**Presentation of the Final Report**

# Compositions of Aqueous Environments

***Presented by***

**Peer Panel on Waste Package Materials Performance**

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***Presented to***

U.S. Department of Energy (DOE)

Bechtel SAIC Company, LLC (BSC)

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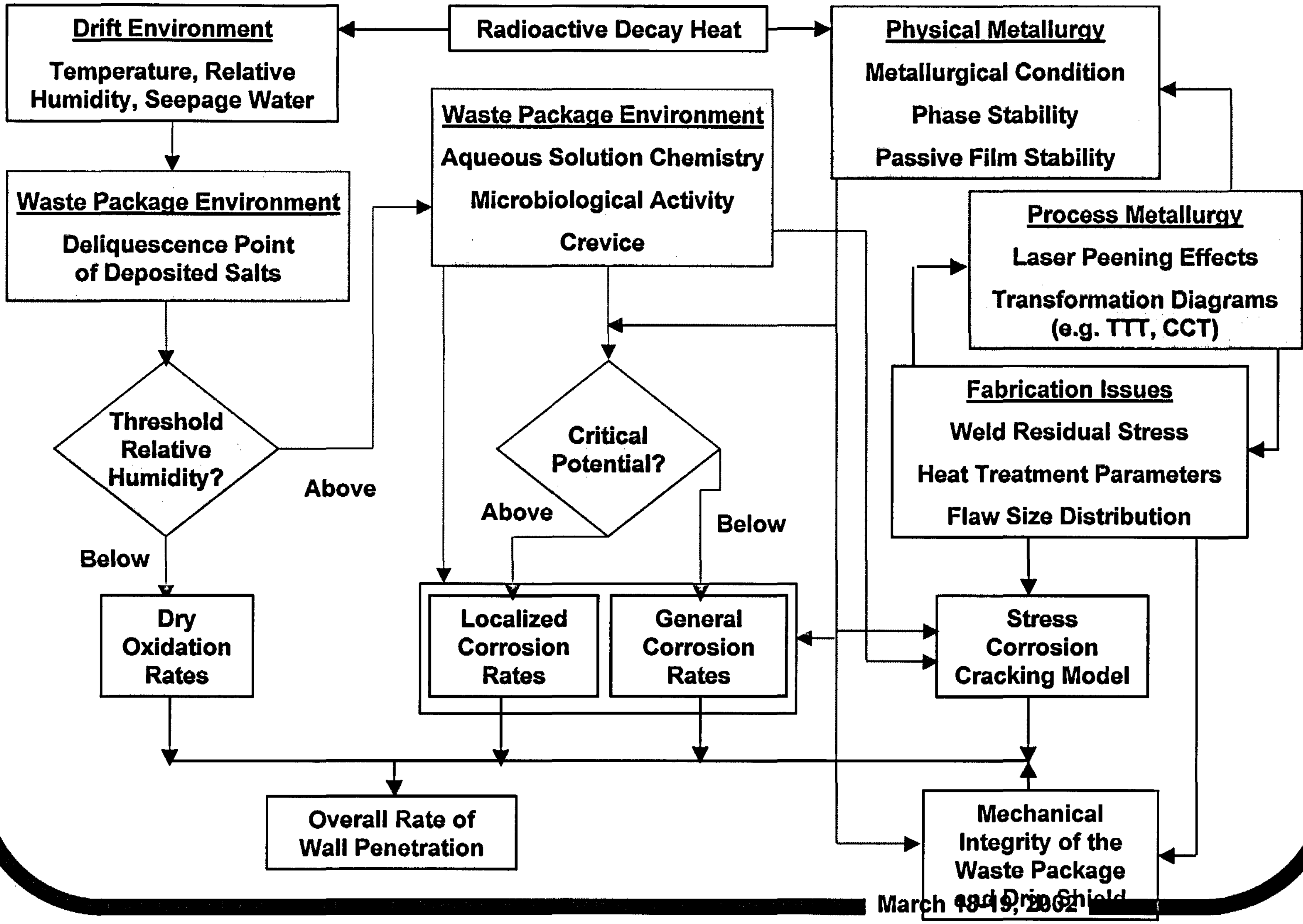
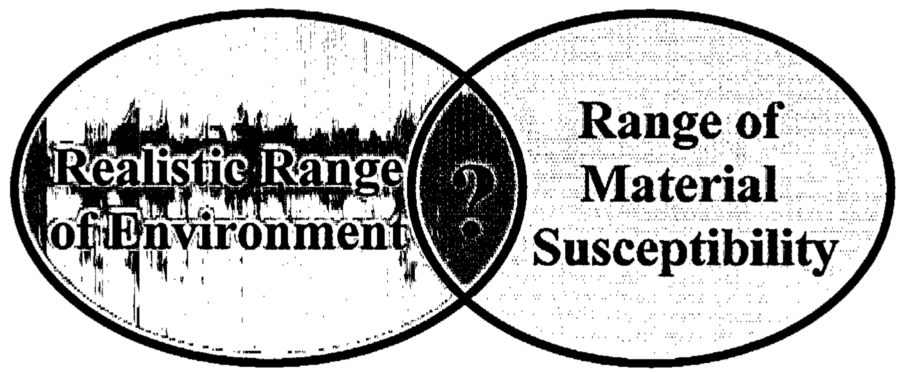
Main - 20

