U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Thermal-hydrologic-chemical Modeling for Experiment Comparison

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Nuclear Energy

FEHM Model Development for WIPP Site Simulations

Model Development Objectives

1. Build confidence in the safety case
2. Validate model results on simple experiments
3. Support the planning, design, and interpretation of laboratory and field thermal tests
4. Optimize instrument placement and data collection in field testing with sensitivity analysis
5. Reduce uncertainty in simulated performance under full scale repository conditions
6. Code comparisons (FEHM, PFLOTRAN, TOUGH2, CODEBRIGHT)

FEHM Model Development for WIPP Site Simulations

New code developments have allowed for additional physics to be represented in FEHM simulations, new experiments include:

- Thermal conductivity comparison to Bechthold (2004) equation (aka BAMBUSII)
  - Experiment and model design
  - Additional FEHM abilities
- Olivella experiment and comparison of FEHM results to CODE-BRIGHT and TOUGH2
  - Experiment
  - FEHM Modeling
  - Code Comparison
- Salt pan evaporation experiment
  - Mass change with relative humidity
  - FEHM code development for appropriate vapor pressure lowering

Determining thermal conductivity for WIPP Site RoM salt

- Thermal conductivity of a material is an important control on how efficiently heat conducts in a system
- Complicated physics occurring around heat source in RoM salt which is controlled to some extent by thermal conductivity
- Goal is to use experimental and modeled data to lock down values of thermal conductivity for WIPP salt for future modeling

(from Jordan et al., 2015)

Determining thermal conductivity for WIPP Site RoM salt

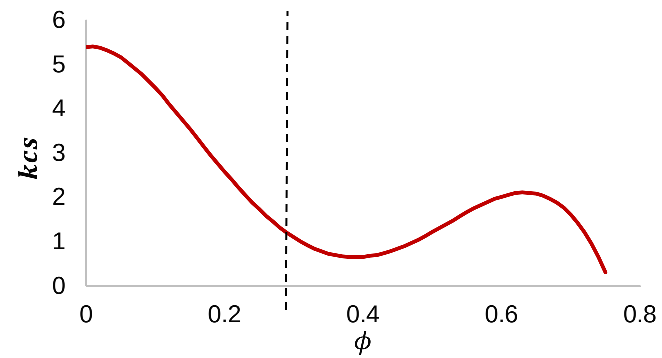
- May need to improve thermal conductivity for WIPP RoM salt for improved simulation of salt behavior to a heat source
- Currently FEHM uses thermal conductivity calculated from porosity based on a relationship from the BAMBUSII study
- Relationship may not be appropriate for WIPP site salt – determined from field experiments of drift-backfilled and crushed salt

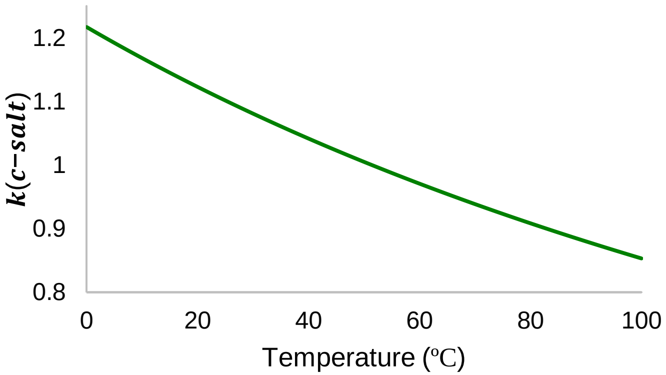
$$\boldsymbol{k_{cs}(\phi) = \begin{pmatrix} -270\phi^4 + 370\phi^3 + \cdots \\ 136\phi^2 + 1.5\phi + 5 \end{pmatrix} \cdot f}$$

$$\boldsymbol{k_{c-salt}(T) = k_{cs}(\phi)\left(\frac{300}{T}\right)^{\gamma}}$$

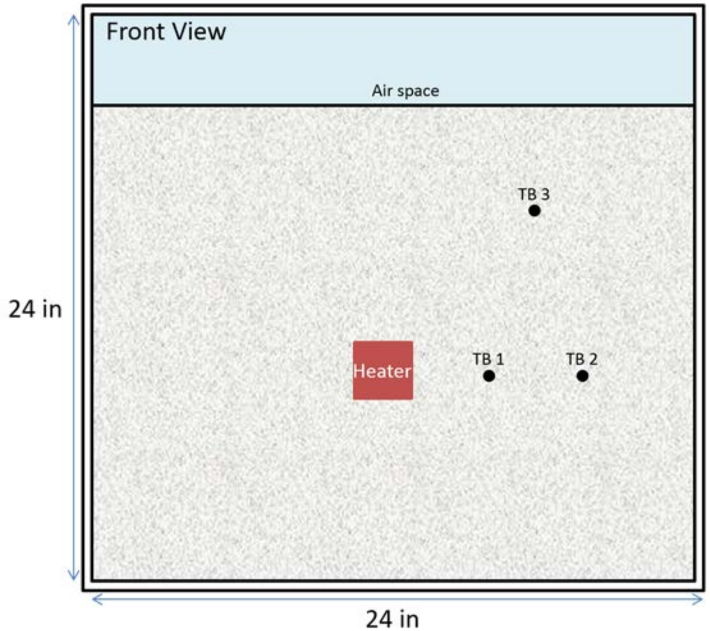
$\boldsymbol{k_{cs} = thermal\ conductivity\ (crushed\ salt),}$
$\boldsymbol{\phi = \text{porosity}, f = fitting\ factor,}$
$\boldsymbol{T = temperature, \gamma = material\ constant}$

