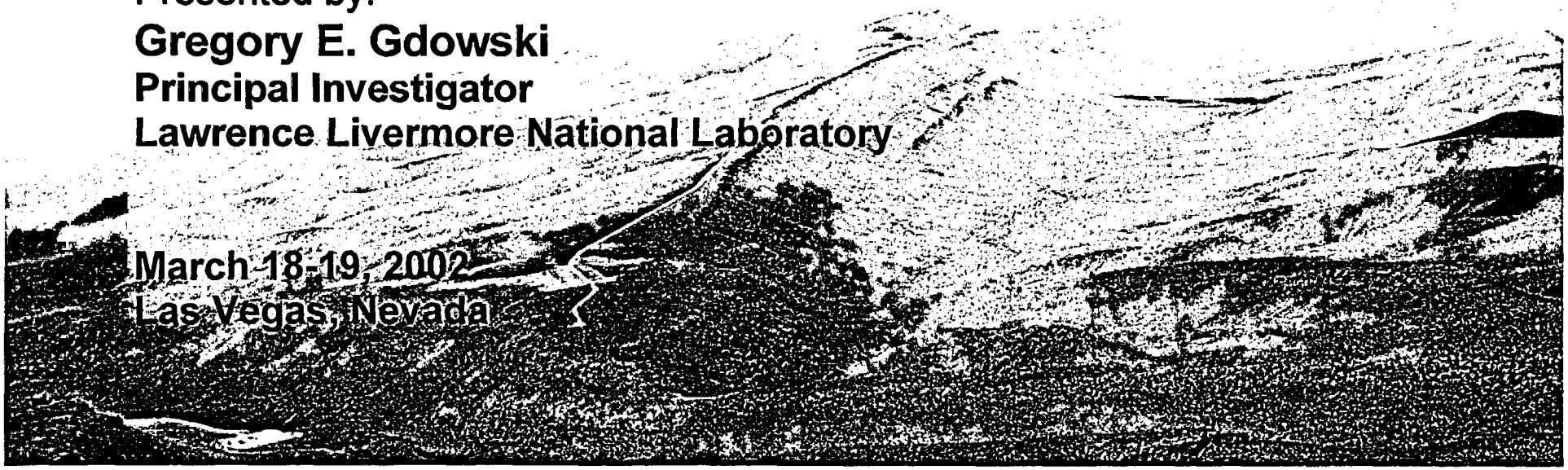
U.S. Department of Energy
Office of Civilian Radioactive Waste Management

YUCCA MOUNTAIN PROJECT

Composition of Aqueous Environments

Presented to:
Waste Package Materials Performance Peer Review Panel

Presented by:
Gregory E. Gdowski
Principal Investigator
Lawrence Livermore National Laboratory



