Nye County Department
of Natural Resources and Federal Facilities

Alternate Conceptual Models for EBS Water Chemistry and Performance

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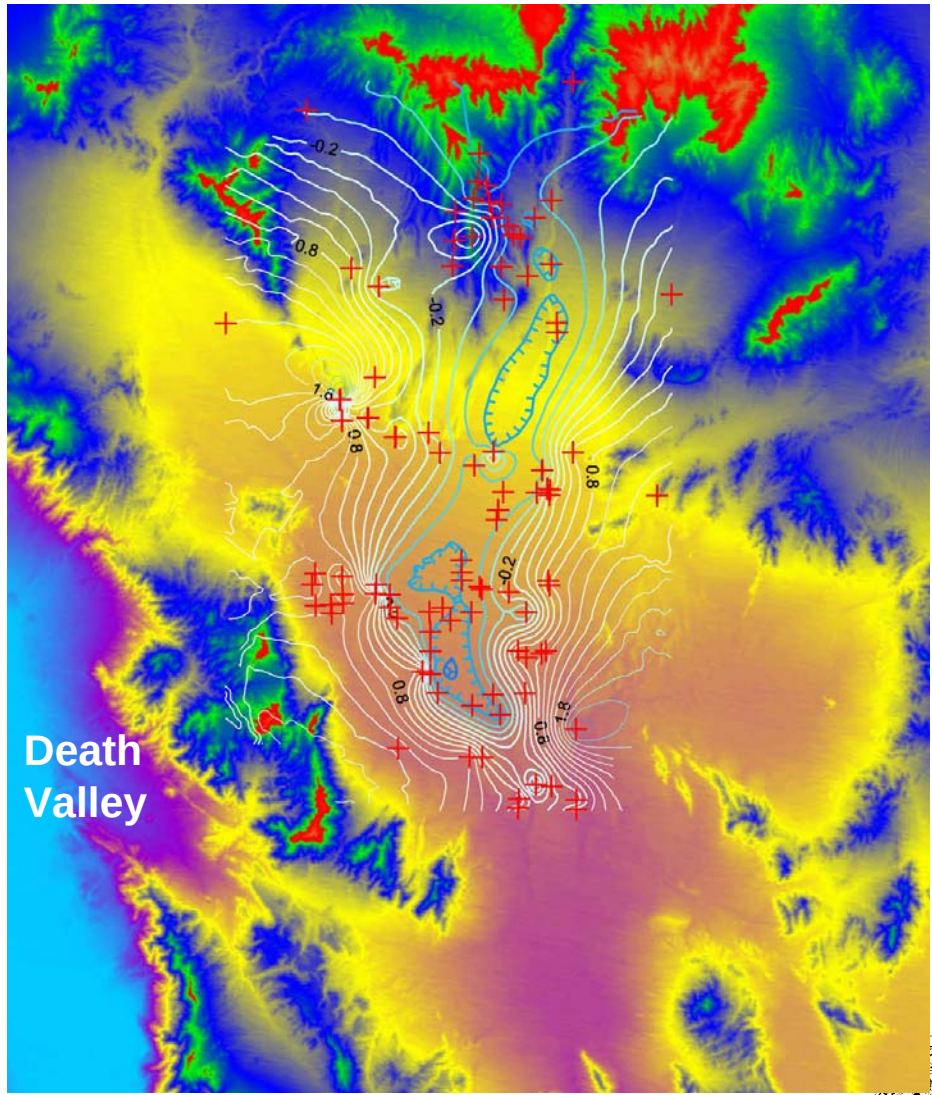
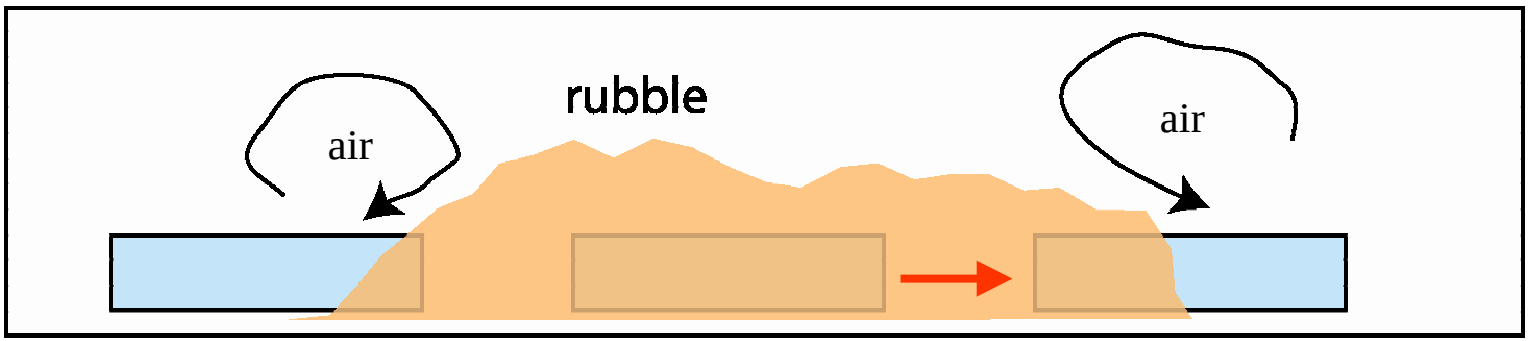
Outline

- Review of physical processes affecting wetting and water chemistry. How does it change in the near field?
- Alternate conceptual model for EBS water chemistry based upon physical separation of soluble salts.
- Performance credit for partially failed waste packages.