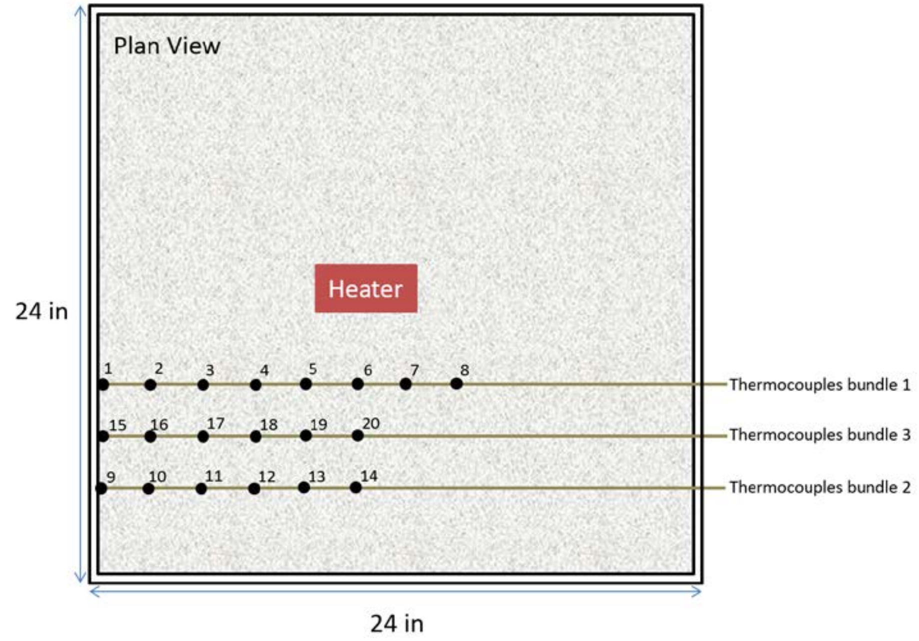
(from Bechthold, 2004)





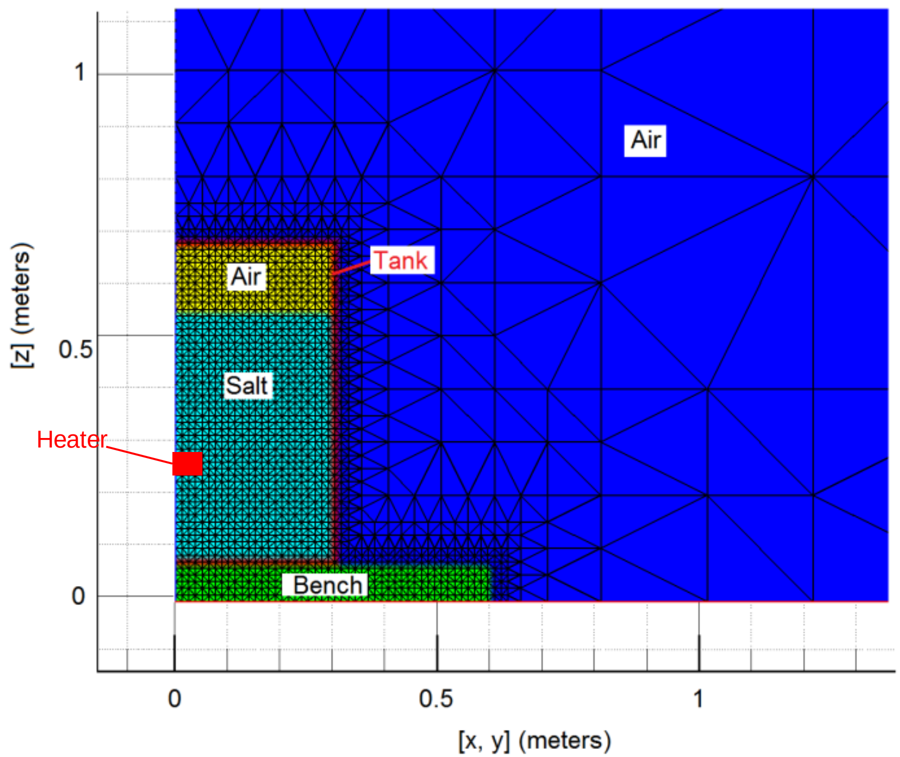
Determining thermal conductivity for WIPP Site RoM salt