# Model for Waste Package Degradation



# Necessary Conditions for Significant Corrosion to Occur on Waste Packages

- Water must contact WP
- Water must remain on WP
- Corrosive species must be present to form electrolyte
- Material must be susceptible to corrosion under these conditions
- Conditions must persist over sufficiently long time

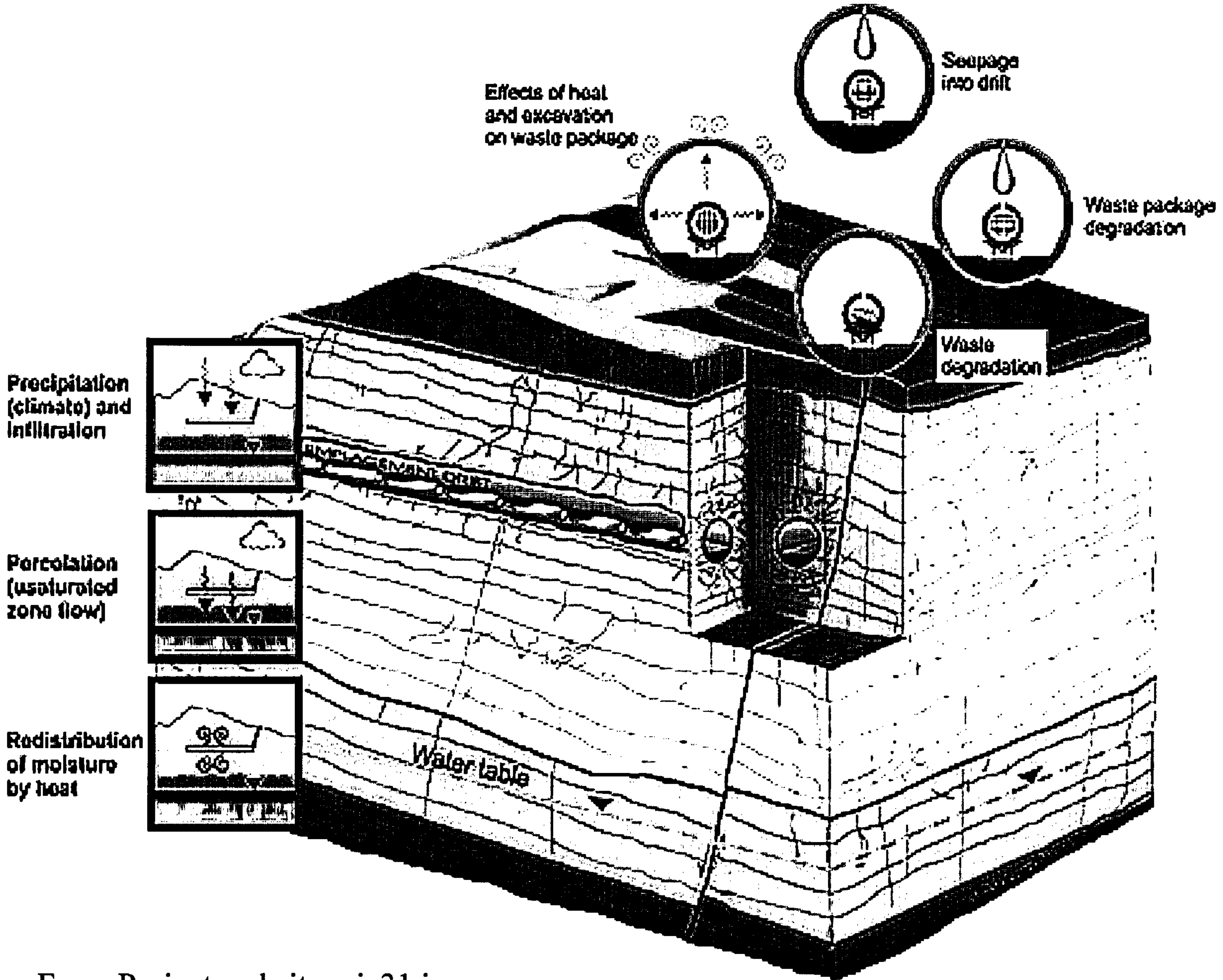


# Importance of the Composition of Aqueous Environments

**For a given material, the characteristics of the aqueous environment control corrosion behavior**

- Presence of water
- Temperature
- Ionic composition (incl. pH), radiolysis, oxidizing species
- Deliquescence of salts and introduced materials
- Deposits

**Prediction of corrosion behavior depends on prediction of environment**




From Project website: via31.jpg

# EBS Chemical Environments

**Incoming** Gas, water, colloids

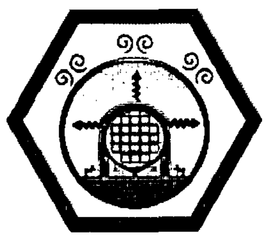
**In-Drift**
- Gas
- Water-solids chemistry
- Colloids
- Microbial communities
- Water-invert chemistry
- Water-cement chemistry