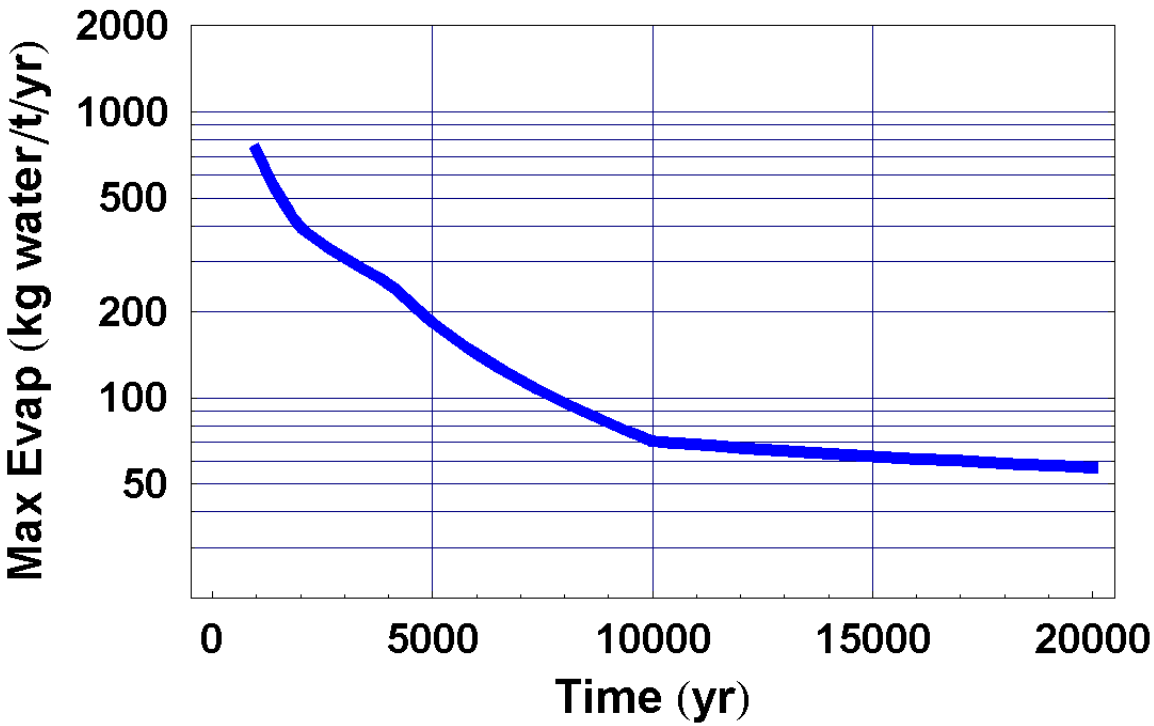
Evaporation and Condensation

- Evaporation and condensation work at many scales.
  - Repository, drift, waste package, inside failed waste package.
- Rubble may cause sustained temperature gradients and/or elevated temperatures.
  - k_{rock} ~ 2 W/m/C
  - k_{soil} ~ 0.15 W/m/C
  - k_{rubble} = ?
  - $k_{corrosion\ products}$ = ?
- Temperature drops proportional to thermal conductivity and heat generation rate.
- When convection is considered the repository becomes more heterogeneous and condensation is anticipated to occur more frequently.

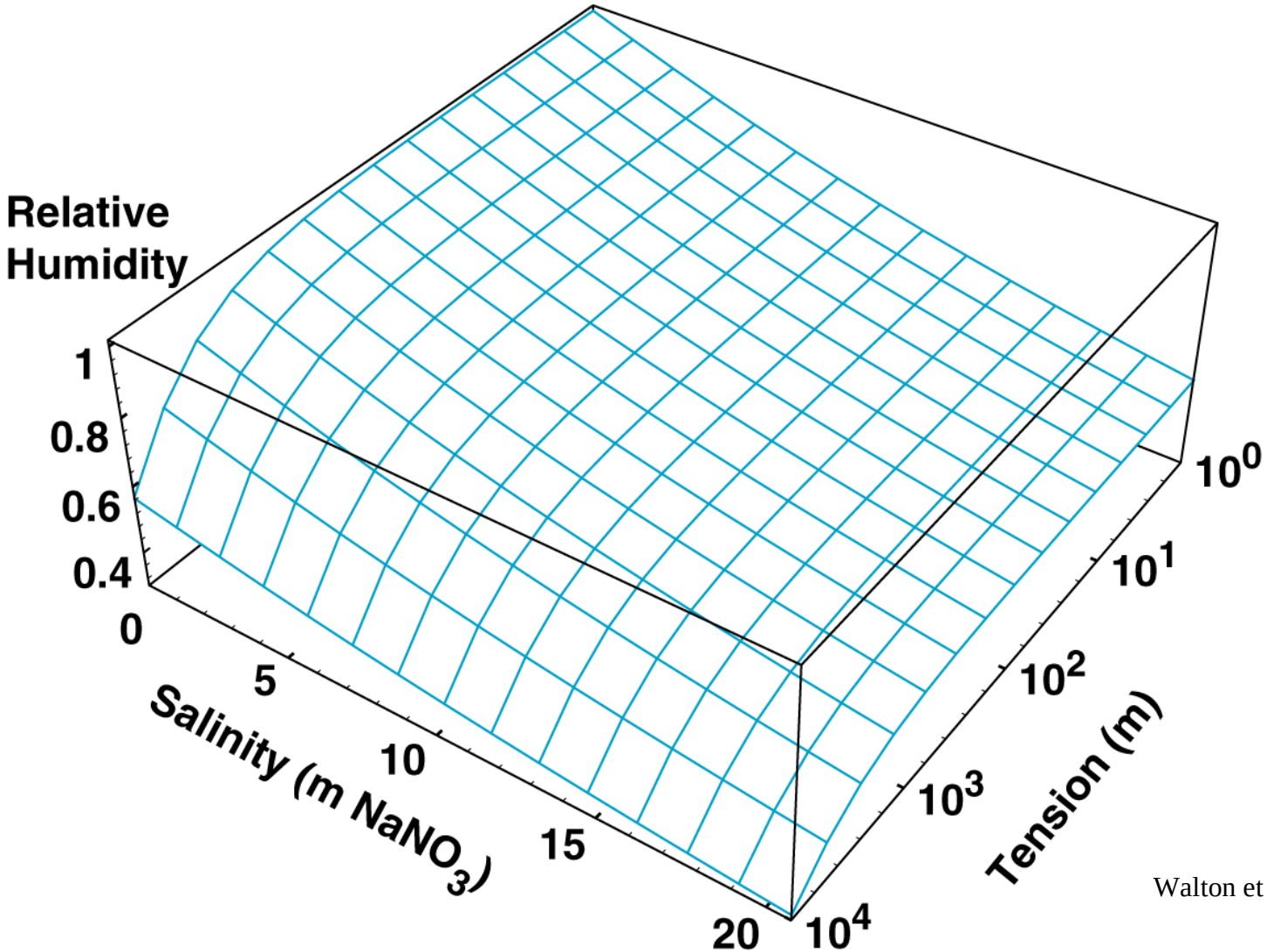


Heat Generation Rate Divided by Latent Heat of Vaporization

- Heat generation extends indefinitely.
- Evaporation and condensation decrease with time but remain significant.
- Heat stored in rock remains important when ventilation is considered.



Vapor Pressure: Solutes and Small Pores



Walton et al., 1994

Alternative Conceptual Model for EBS Water Chemistry

- Many processes (physical, chemical, biological) may be important.
- Most not in codes and not in experiments.
- We have chosen to illustrate one physical process.
- Physical separation of soluble salts based upon differential solubility.

Alternative Conceptual Model for EBS Water Chemistry (continued)

- Common in real world environments:
  - Playa deposits,
  - Near springs in arid regions.
- Water generally moves while evaporating.
- Lower solubility salts precipitate prior to more soluble salts, often at different locations.
- Deliquescence in cooling repository creates new aqueous solutions from the spatially separated precipitates.