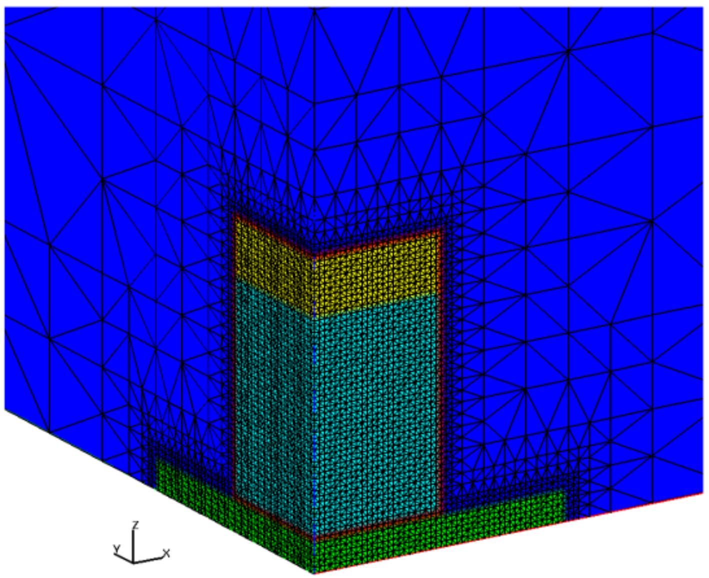




- Total mass of salt = 500 lb +- 20
- Moisture content = 0.2 wt. %
- 24” by 24” Plexiglas Box in laboratory
- Three thermocouple bundles with total of 20 sampling locations
- Tested three heater temperatures (80ºC, 160ºC, and 260ºC)

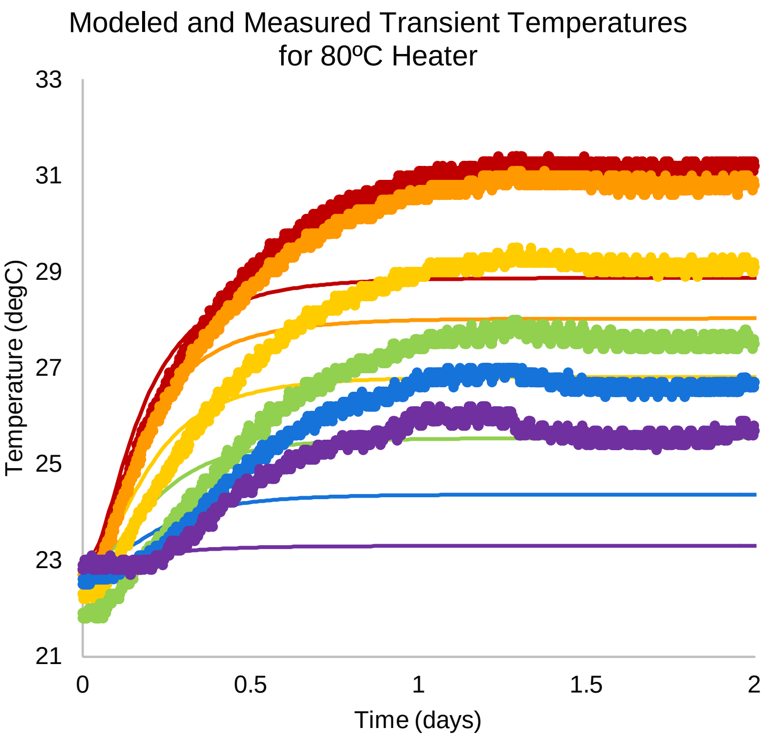
Determining thermal conductivity for WIPP Site RoM salt