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Main-20

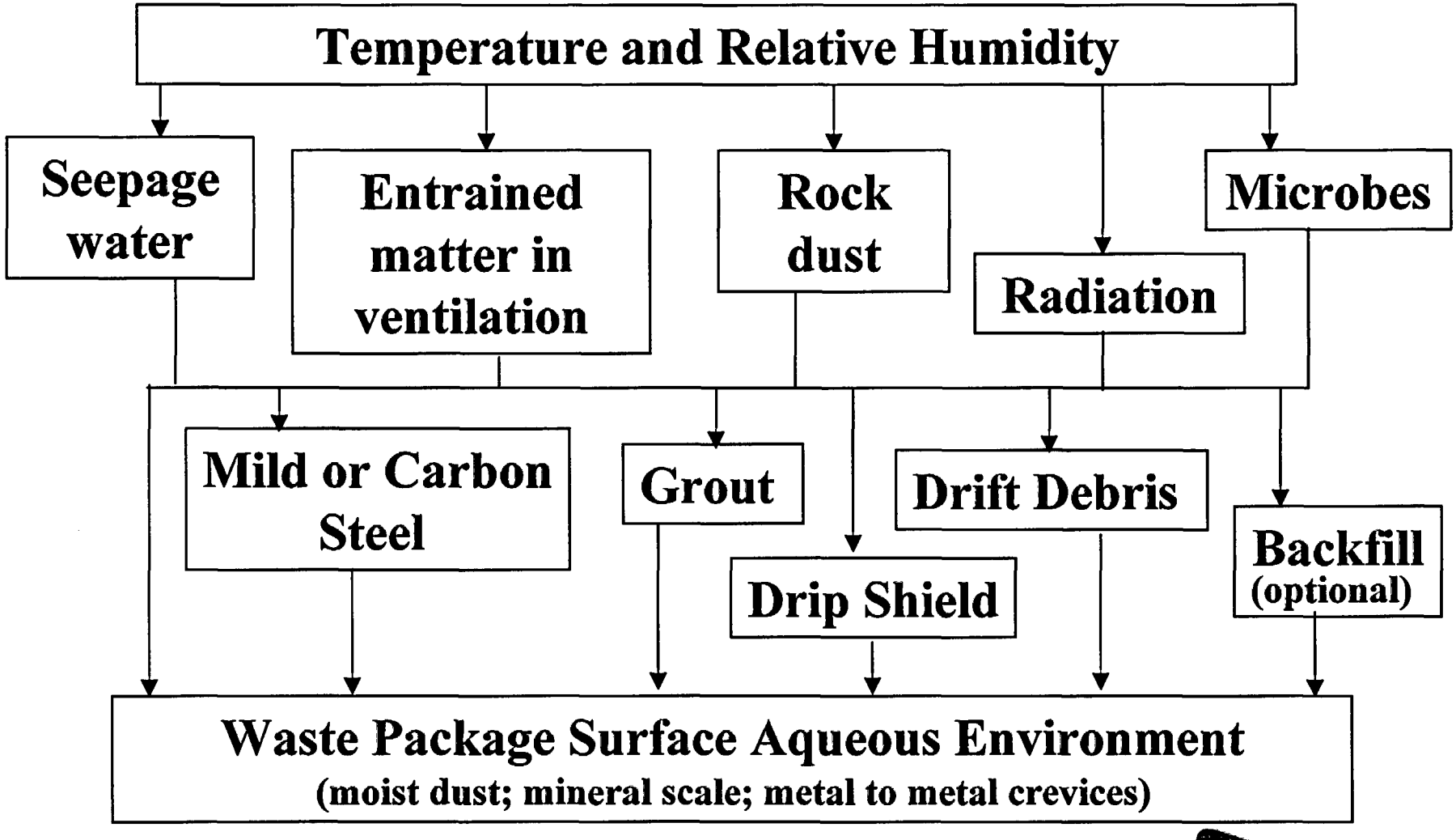
Strategy

- **Characterize the aqueous environments in contact with the Waste Package (WP) into aqueous solution "types" that can be classified according to their "corrosive nature"**
  - **Establish bounds on parameters given the constraints of the system**

Aqueous Solution Parameters Important for Corrosion

- Dripping water including transient behavior
- Deliquescence of deposited salts
- Ionic composition as a function of relative humidity
- Minor constituents
- Electrochemical potential, Eh; Thermodynamic and kinetic considerations
- pH
- Crevices: Metal-to-metal, under-deposit, & dust
- Microbes
- Thermal gradients on surfaces due to mineral scale deposits