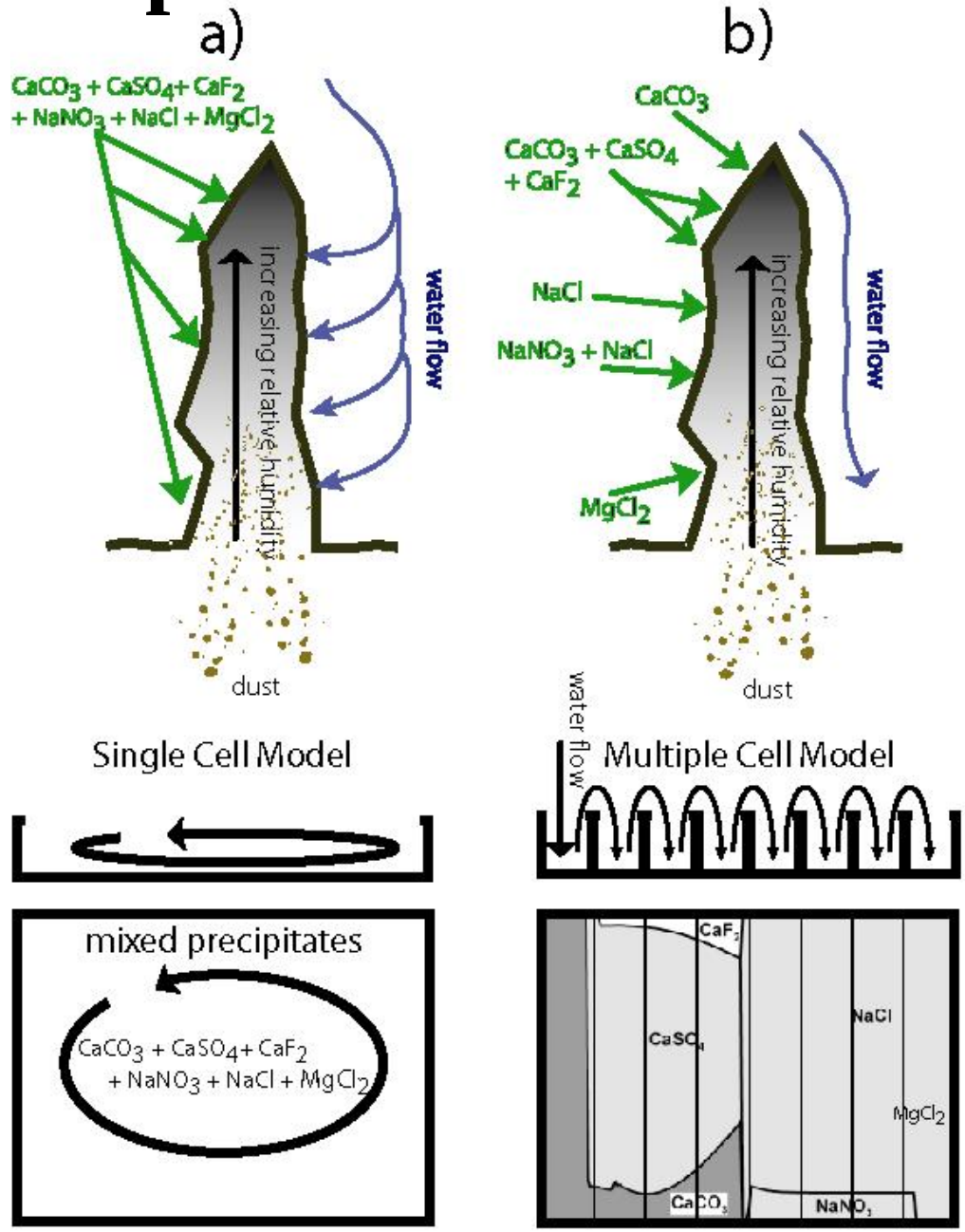
Sidewalk Example

Physical Separation in a Fracture

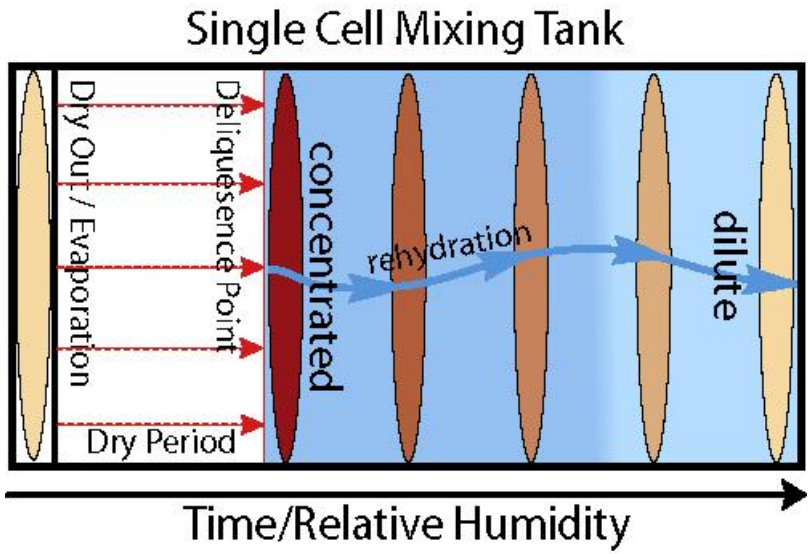
conceptual model

mathematical model

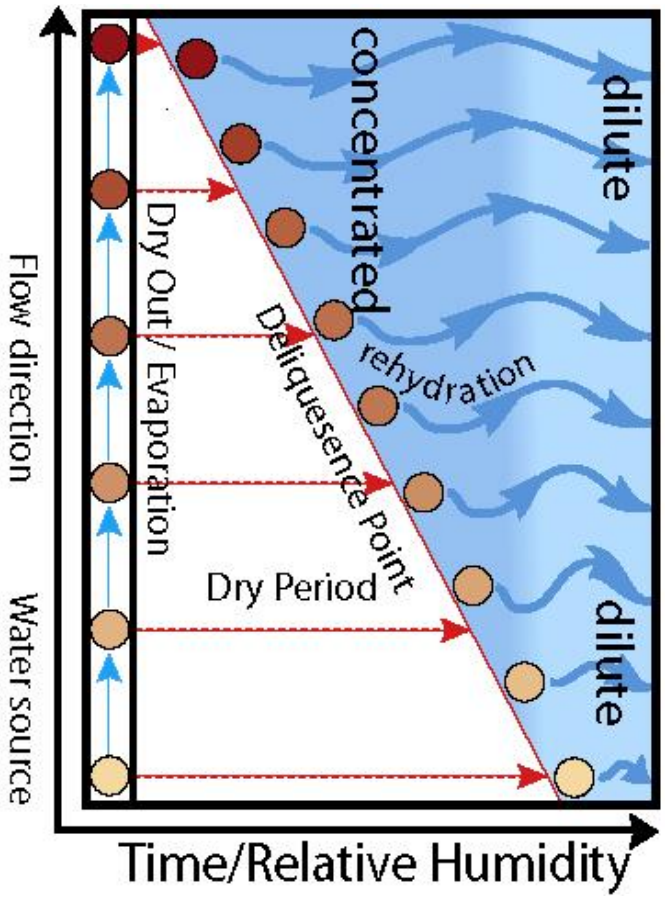
prediction



Precipitation and Deliquescence



Infinite Cell Mixing Tank

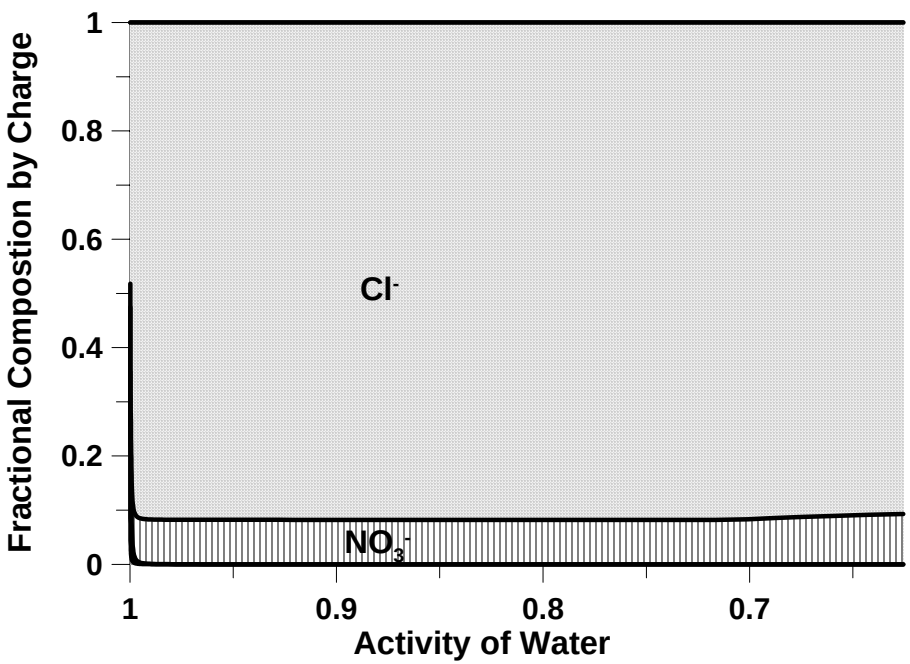


Numerical Model Description

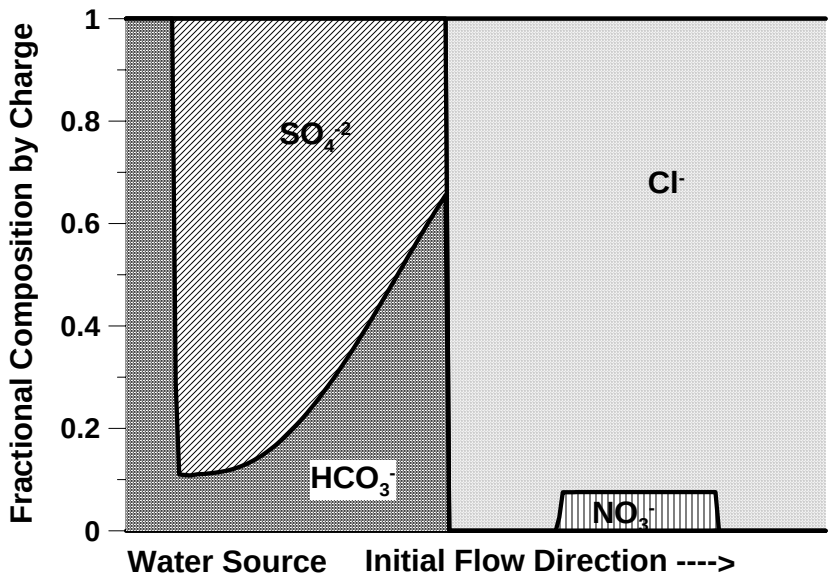
- Simple equilibrium model.
- Suitable for first look semi-quantitative analysis.
- Two endpoints:
  - Single mixing cell (no separation),
  - Infinite series of mixing cells (maximum possible degree of separation by this process).
- Reality likely to be intermediate and highly variable.