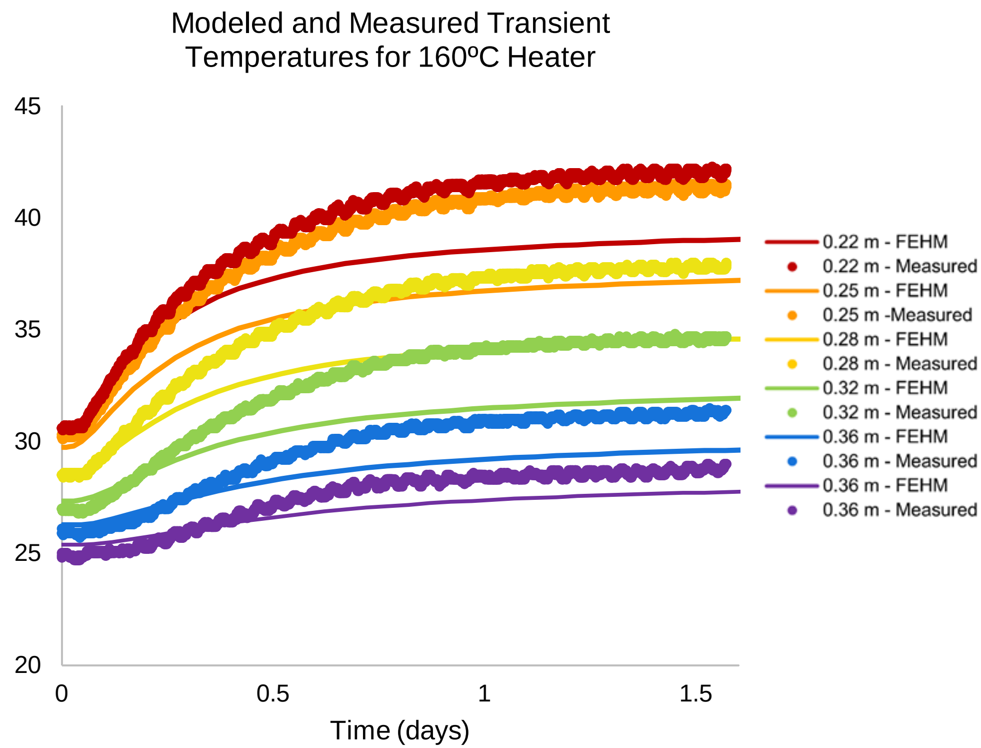




- Three dimensional model, quarter-space model includes RoM salt, air inside and outside of the box, Plexiglas walls, and lab bench
- Used BAMBUSII relationship for thermal conductivity
- Ran 3 simulations of heater temperature set to 80ºC, 160ºC, and 260ºC

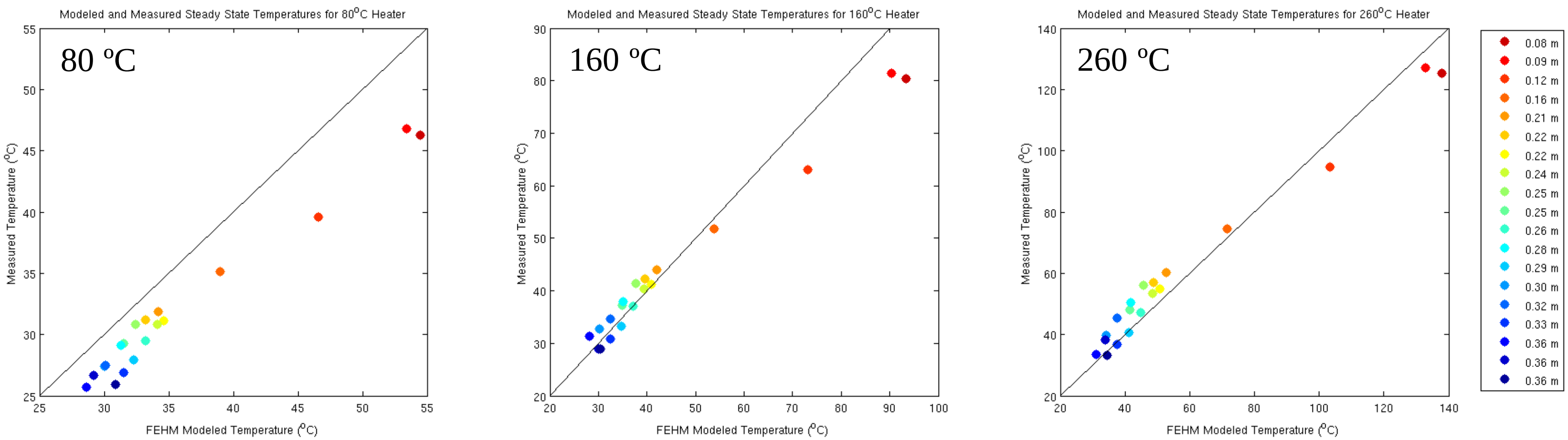
FEHM Model Development for WIPP Site Simulations





- BAMBUSII function of thermal conductivity:
  - Over predicts time of heat equilibration for 80ºC case, under predicts for 160ºC case
  - Under predicts steady-state temperature for both cases

FEHM Model Development for WIPP Site Simulations



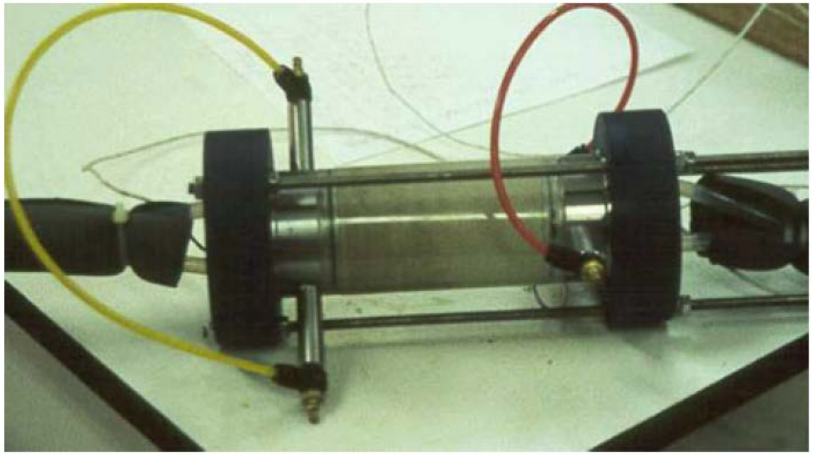
- Steady state measured and modeled temperatures from salt box experiment show the thermal conductivity derived from BAMBUSII does not work well for all temperatures:
  - Poor fit to 80 ºC test
  - Poor fit close to heater
  - Gas tracer data may give clues to change in behavior for different temperatures