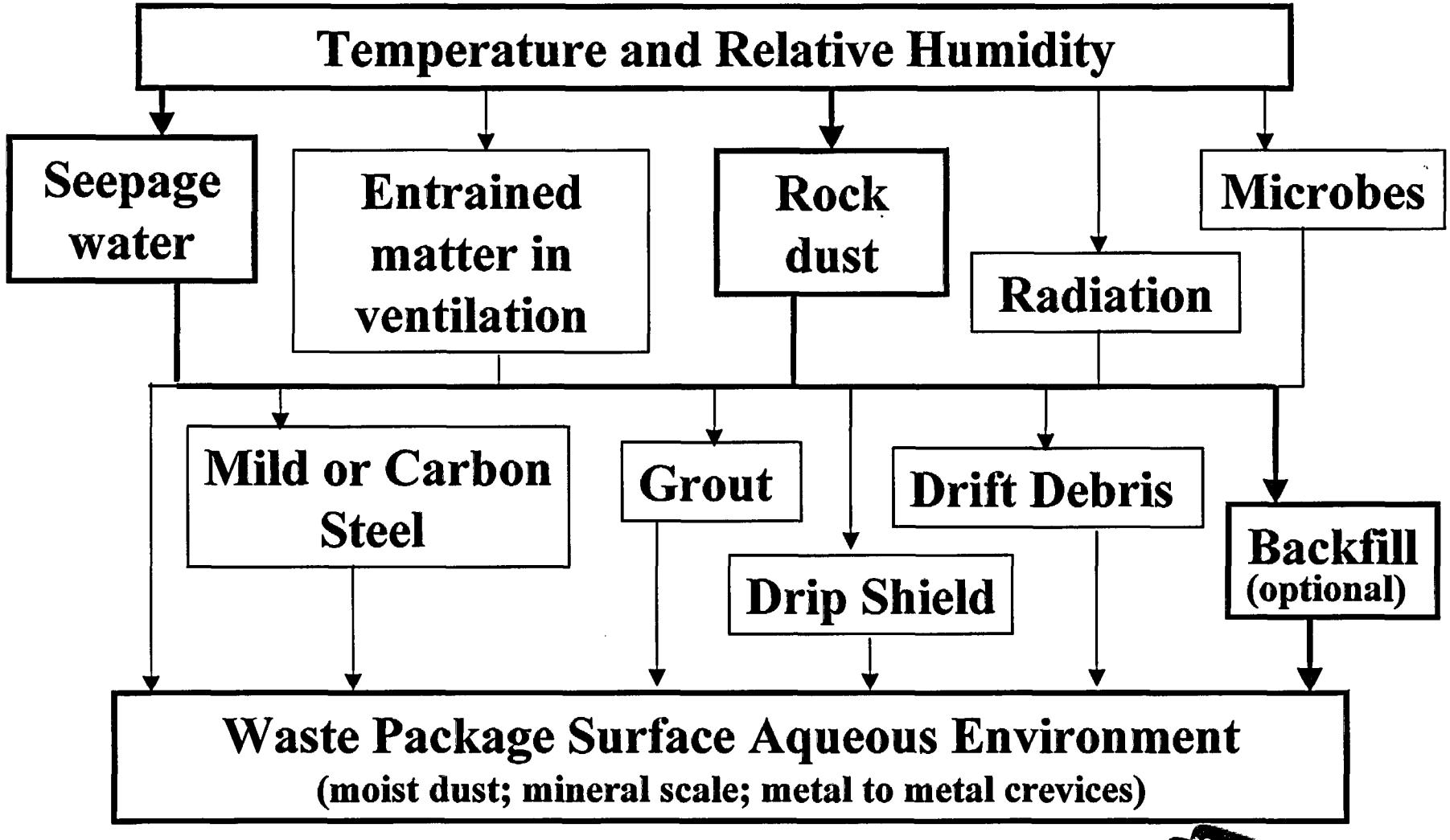
Aqueous Environment Evolution Characterization Strategy



Illustrative Example of Aqueous Environment Evolution

- Seepage water contacting silicate base materials before contacting a waste package
- Silicate base materials:
  - Rock dust
  - Backfill (optional)

Aqueous Environment Evolution Characterization Strategy



Illustrative Example: Seepage Water - Rock Dust - Interaction

- Seepage water reacts with rock dust before contacting the Waste Package
- Considerations
  - Three types of brine
    - Na-Cl-F-NO3-SO4-CO3
    - Na-Ca-Mg-Cl-NO3
    - Na-Mg-Cl-SO4-NO3
  - Rock dust is silicate base
  - Temperature and relative humidity effect on aqueous solutions composition