Paintbrush Non-welded Tuff Pore Water

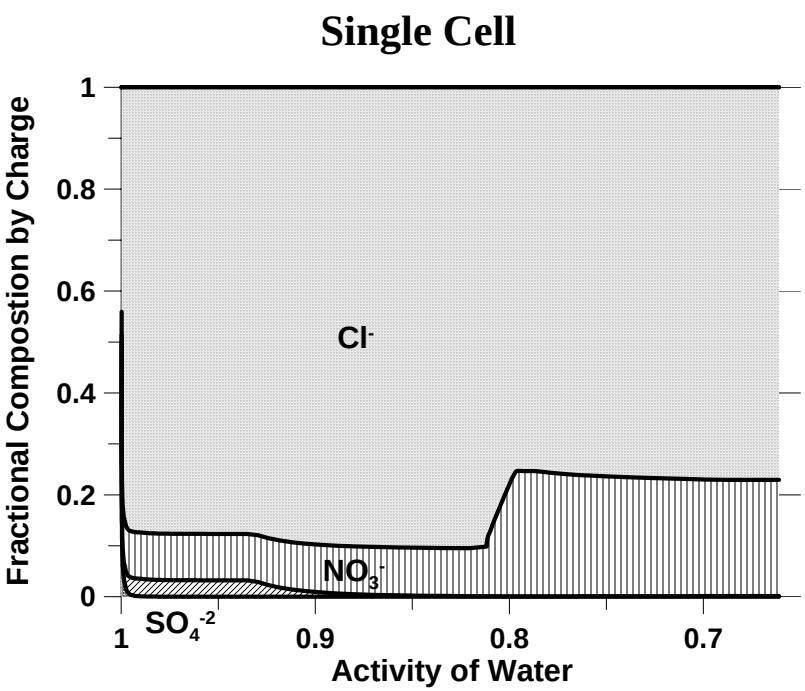
Single Cell

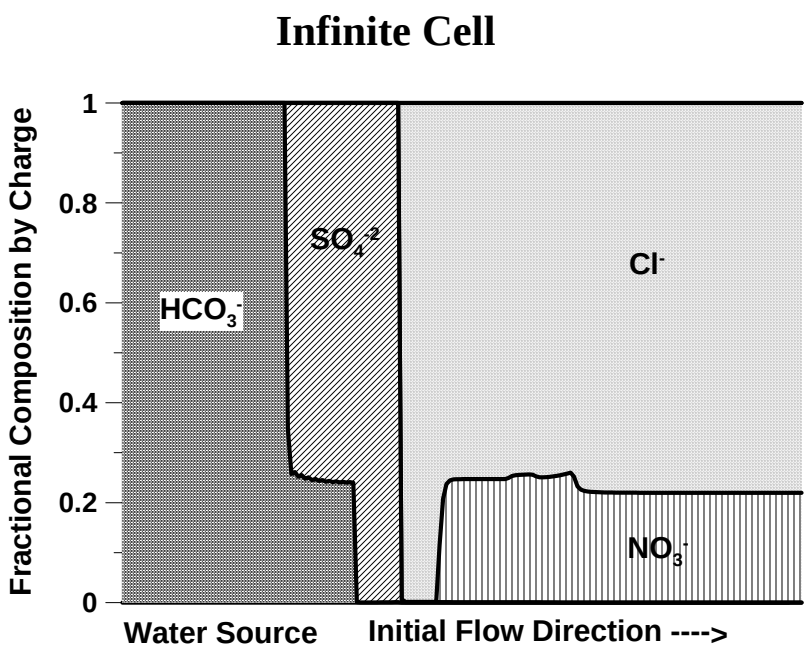


Infinite Cell



Topopah Spring





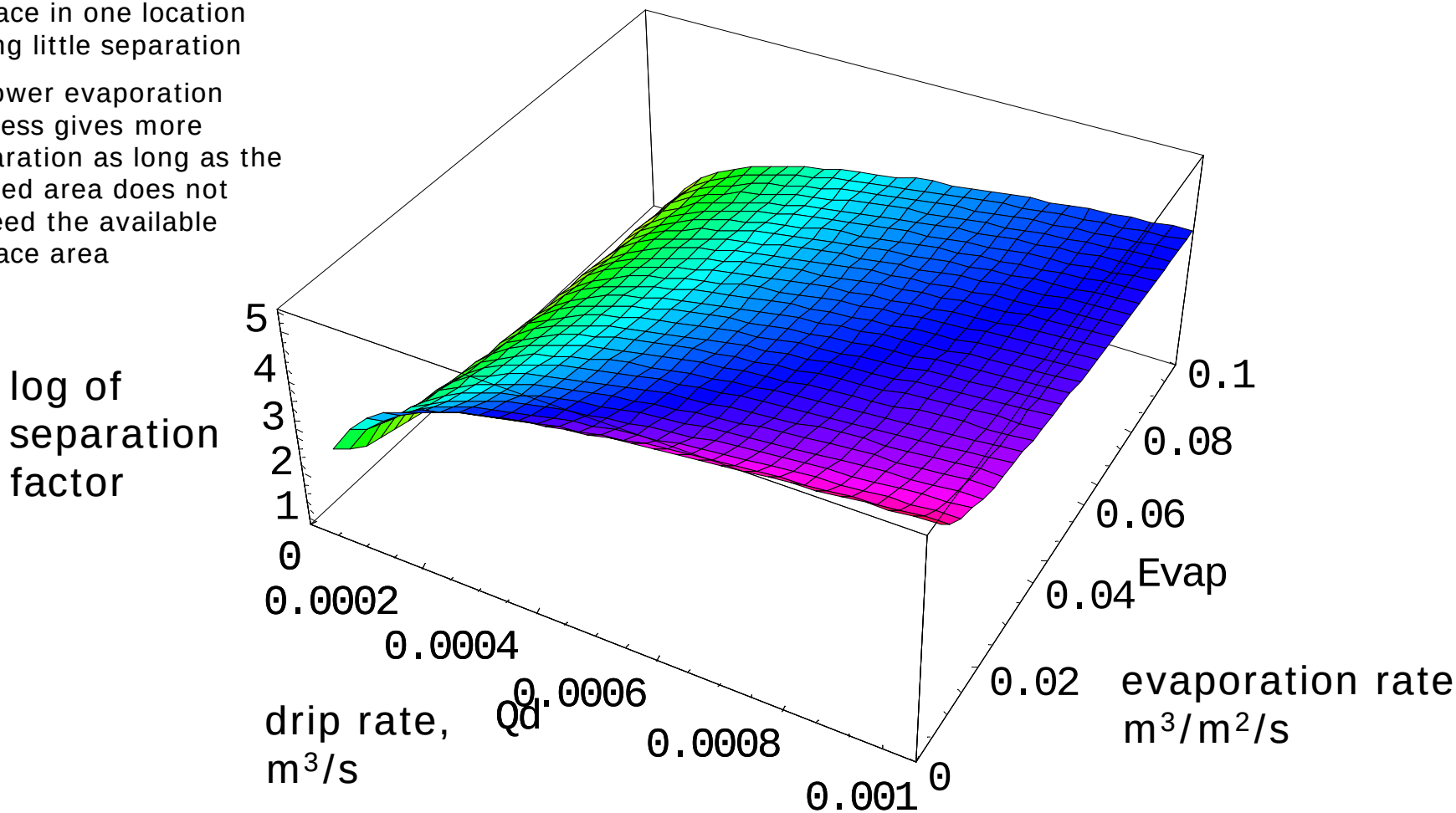
Physical Separation: When will it occur?

- Diffusion equalizes concentrations as water moves.
- If diffusion > advection, no physical separation.
- Advection > diffusion conducive to physical separation.
- Derive and examine ratio of advective to diffusive transport (form of Peclet number) called separation factor.