FEHM Model Development for WIPP Site Simulations

The poor fit to the data indicates a new function is needed for WIPP-site simulations

- BAMBUSII determined salt based on different site with possibly different humidity, saturation, impurities in salt, and other environmental conditions
- We will use parameter optimization techniques to determine a new function for thermal conductivity to better fit for the RoM salt from WIPP site
  - PEST is a flexible parameter estimation software we can use to optimize a new thermal conductivity function to best reproduce the temperature changes for all 20 measurements for the three temperature experiments

Olivella 2011 Experiment



Sample	Cylindrical with horizontal axis
Diameter	50 mm
Length	100 mm
Initial porosity	30%
Initial saturation degree of brine	40%
Grain size	1–2 mm
Hot side temperature	85°C
Cold side temperature	5°C
Testing time	15 days

Goal is to develop new capabilities for FEHM for salt problems and validate FEHM against experimental data and other codes (CODE-BRIGHT, TOUGH2)

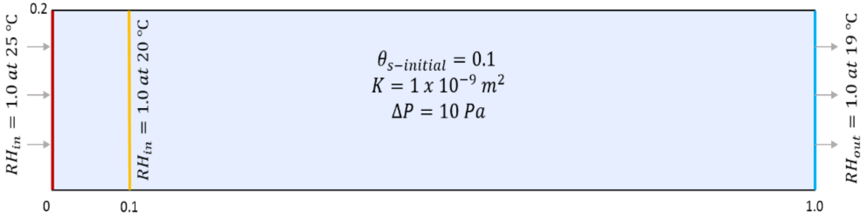
Canister experiment (Olivella et al., 2011)

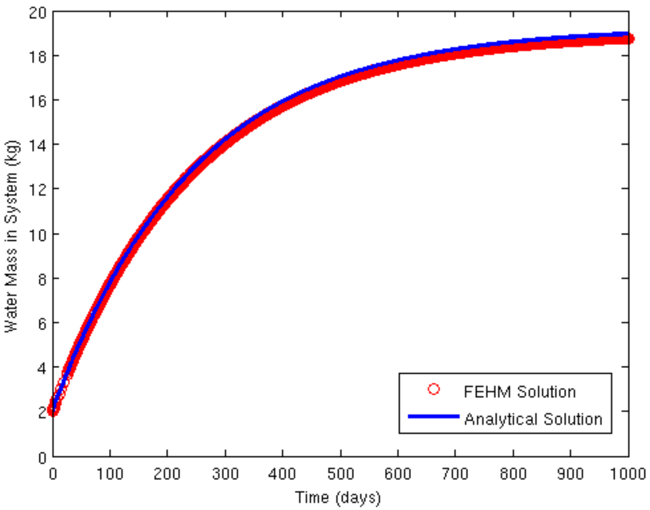
- 0.1 m canister of salt, heated ends to 85ºC and 5ºC
- Characterized salt matrix properties at 4 times following heating
- Used CODE-BRIGHT to model system and compare experimental results

Olivella 2011 Experiment

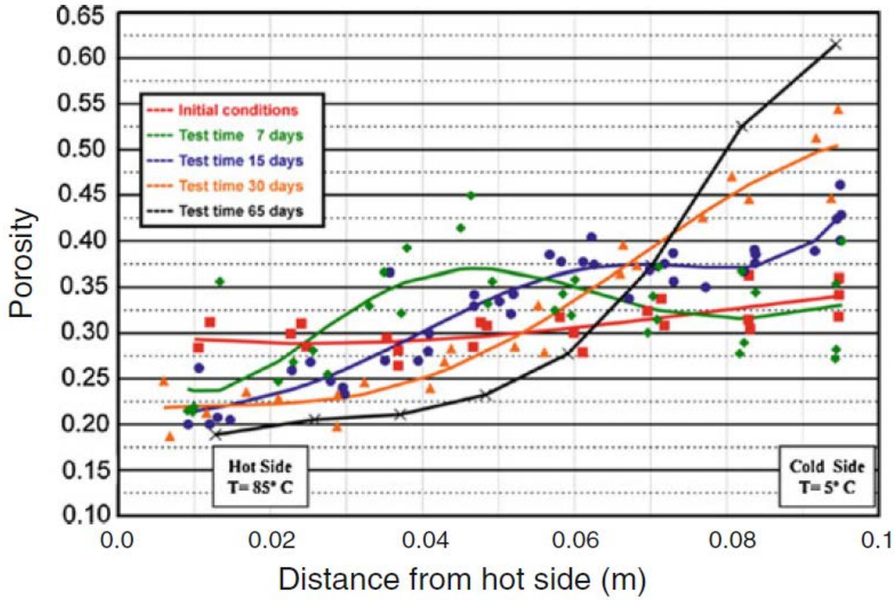
- Interested in porosity changes, brine migration due to large temperature gradient
- Equations used for modeling using CODE_BRIGHT (Olivella et al., 2011) are newly incorporated into FEHM salt modeling capabilities