Illustrative Example: Seepage Water - Rock Dust - Interaction

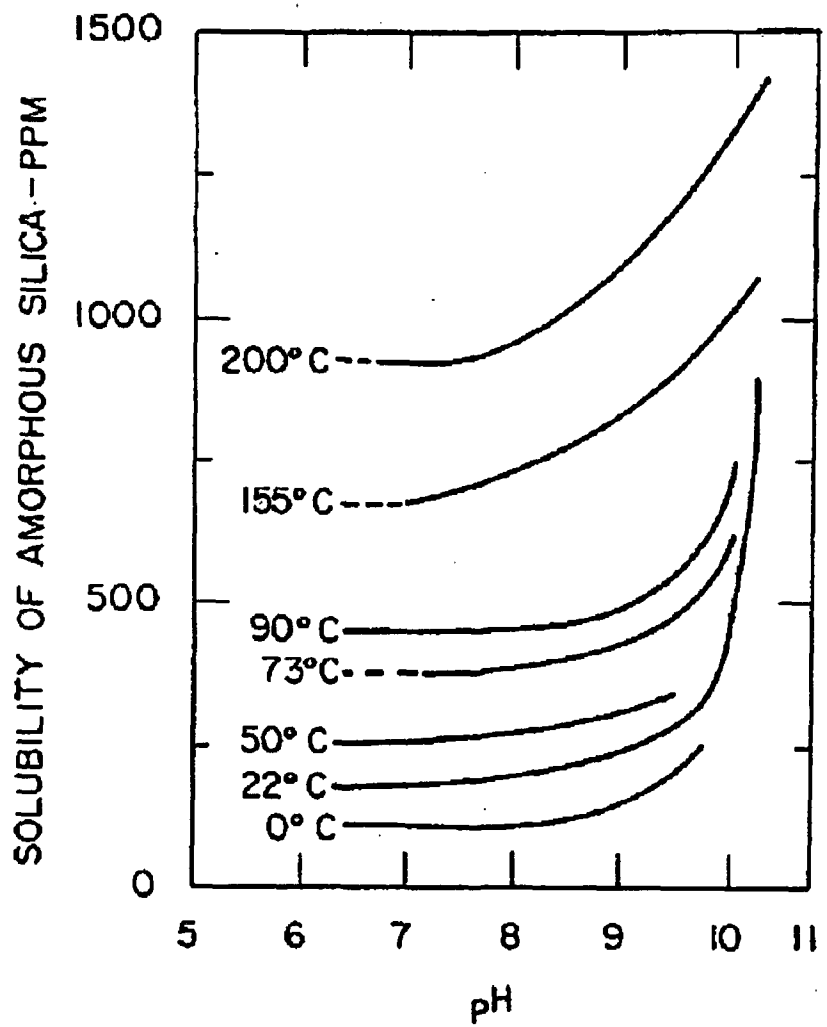
(continued)

- Na-Ca-Mg-Cl-NO3 + "silicates"
  - Clay mineral formation
    - Mg-smectite ($Na_{0.3}(Al,Mg)_2Si_4O_{10}(F,OH)_2$)
  - "Silicate" deposition on the metal surface
- Na-Mg-Cl-NO3-SO4 + "silicates"
  - Clay mineral formation
  - "Silicate" deposition on the metal surface

Seepage Water - Rock Dust or Silica Backfill - Interaction

- $Na\text{-}Cl\text{-}NO_3\text{-}SO_4\text{-}CO_3$ + "silicates"
  - High pH of brine moderated by silica dissolution
  - "Silicate" deposition on the metal surface; more prevalent under higher pH conditions
  - Clay mineral formation
    - Mg-smectite ($Na_{0.3}(Al,Mg)_2Si_4O_{10}(F,OH)_2$)
    - Kanyataite ($NaSi_{11}O_{20.5}(OH)_4 \cdot 3H_2O$)

Silica Solubility Dependence on pH



RK Iler, The Chemistry of Silica, John Wiley & Sons, Inc., New York, 1979.