  - Water film, function of drip rate, evaporation rate, film thickness.
  - Porous media, function of tension and constitutive properties.
- Calculations support likelihood of physical separation.

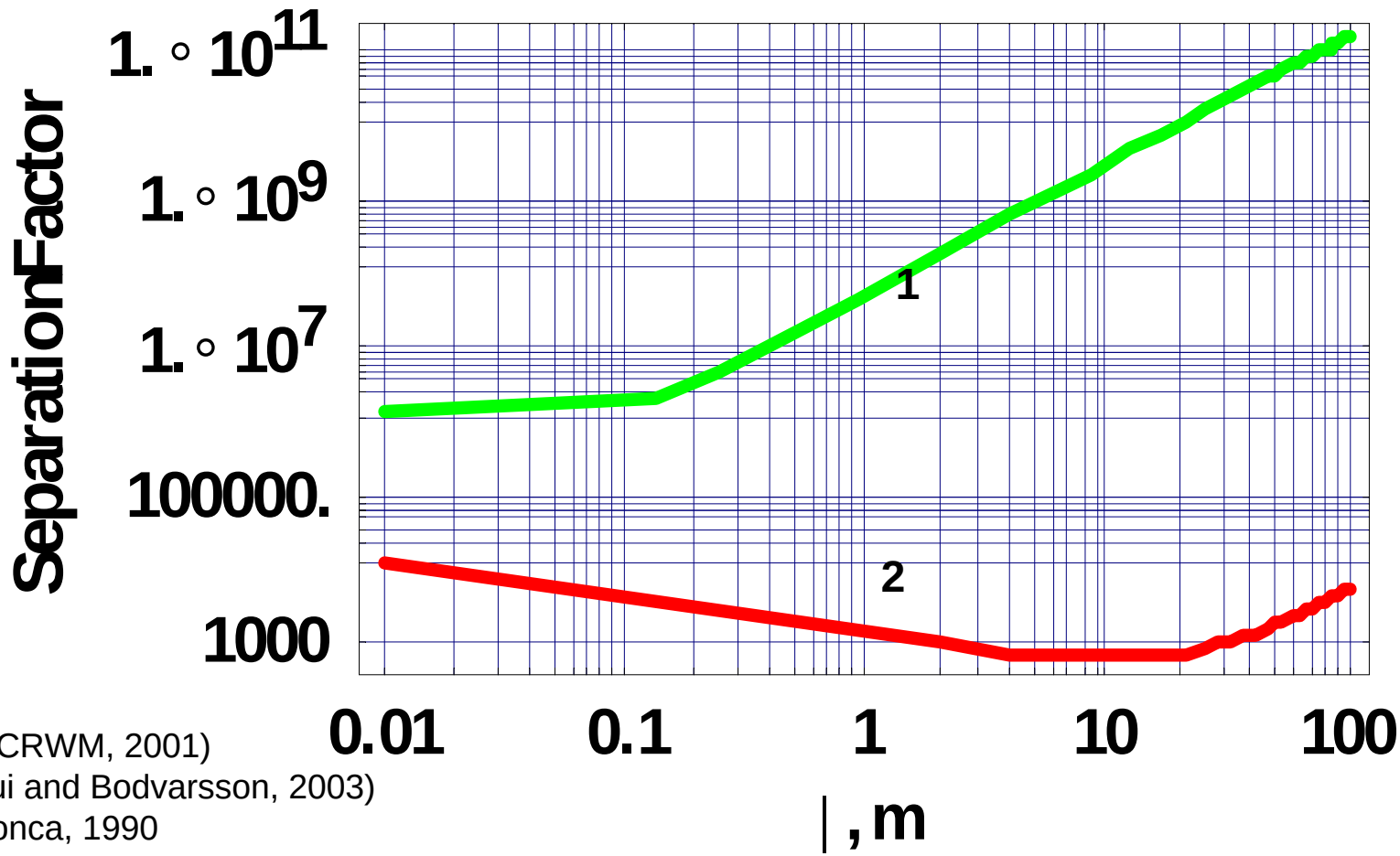
Physical Separation in a Water Film

when drip rates are low the water “flashes off” a hot surface in one location giving little separation

a slower evaporation process gives more separation as long as the wetted area does not exceed the available surface area