- Corrosion chemistry

**Near-Field Environment**
- Incoming water composition
- Incoming gas composition
- Incoming water rate

**Thermal Hydrologic Environments**
- Temperature
- Relative humidity
- Incoming water flow rate
- Water evaporation rate
- Evaporation rate

**Design**
- Repository
- Waste Package

*Inputs*



*Outputs*

**On Drip Shield**
- Water composition
- Microbe quantity

**On Waste Package**
- Water composition
- Microbe quantity

**In Invert**
- Water composition
- Colloid Stability and concentration

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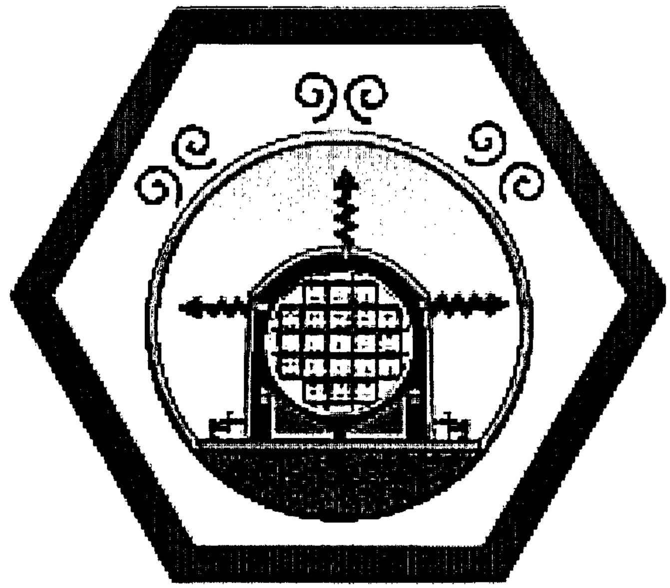
Findings

# Presence of Moisture

- Full immersion of metal surfaces is a highly unlikely condition.

- Two sources of water:
    - o Condensation from the air
    - o Seepage from the rock



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**Findings**

# TECHNICAL ISSUES TO BE RESOLVED

Nominal waters at Yucca Mountain are fairly benign, **but** water composition will change at the metal surface

Needed Information:

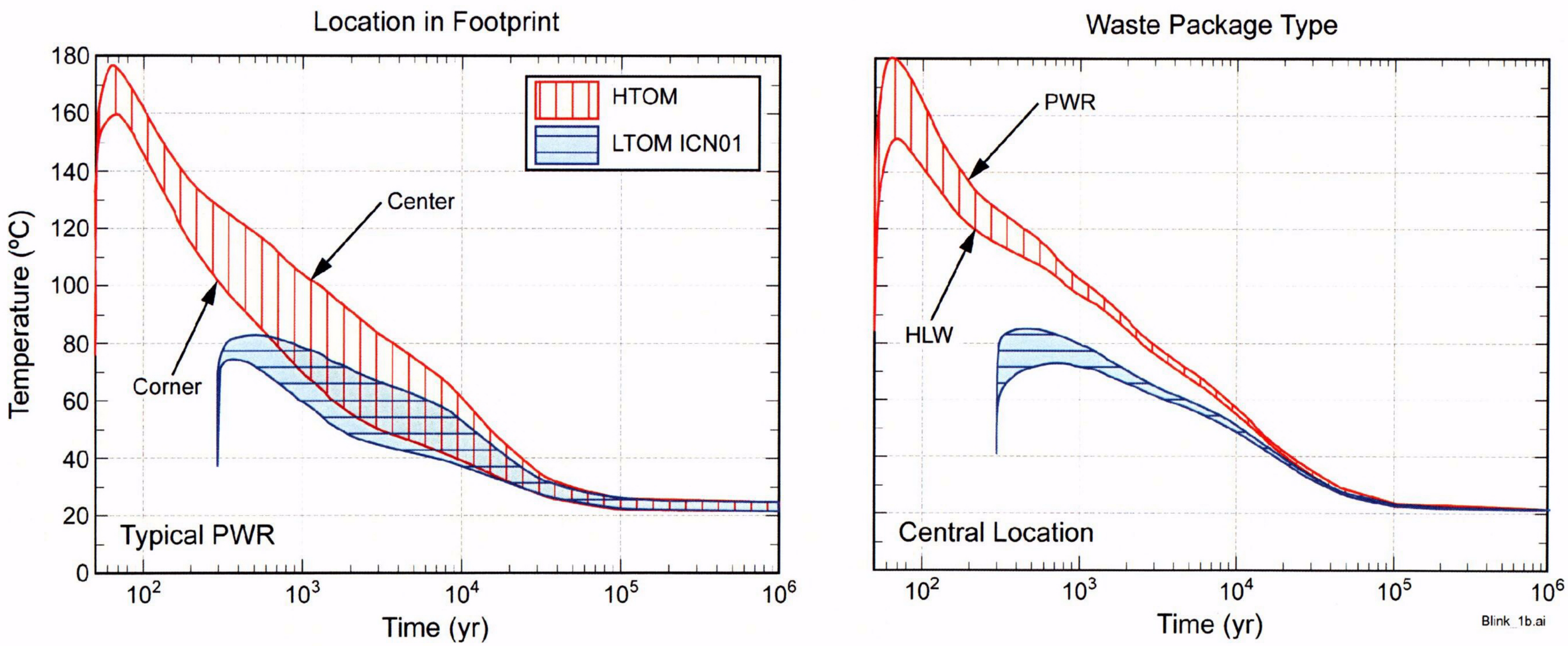
- **Realistic boundaries for environmental conditions**
- **Corrosion behavior within the range of realistic environmental conditions**
- **Radiolysis from gamma radiation at realistic levels**

# Influence of Operating Mode on Time, Temperature, Environment

Two operational modes are now under consideration.

- A higher-temperature operating mode
  - waste package surface temperature could reach 180°C
  - surrounding rock would be heated above boiling
  - rock would be initially dried out near the drifts.
- A lower-temperature operating mode
  - waste package surface would be maintained below 85°C
  - surrounding rock not heated above boiling
  - minimal dry-out zone in the rock.

