U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Engineered Barrier System - Chemical Environments and Transport

Presented to:
NRC/DOE Technical Exchange on Total System Performance Assessment (TSPA) for Yucca Mountain
San Antonio, Texas

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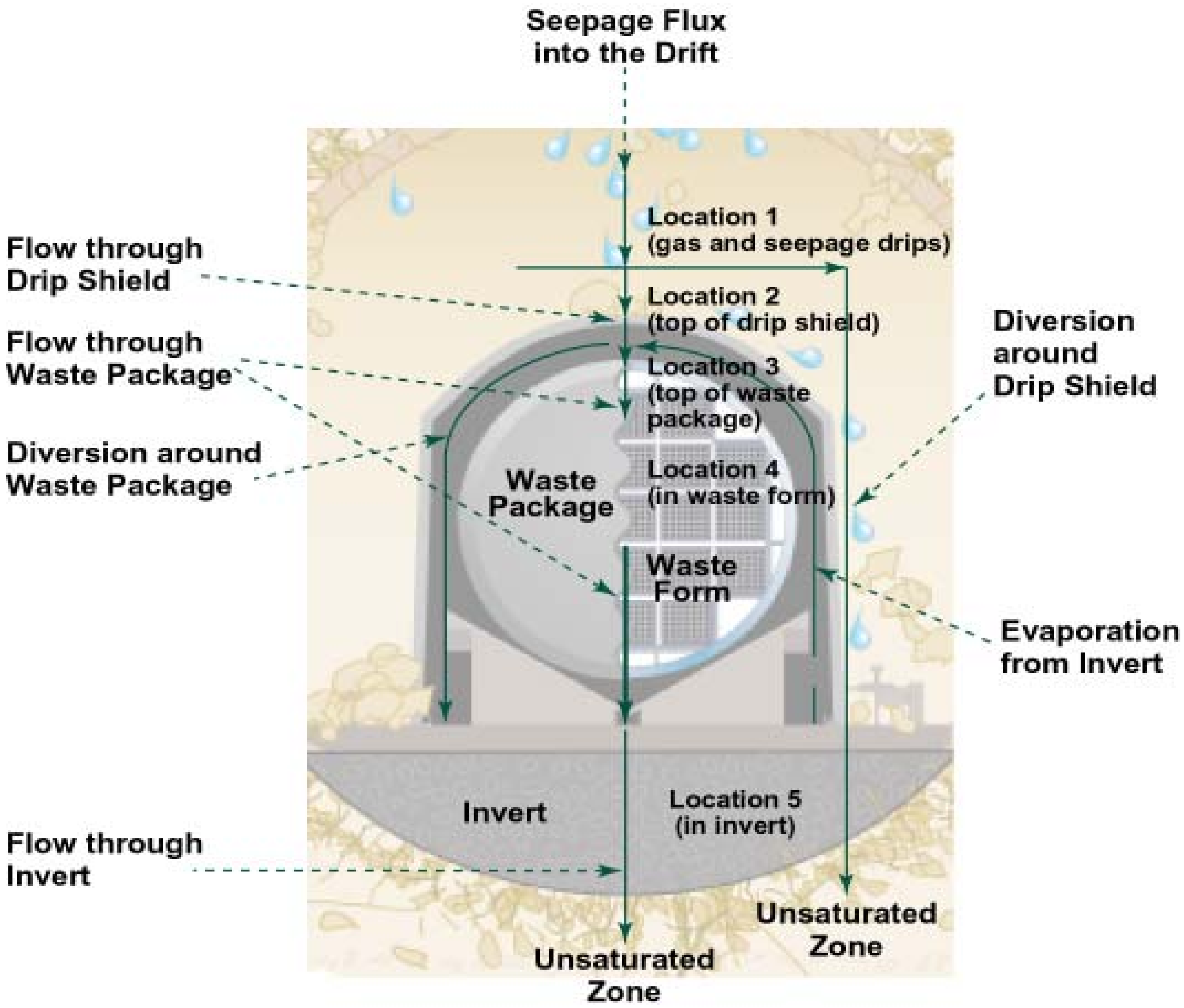
YUCCA MOUNTAIN PROJECT

Chemical Environments and Transport - Paths and Locations



Engineered Barrier System Chemical Environments and Transport Feed TSPA

- **Chemical environment on drip shield affects drip shield corrosion, degradation**
- **Chemical environment on waste package affects waste package corrosion, degradation**
- **Chemical environment in invert affects the mobile radionuclide concentrations and species transported to unsaturated zone**
- **Transport of radionuclides in fluids within Engineered Barrier System (EBS) affects quantities of radionuclides entering the unsaturated zone**
  - **Diffusion and advection, waste package to invert and invert to unsaturated zone**