Porous Media: Two Examples

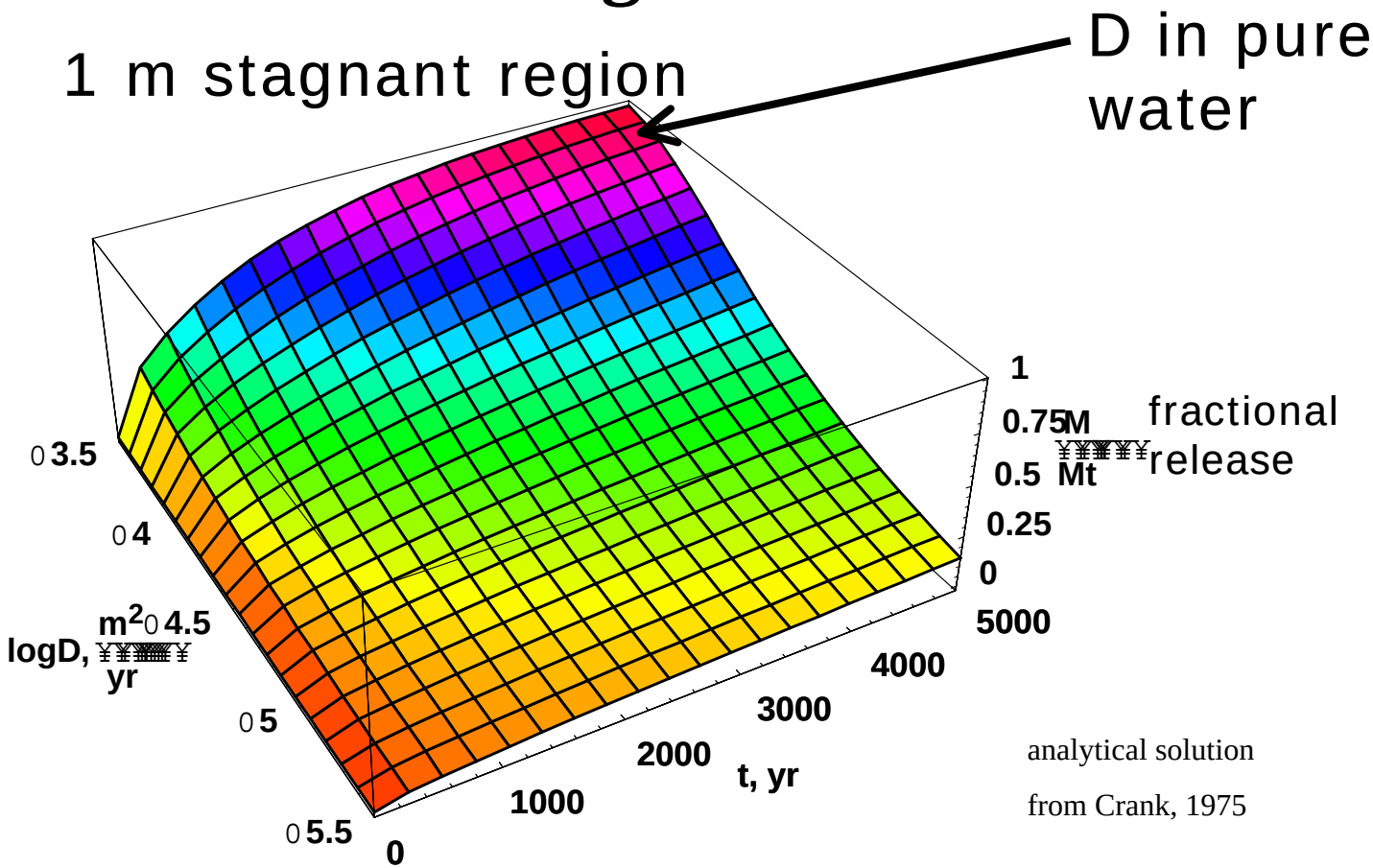


1.(OCRWM, 2001)
2.(Lui and Bodvarsson, 2003)
J. Conca, 1990

Partial Waste Package Failure Credit – Simple Diffusion

- Localized waste package failures (aggressive solution) generally not aligned with seepage (generally less aggressive).
- Diffusion from stagnant zones out to advective transport areas.
- Example calculation without retardation.
- One meter region, analytical solution (Crank), variable effective diffusion coefficient.

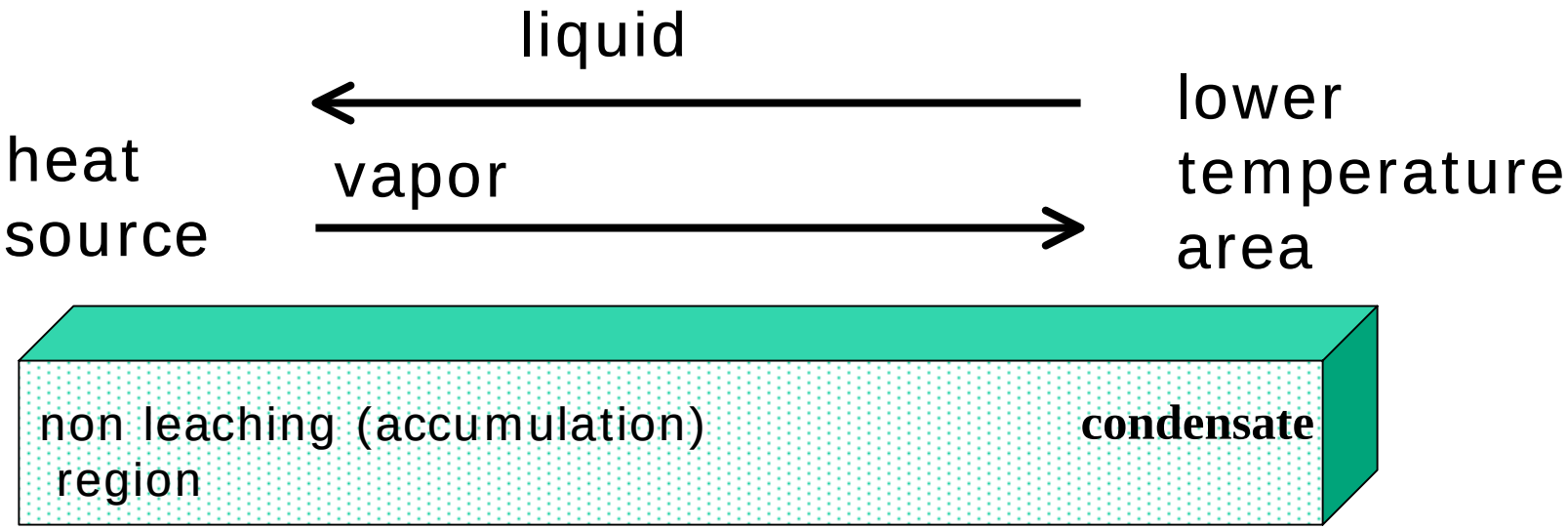
Diffusion from Stagnant Zones in Waste Packages



