help verify the minimum estimates
  - Necessary modifications
Expert Panel on Radionuclide Retardation in the Culebra, Proposed for FY 1992 (cont.)

Selection of panelists

- Nominations
  - Initial nominees from Sandia staff, review groups, intervener groups, public agencies, and literature
  - Additional nominations from all those contacted

- Selection criteria

- Selection committee
  - Taken from the pool of nominees
  - Removed from consideration as nominees
Expert Panel on Radionuclide Retardation in the Culebra, Proposed for FY 1992 (cont.)

1st meeting
• Issue statement
• Background presentations
• Expert judgment training

Between meetings
• Develop approach for determining minimum values for the coefficients
• Review proposed experimental plan
• Prepare draft text explaining approach

2nd meeting
• Discussion of approaches
  - Analyzing/interpreting existing data
  - Outlining necessary research
• Elicitation sessions
• Discussion between panel and Division 6344 regarding modifications to proposed experimental plan
Expert Panel on Radionuclide Retardation in the Culebra, Proposed for FY 1992 (cont.)

After meeting
• Final text explaining $K_d$ estimates and the reasoning behind the modifications to the experimental plan
Expert Panel Summary

**Human Intrusion** -
- Expert panel on future societies: Document in preparation
- Expert panel on markers: Restart October 1
- Expert panel on barriers to HI: Begin FY92

**Radionuclide Source Term and Transport** -
- Source term panel (external): Elicitation complete and document in preparation
- Retardation (Culebra) panel (internal): Elicitation complete and document in preparation
- Retardation (Culebra) panel (external): Proposed for FY92
Expert Panel Summary, Cont.

Geostatistics Working Group -

- Conditional Simulations of T fields using present CAMCON module completed for 91 Assessment
- Automated SWIFT II/GRASP II calibration/conditional-simulation approach using pilot point method to be used for 92 assessment available by 3/92
- T field comparison study to be completed by 3/92

Future Panels -

- Will depend on results of 91 Sensitivity Analysis and project priorities