Key Technical Issues

- **Evolution of the Near-Field Environment**
  - Effects of THC on waste package chemical environment
  - Effects of THC on chemical environment for radionuclide release
  - Effects of THC on radionuclide transport through EBS
- **Relevant integrated subissues from the Total System Performance Assessment and Integration Issue Resolution Status Report Rev. 2 include:**
  - Engineered barrier degradation
  - Quantity and chemistry of water contacting waste packages and waste form

Key Technical Issues
(continued)

- The Engineered Barrier System Degradation, Flow and Transport Process Model Report (PMR) and Near-Field Environment PMR addresses acceptance criteria related to this topic and will be discussed at a Technical Exchange scheduled for September 7, 2000

Processes considered in EBS Chemical Environments and Transport Models

- Gas-water interactions
- Evaporation of water and condensation of water vapor
- Salts precipitation and salts dissolution
- Microbial activity and effects
- Water-cement interactions
- Corrosion and degradation of EBS components
- Water-invert interactions
- Water-colloids interactions
- Transport by advection and diffusion
- Colloidal radionuclide transport

Basis is in Analysis Model Reports (AMRs)

- **EBS chemical environments**
  - Integration of models into TSPA given in
    - Physical and Chemical Environmental Abstraction Model, ANL-EBS-MD-000046 Rev00
    - Several sub-model AMRs and Feature, Events and Processes (FEPs) AMR cited in the above AMR
- **EBS transport**
  - Abstraction and integration into TSPA given in
    - EBS Radionuclide Transport Abstraction, ANL-WIS-PA-000001 Rev 00
- **Model uncertainties, assumptions, and integration regarding design features, physical phenomena, and couplings are treated in these AMRs**

Several Improvements Have Been Added

- **Solution chemistry**
  - Pitzer approach
  - Response surfaces
- **Colloids model**
  - New data incorporated
  - Improved relationships with solution chemistry
- **Transport model**
  - Improved diffusion model for invert
- **Additional interactions considered**
  - Water-invert, corrosion
- **All analyses and codes are QA**

Inputs from Thermal Hydrologic Environments Were Used with the Models

- **Incoming water composition**
- **Incoming water flow rate**
- **Incoming gas composition**
- **Temperatures in drifts**
- **Relative humidity values in drifts**
- **Water evaporation rates in drifts**