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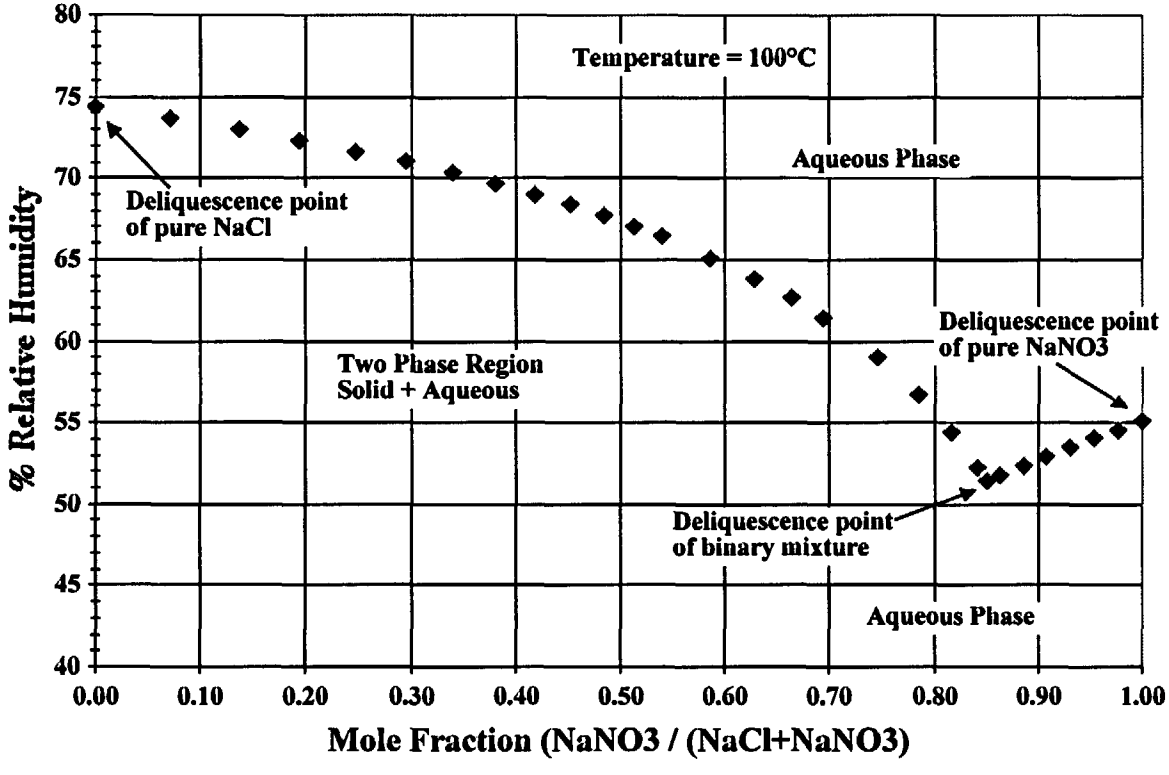
- Microbes

Solution Composition Dependence on Relative Humidity

- Type of corrosion process that occurs is dependent on solution composition
  - Localized corrosion (e.g. crevice corrosion) susceptibility in concentrated solutions is a function of occurs ratio of aggressive ion concentration to inhibitor ion concentration
- Thermodynamic database based on the Pitzer formulation is being developed for relevant species at high temperatures
  - Database for sodium species is nearing completion
  - Database for calcium and magnesium is being developed