# Example Thermal Load Time Profiles

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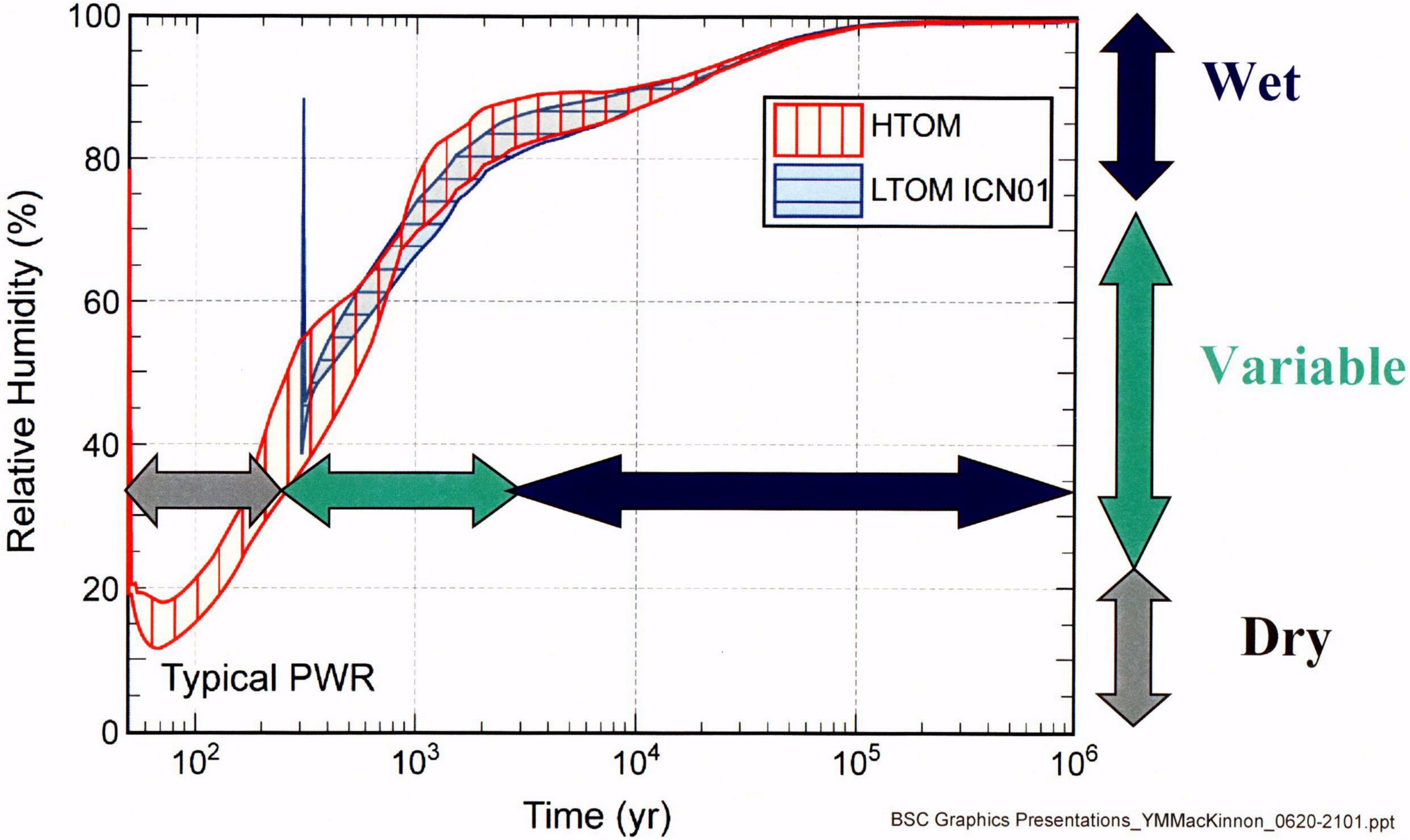
# Example of Equilibrium Humidity and Its Connection to Moisture on Surfaces

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**Findings**

## Presence of Moisture

Water composition **in** Yucca Mountain

- naturally occurring
- major source of water and ionic species

Aqueous environments **on** metal surfaces

- alteration of natural environment due to thermal and chemical conditions

Findings

## Composition of Waters in Yucca Mt.

- Dilute
  - Dominated by Na-Ca-Mg-$HCO_3$-$CO_3$-Cl-$NO_3$-$SO_4$
  - pH 5.6-7.4

- Can be modified during movement:
  - through interactions with surfaces of fractures
  - by thermal-chemical processes