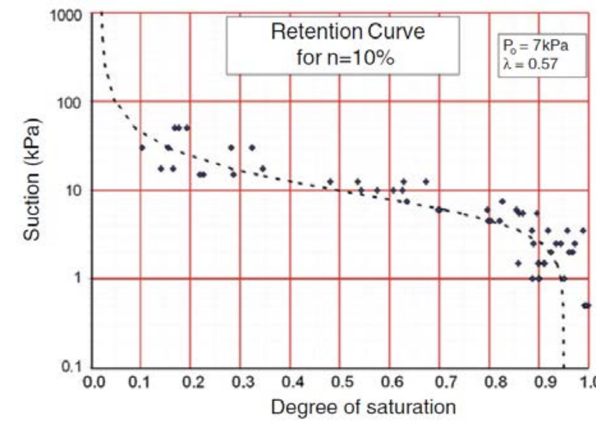
  - Similarities to test problem – ngas macro improvement
  - The outflow fluid mixture with constant pressure was corrected to include the correct mixture of air and water
  - Condensation and evaporation controlled by temperature gradient

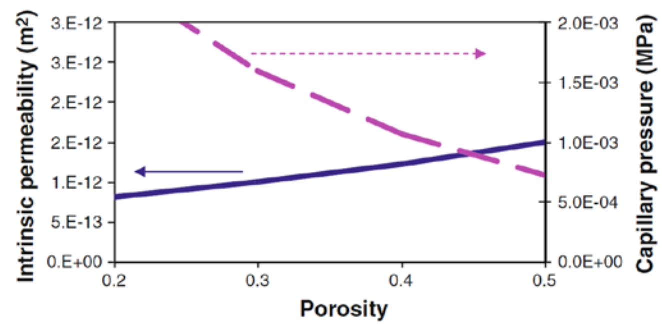




Olivella 2011 Experiment



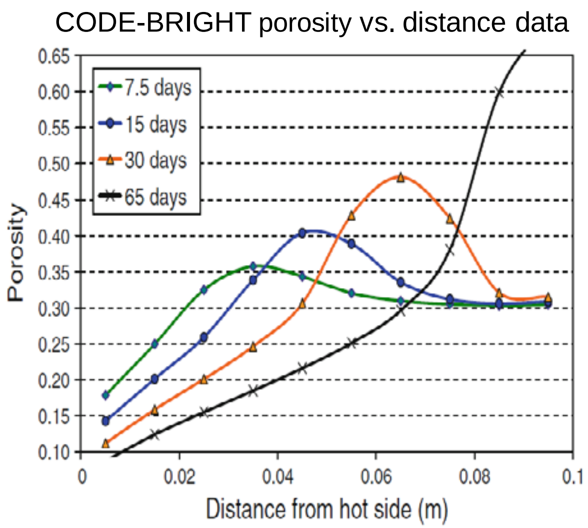


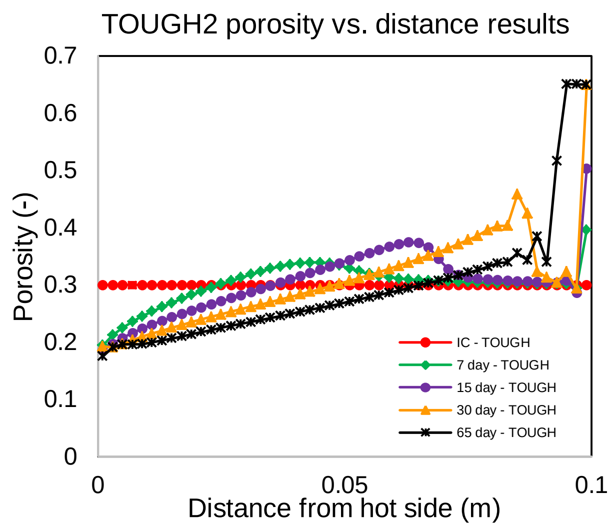


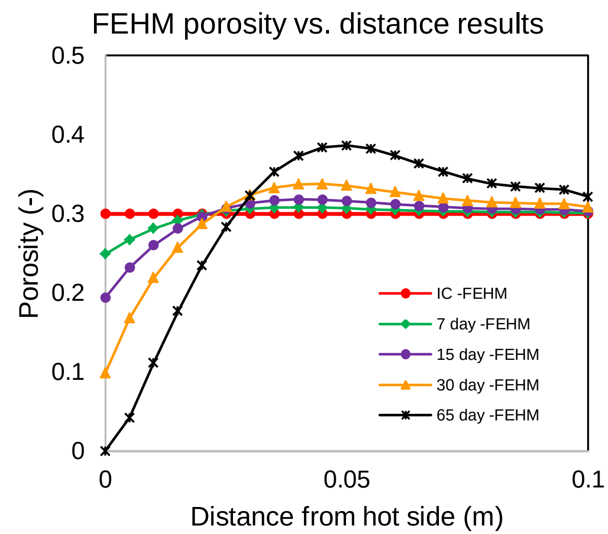
Figures from Olivella et al. (2011)