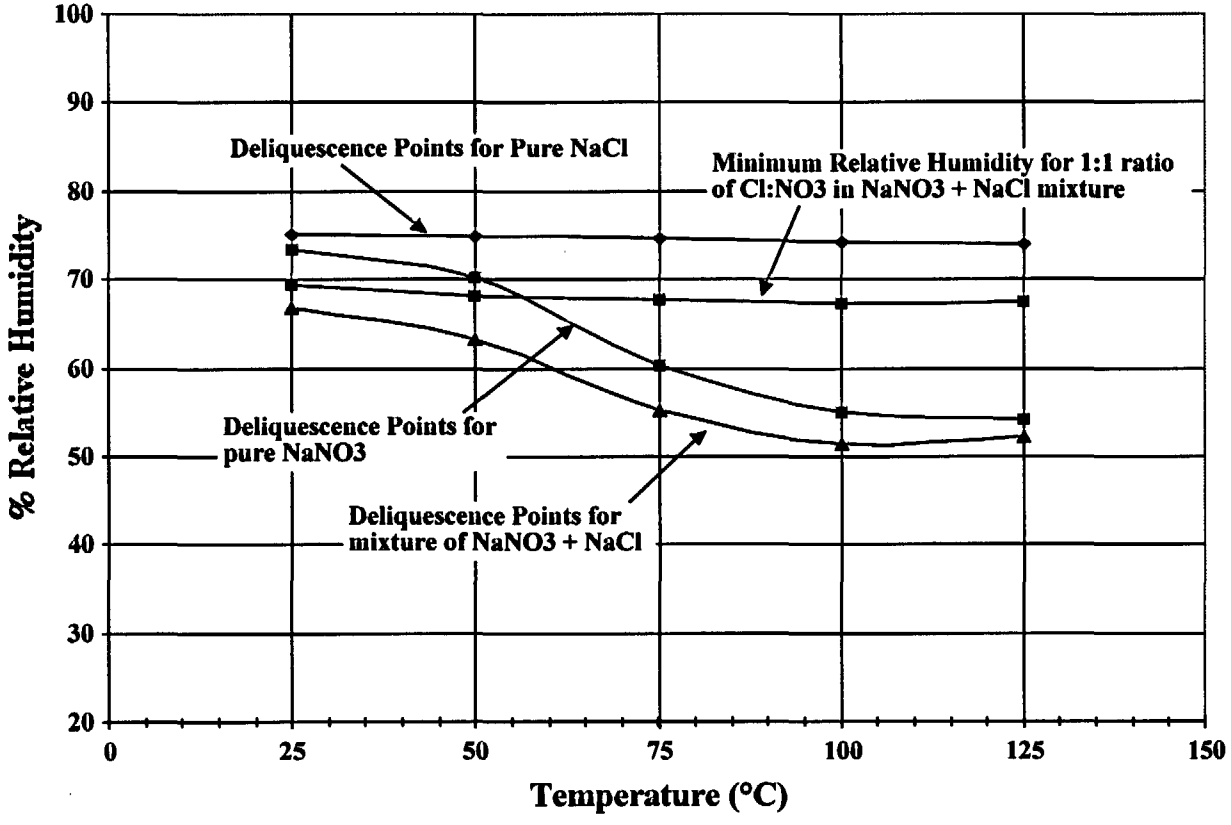
Phase Diagram for Mixture of NaCl + $NaNO_3$



- Deliquescence point of any salt mixture is lower than the deliquescence point of any pure salt in the mixture
- Pitzer database developed to model high ionic strength aqueous solutions