Findings

# Composition of Aqueous Environments on Waste Packages

Solutions on the waste package will evolve into

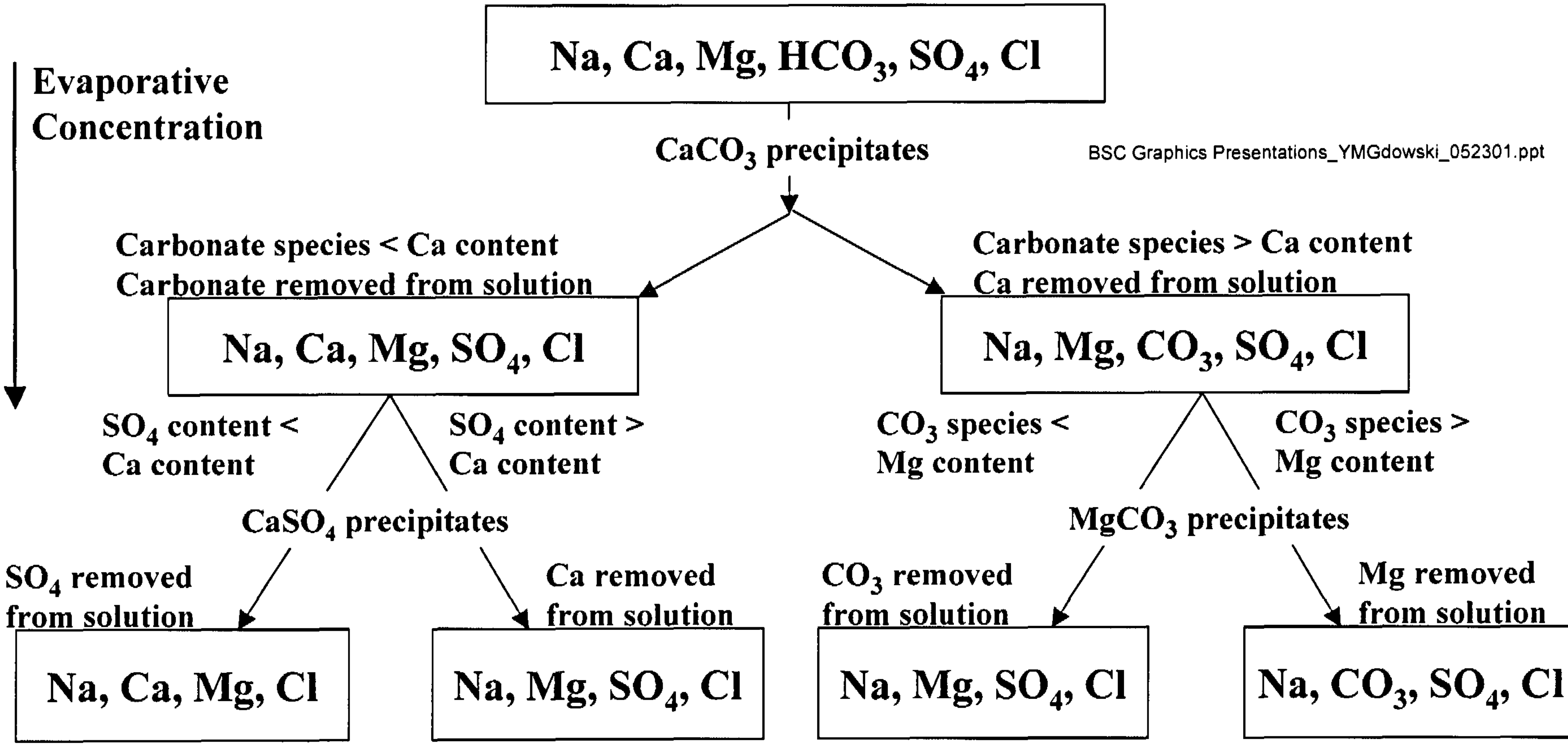
- An alkaline solution (pH 11-12) containing high concentrations of sulfate, carbonate, nitrate, and chloride

OR

- A near-neutral solution (pH ca. 6) containing high concentrations of chloride and nitrate with or without sulfate.

As the temperature of the metal surface decreases, dilution of the aqueous solution on the waste package occurs.

# The Project Approach: The Chemical Divide Principle Applied to YM Waters




Death Valley, CA (Na)*
Bristol Dry Lake, CA (Na, Ca)
Cadiz Lake, CA (Na, Ca)
Carson Sink, NV (Na)

Saline Valley, CA (Na)*
Danby Lake, CA (Na)
Salton Sea, CA (Na)

Surprise Valley, CA
Mono Lake, CA
Owens Lake, CA
Soda Lake, CA
Pyramid Lake, NV
Winnemucca Lake, NV

* dominant cation(s) in brine

Findings

# Range of Seepage Water Compositions

## Near Neutral pH Brines

- Some Ca & Mg removed by precipitation of insoluble carbonates and silicates
- Mg & Ca chloride precipitates may form which are very hygroscopic
- pH near 7

## High pH Brines

- All Ca & Mg removed by precipitation of insoluble carbonates and silicates
- Under very low $P_{CO2}$ very high pHs possible (pH 12)
- Very concentrated solutions are mixtures of chloride and nitrate

***Project has confirmed these pH values with simulated YM waters***

# Composition of Waters and Corrosive Environments

***Other species*** to consider include

- Lead, mercury, arsenic, bromide
- These types of species can have effects at low levels