analytical solution from Crank, 1975

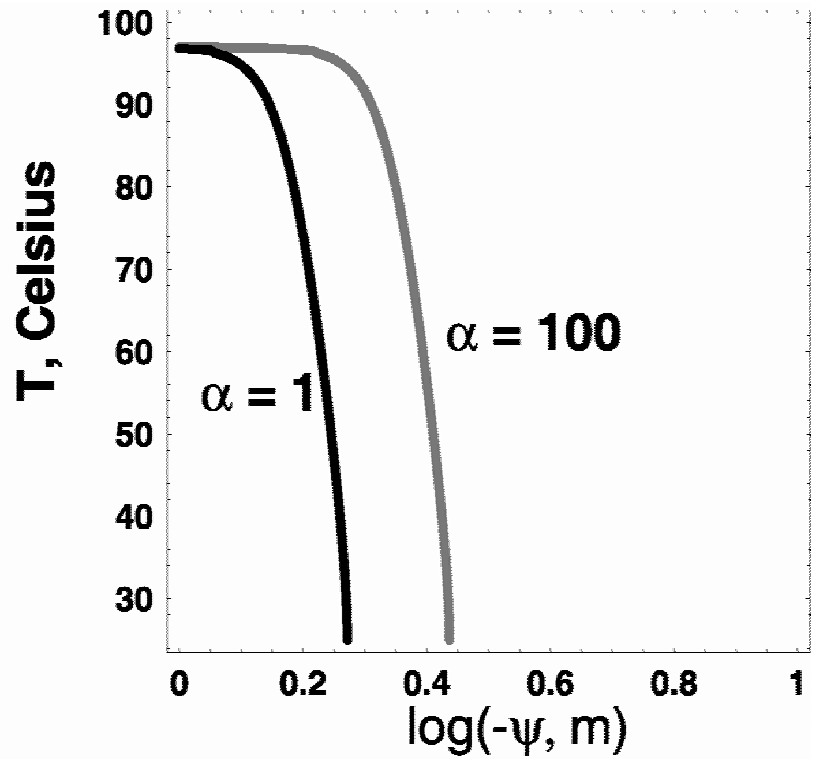
Evaporation in Intact Areas of Failed Waste Packages

- Long term heat generation protects portions of the WP.



Evaporation Protects Areas from Release

- α is the ratio of potential vapor diffusion to liquid advection.
- At $\alpha > 1$ liquid flow is towards the heat source.
- Effectively prevents liquid release.
- Assumes rubble and corrosion products have properties of sand.



Lichtner and Walton; CNWRA 94-022, 1994

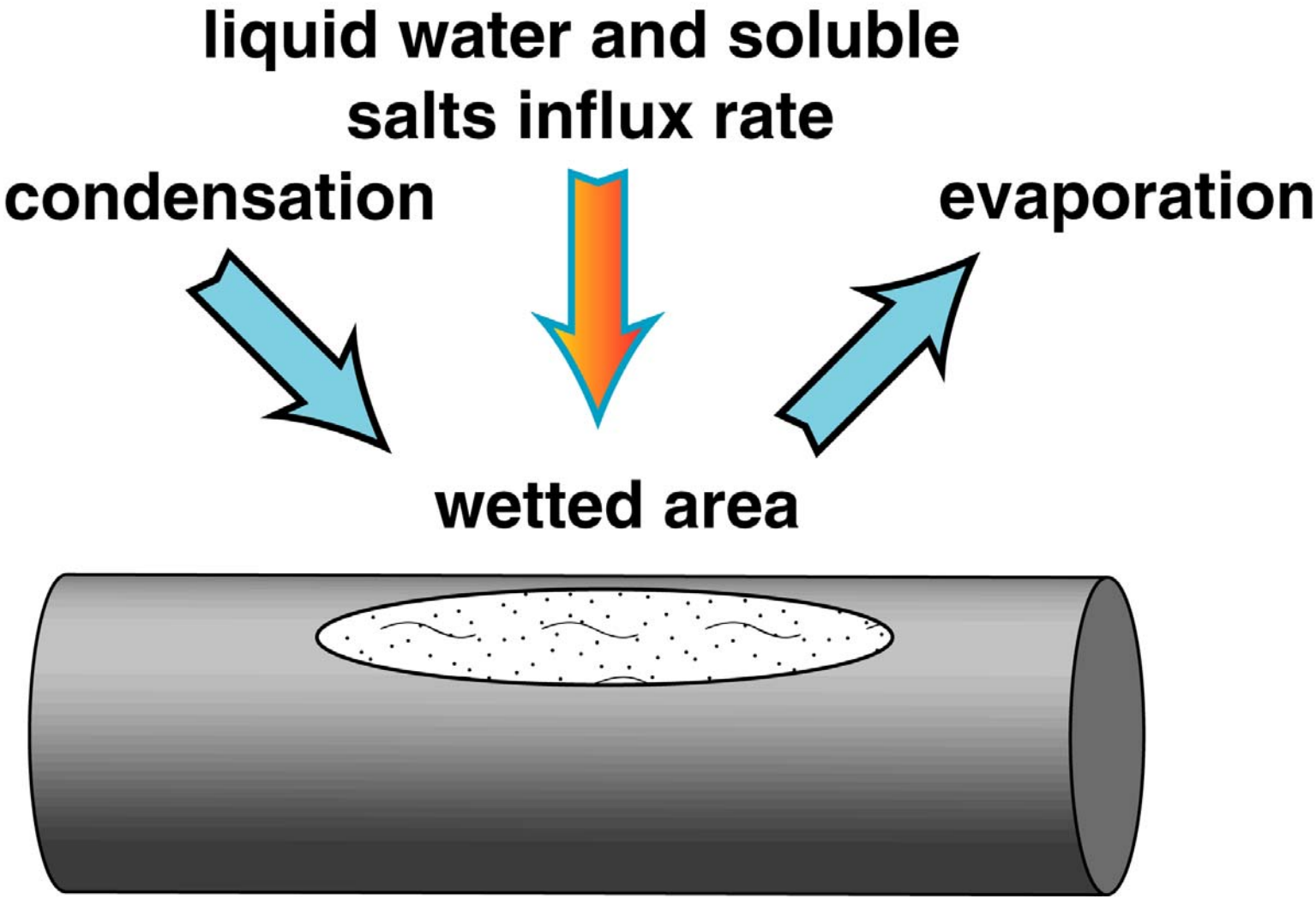
Conclusions

- EBS chemistry more variable than has been assumed.
- Nitrate will sometimes be separated from chloride.
- Changes in design could make this less important (e.g., lower average temperature).
- Some high temperatures will occur in “cold” repository with partial roof collapse.
- Microenvironments persist for > 10,000 years.
- Other defensible factors could be considered for performance credit:
  - Evaporation driven flow system within failed containers,
  - Diffusion in partially failed containers.