Calculated with EQ3/6 Thermodynamic Code; Tom Wolery, LLNL

Relative Humidity - Temperature Dependence of Aqueous Solution Properties



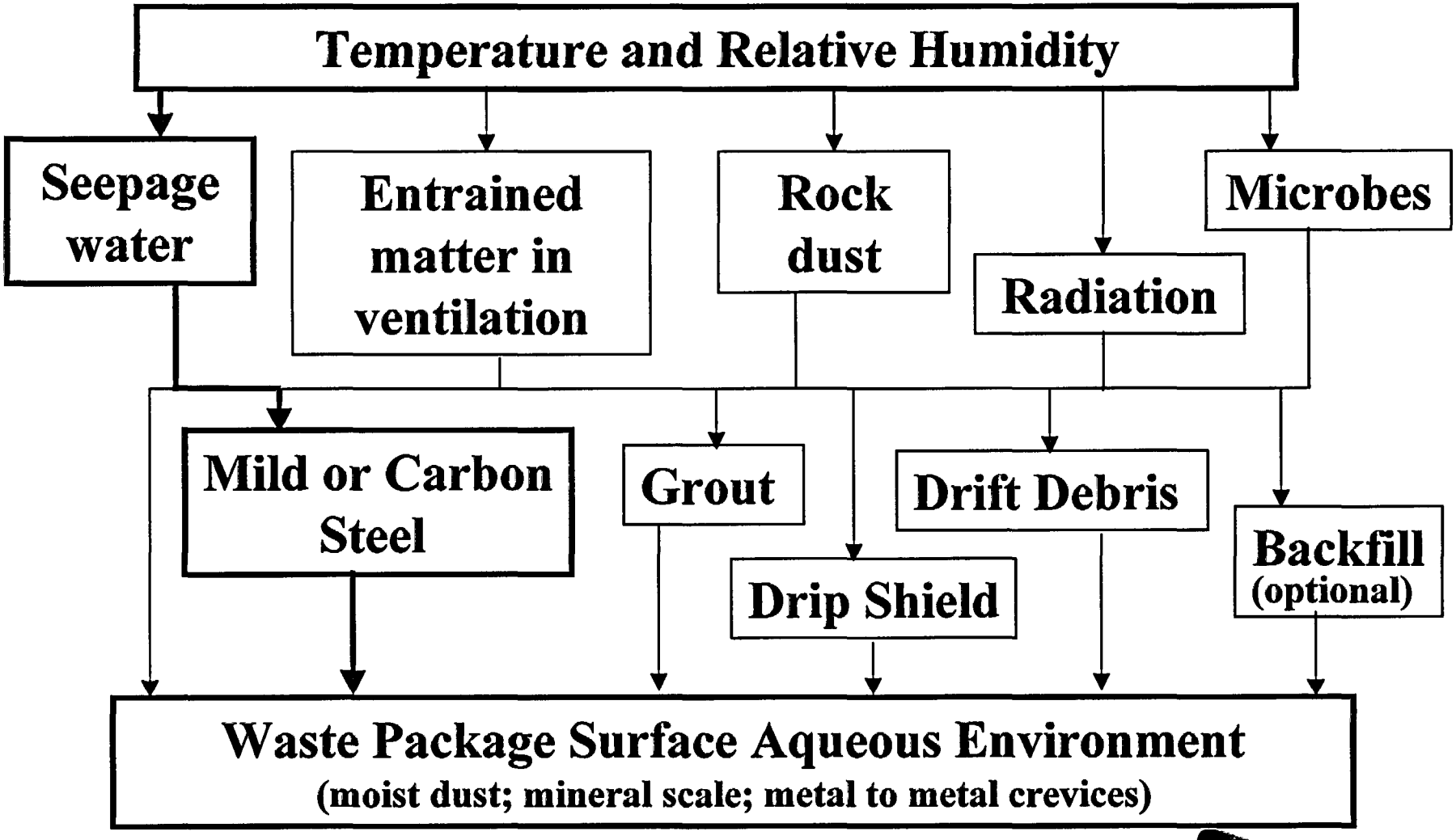
- General corrosion susceptibility at deliquescence of salt mixture
- Localized corrosion susceptibility for sodium base salt may occur at relative humidities much higher than mixture deliquescence