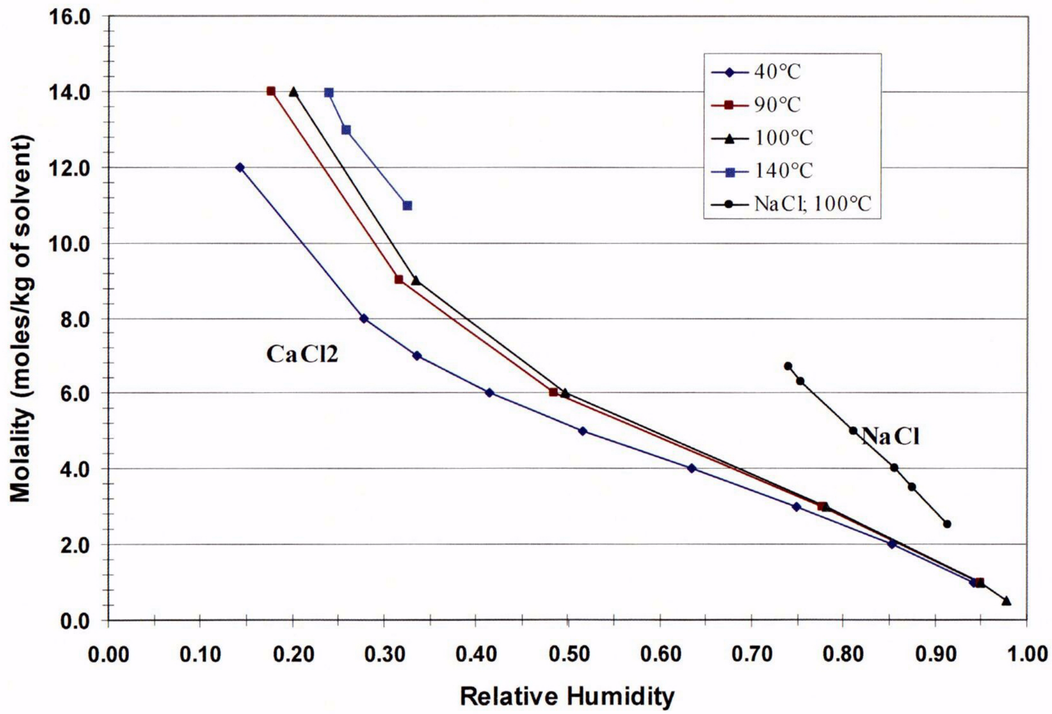
***Mixture of all of the salts present on the surface***

- Solution will be comprised of mixed ionic solutions
- Most anions tend to inhibit the localized corrosion of metals in the presence of chloride, for example nitrate and sulfate

# Drift Environmental Conditions Can Lead to Three Types of Surface Conditions

- **Condensation leads to moist dust**
  - Dust includes entrained matter in ventilation air
  - Condensation enhanced due to capillary action
- **Dripping seepage water forms mineral scale**
  - Expected to be variable in time and location
- **Crevice areas entrap environments**
  - From deposits as well as engineered structural details
  - Can entrap water and concentrate ionic species if there exists external cathode

# Findings
# Moist Dust Scenario




Capillary condensation and deliquescence combine to form a solution at RH < 100 %