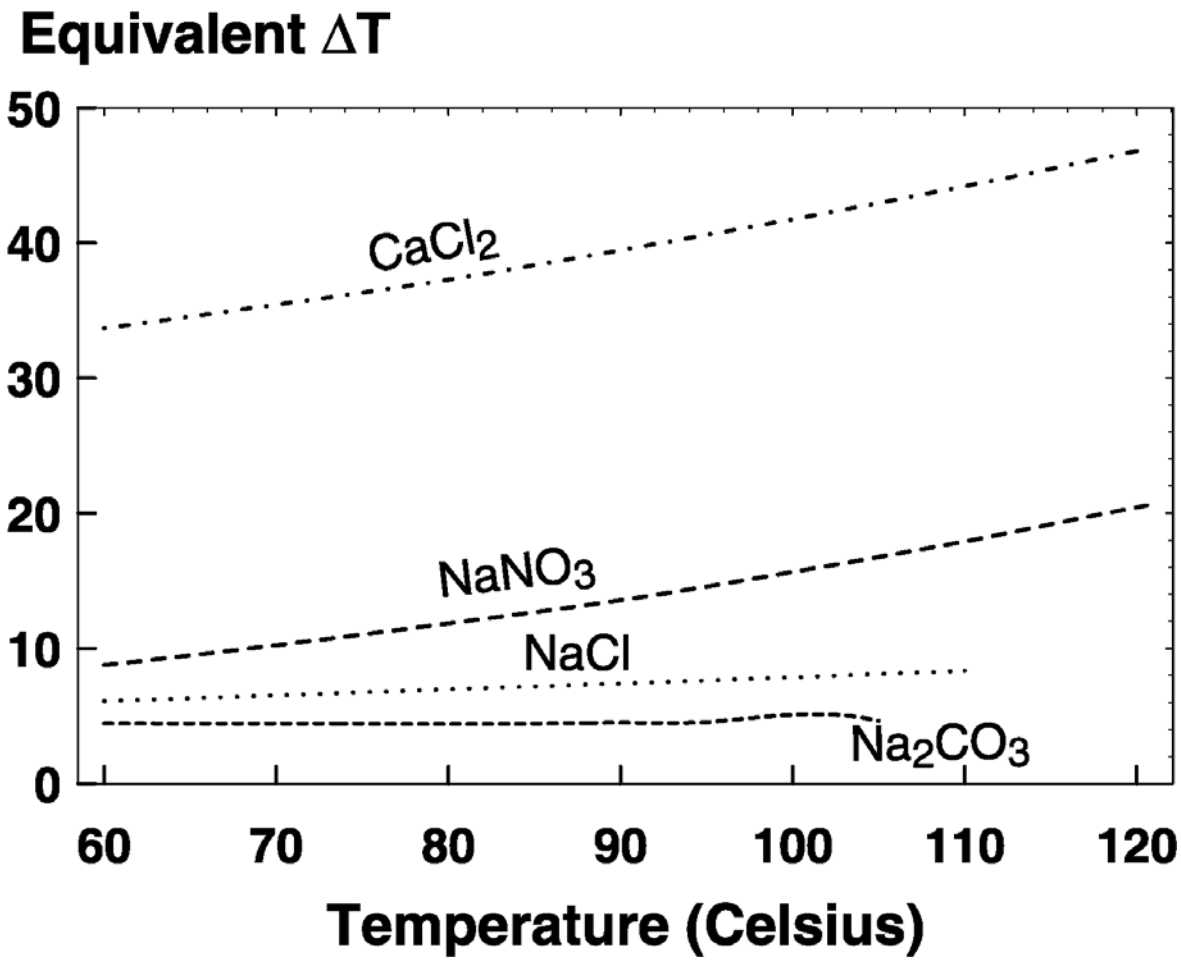
desert spring

Backup Slides

Liquid Film


liquid water and soluble salts influx rate
condensation
evaporation
wetted area

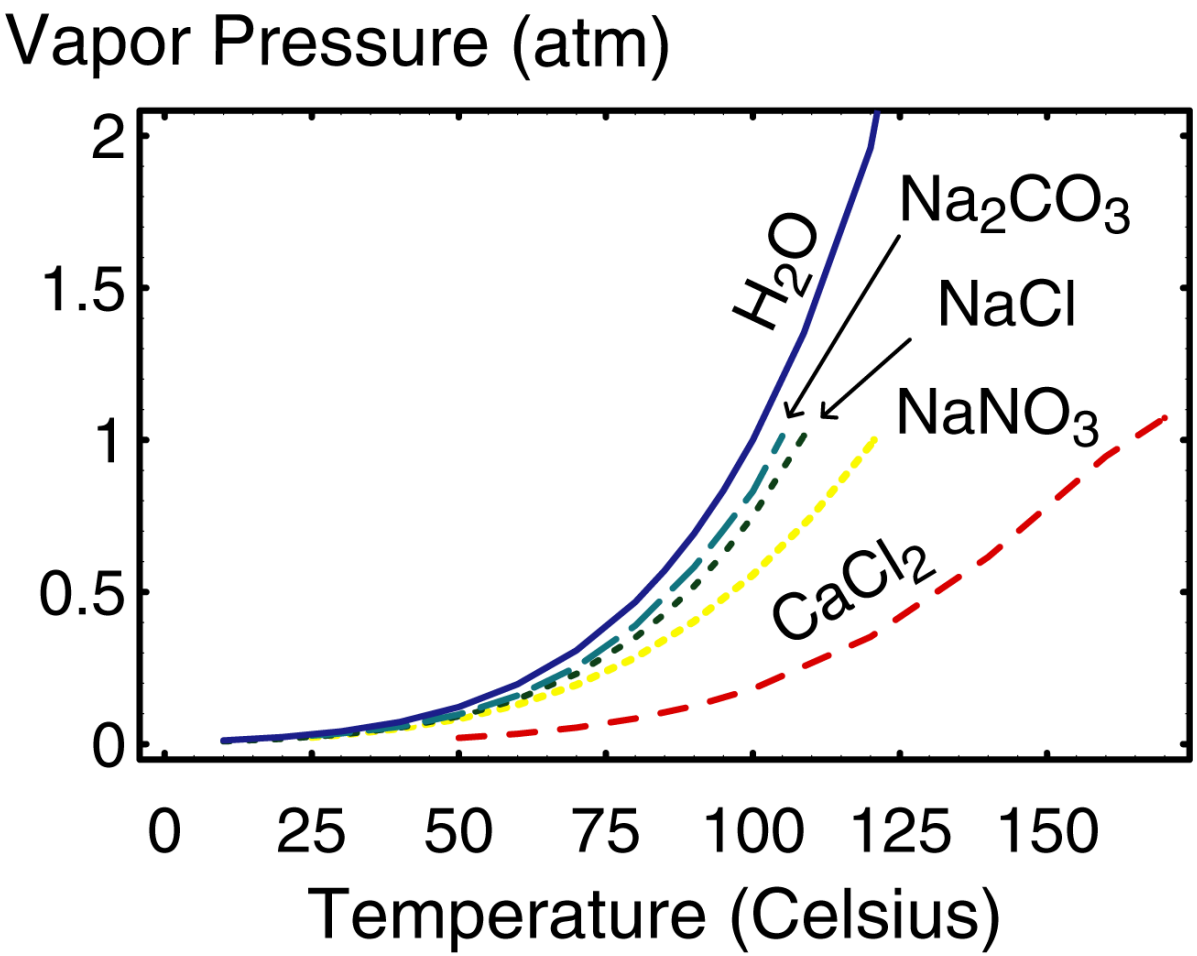
Temperature Gradients



temperature difference between saturated solutions and pure water at same vapor pressure

Walton, 1993

Vapor Pressure of Saturated Solutions



Walton, 1993