- FEHM improvements for simulations:
  - retention curves in FEHM runs to correspond with data from Olivella (2011)
  - salt module includes equations used in CODE-BRIGHT simulations
  - FEHM does not accommodate a relationship between capillary and porosity

Olivella 2011 Experiment





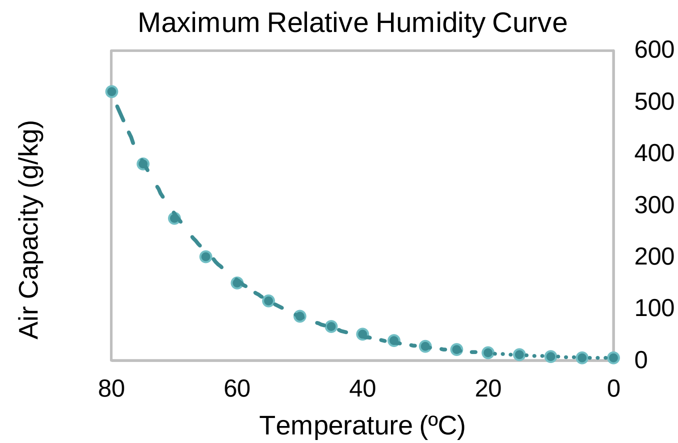


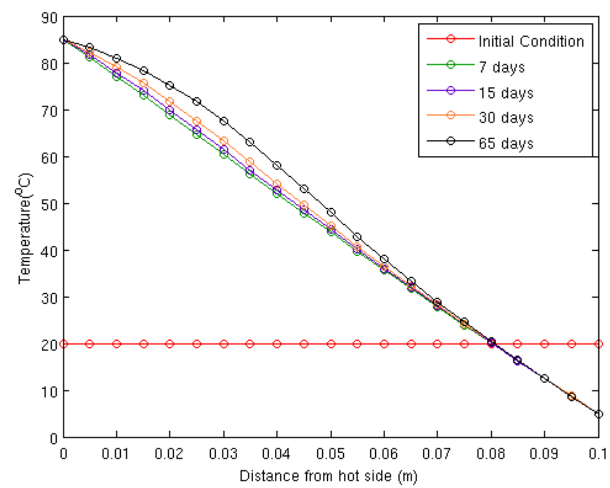
- All data show decrease in porosity on the hot side where evaporation is greatest, increased porosity on cold side due to condensation
- FEHM not producing porosity change on the cold side that other codes are replicating:

Olivella 2011 Experiment

What is driving the observed increase in porosity?

- Air holding capacity gradient not large enough to drive at cold end to drive such high condensation (dissolution of salt)
- Other simulation we ran with higher ‘cold-end’ temperatures do show high porosity