N.B. Limit on total pressure

As T falls, RH increases, concentrations decrease

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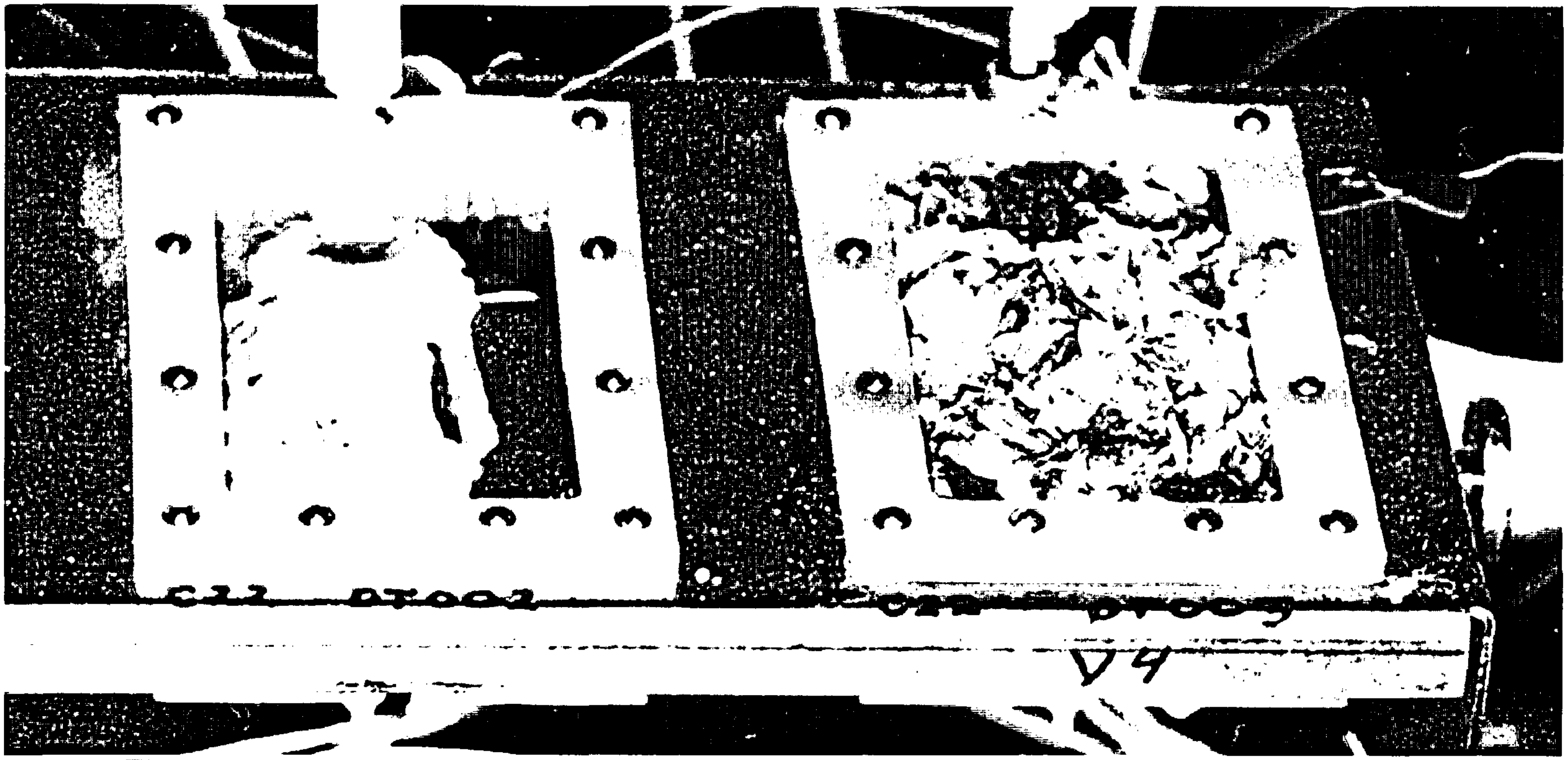
# Findings
# Mineral Deposit Scenario



***Examples of Deposits from Dripping Experiments***

***Gdowski, Presentation to Peer Panel, May, 2001***

## *Findings*
## Crevice Scenario

- An occluded geometry limits mass transport
  - *e.g.*, pallet/package contact areas
- Entrap moisture
- Can increase corrosion rates within crevices
  - Depends strongly on interaction between crevice area and external surface

Findings

# Composition of Waters and Aqueous Environments

## Direct Factors

- pH of Surface Environment
- pH buffering species
- Ratio of chlorides:all other anions
- Oxidizing potential
- Dust and scale deposits
- Radiation

## Contributing Factors

- Microbiological Influences
- Atmospheric chemistry
- Atmospheric pressure in repository is fixed at 0.89 atm
  - Unlimited supply of oxygen
  - Partial pressure of volatile gases is limited to the atmospheric pressure

# *Findings*
# Possible Effects of Microbial Activity

- Microbial activity can affect corrosion processes
- Bacteria are present at YM, will be introduced, and cannot be disregarded
- Nonetheless, there are limitations on growth
  - need condensed water and carbon source
  - limited temperature (ca. < 140 C)
- Challenge in predicting microbial effects on aqueous environments due to adaptations
- Presence of microbes is necessary, but not sufficient for microbiologically influenced corrosion
- Data required for modeling must be from measurements in more realistic environments

*Recommendations*

# Aqueous Environments on Metal surfaces

- Form a task group of Project technical experts to coordinate and guide both the experimental determination and analytical modeling of the environment.
  - Requires authority and responsibility to determine directions
- Undertake comprehensive experimental and analytical modeling program for the three environmental scenarios cited
  - Develop technical basis for realistic environmental extremes for each
- Continue work on interactions between seepage water and hot metal surfaces
- Continue current studies of entrained material deposition composition and rate

## *Recommendations*
## Microbiological Influenced Corrosion

- Move focus microbiological work from viability assessment to understanding:
  - Effects of microbe metabolites on engineered materials (including steel) especially at welds and crevices
  - Growth and corrosion effects in more realistic environments
- Do not use a simple "rate enhancement factor" in model as microbial effects change corrosion from uniform to localized

## *Recommendations*
## Corrosion Testing Environments

- Better connect work on aqueous environment determination to long-term corrosion testing
  - Extend measurements to higher temperature (up to 180 C)
  - Use dripping and moist dust configurations to better simulate expected exposure rather than full immersion