Calculated with EQ3/6 Thermodynamic Code; Tom Wolery, LLNL

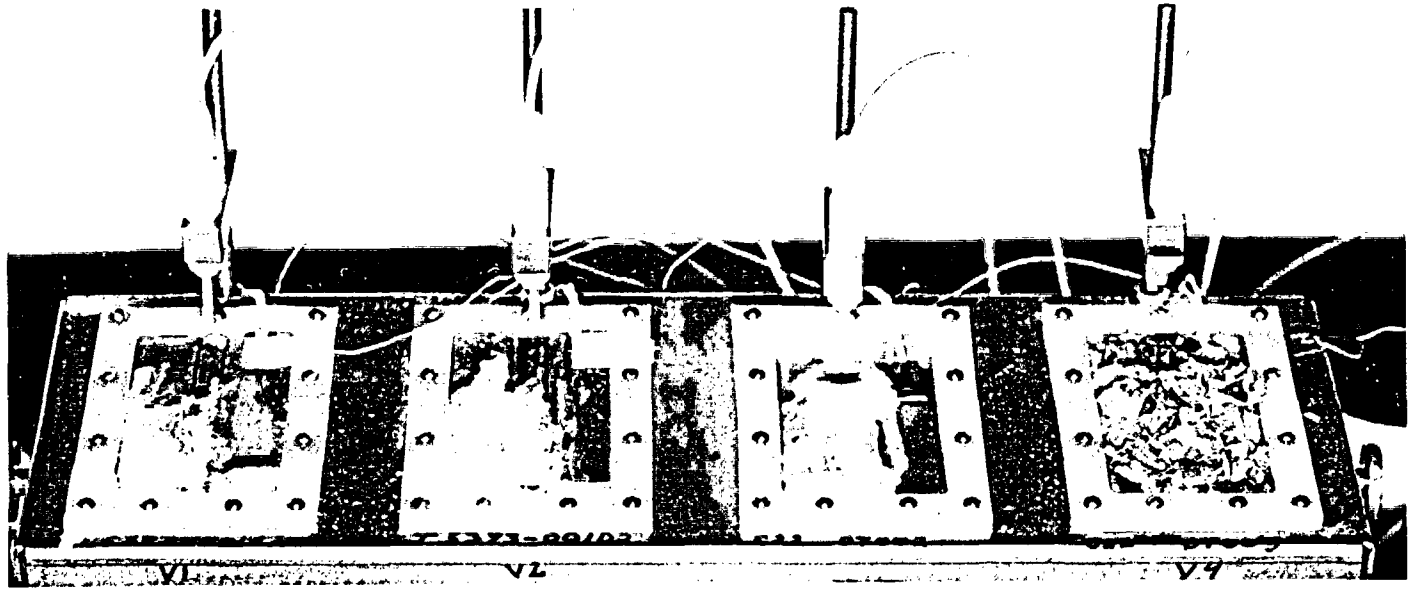
Thin Film Corrosion Testing on Metal Surfaces

- Testing under conditions that result in very high ion strength solutions at temperatures up to 170°C
  - Thermogravimetric analyzer and environmental chamber apparatus modified for elevated temperature testing
  - Analyze corrosion products and mineral scale
- Water drip tests at elevated temperature and constant relative humidity (environmental chamber and heated coupons)
  - Allow evaporation to dryness between drips
- Thermogravimetric analysis (TGA); continuous measurement of weight change vs time
  - Metal coupon with salt deposits (e.g. CaCl2) under constant temperature and relative humidity

Aqueous Environment Evolution Characterization Strategy



Evaporative Drip Testing



- Apparatus modified for higher temperature operation (170°C)
- Testing will include interaction of test aqueous solutions with "grout" and "carbon steel" prior to interacting with waste package candidate material

Summary

- Strategy is to characterize the aqueous environments in contact with the Waste Package (WP) into aqueous solution "types" that can be classified according to their "corrosive nature"
- Identified and consider those parameters that are important for corrosion and potential sources that affect those parameters
- Aqueous solution modeling effort is continuing
- Extending the thin film aqueous solution testing to higher temperatures