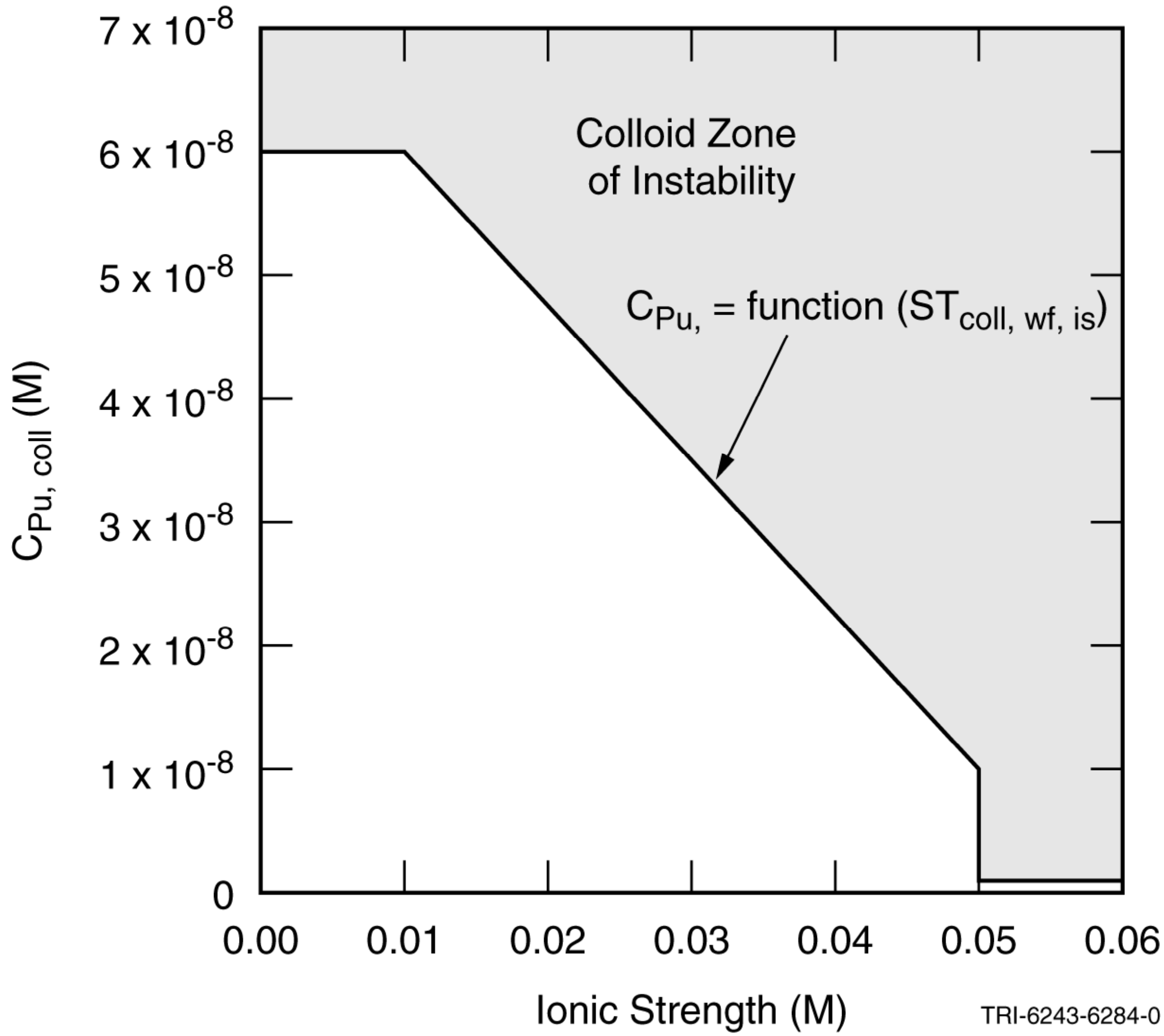
Results and Conclusions

Gas-Water-Precipitates Chemistry for Transition Cooldown Period, 1000 - 2000 yr

Volume fraction carbon dioxide gas = 10^{-3}

Input Parameters			Precipitates/Salts Model Output		
RH **(%)**	***T*** **(°C)**	R^{es}	**pH**	**Cl (molal)**	***I*** **(molal)**
< 50.3%	na [a]	na	dry	dry	dry
50.3%	90	na	7.64	3.73E-03	2.44E+01
51.0%	90	na	7.64	5.70E-02	2.40E+01
53.1%	90	na	7.64	4.06E-01	2.11E+01
55.2%	90	na	7.64	6.77E-01	1.89E+01
60.5%	90	na	7.64	1.63E+00	1.10E+01
65.7%	90	na	7.64	2.28E+00	5.65E+00
71.0%	90	na	7.64	2.49E+00	3.91E+00
76.2%	90	na	7.64	2.53E+00	3.54E+00
81.5%	90	na	7.64	2.48E+00	3.96E+00
85.0%	90	na	7.64	2.41E+00	4.53E+00
> 85%	90	0	7.72	3.19E-03	1.03E-02
> 85%	90	0.1	7.71	3.56E-03	1.14E-02
> 85%	90	0.5	7.64	6.40E-03	1.98E-02
> 85%	90	0.9	7.45	3.20E-02	9.48E-02
> 85%	90	0.99	7.58	3.15E-01	6.60E-01
> 85%	90	0.9988	7.64	2.36E+00	4.69E+00
> 85%	90	> 0.9988	7.64	2.41E+00	4.53E+00

Relationship between Radionuclide-Bearing Colloid Concentration and Ionic Strength



Microbial Communities Effects Are Included

- Microbes are viable
  - MING code available to calculate microbial mass
- Microbial communities may increase corrosion rate
  - Corrosion rate multiplication factor
    - uniform distribution between 1 and 2
- Microbes have negligible effect on water composition

Remaining Chemical Processes Have Negligible Effects

- **Water-cement interactions - negligible**
- **Corrosion and degradation of EBS components - negligible**
- **Water-invert interactions - negligible**

Transport Model Includes

- Flow paths in 1-D model
- Two mixing cells
  - Inside waste package
  - In invert
- Colloid-facilitated transport
  - Advection and diffusion
  - Waste form colloid source term
- Potential for evaporative reflux

Transport Model Provides

- Water flux for advection
- Diffusion areas, lengths, and coefficients
- For the following paths
  - Waste package to invert pathway
    - for stress cracks, corroded patches, and pits
  - Invert to unsaturated zone pathway
    - for void space in invert
- Corrections for porosity, saturation, temperature
- Advection includes
  - No retardation and lateral or forward dispersion
  - Colloidal particle transport