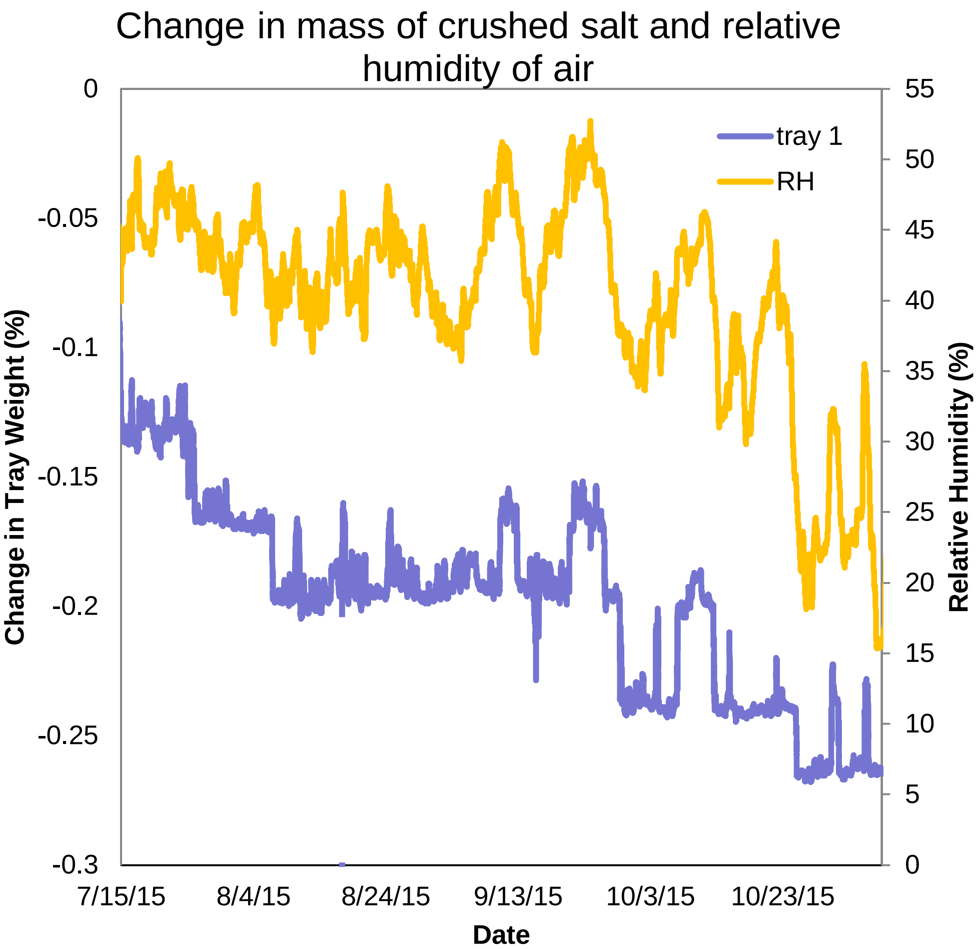




Olivella 2011 Experiment

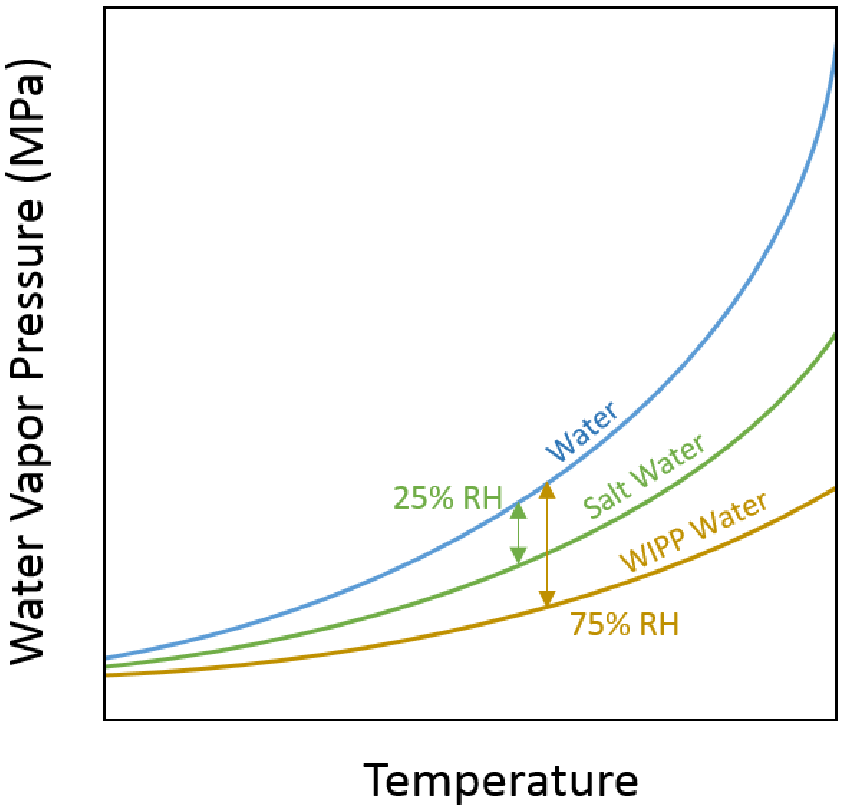
Change in weight of crushed salt shows evaporation and condensation of water from the air

- Increased evaporation when relative humidity drops below ~40%



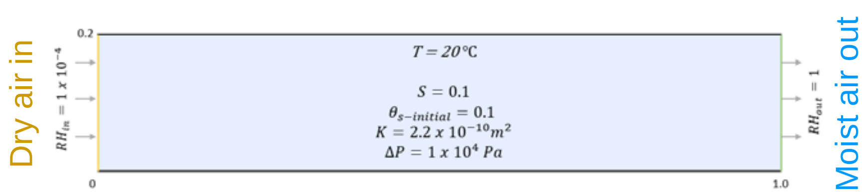
Pan Evaporation Experiment

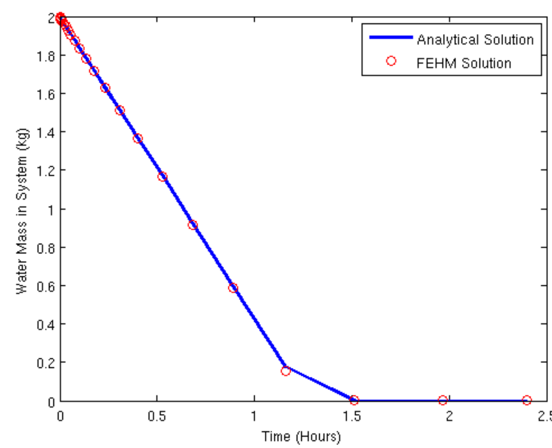
- Salt and other dissolved solids lower water vapor pressure, which increases retention of water in pores spaces
- No established relationship for WIPP site water
- Issues of FEHM using water vapor pressure - temperature relationship not representing the water at the WIPP site
- Performing long-term, on site experiment to determine water vapor pressure lowering for WIPP site
- Match model results to determine WIPP site relationship



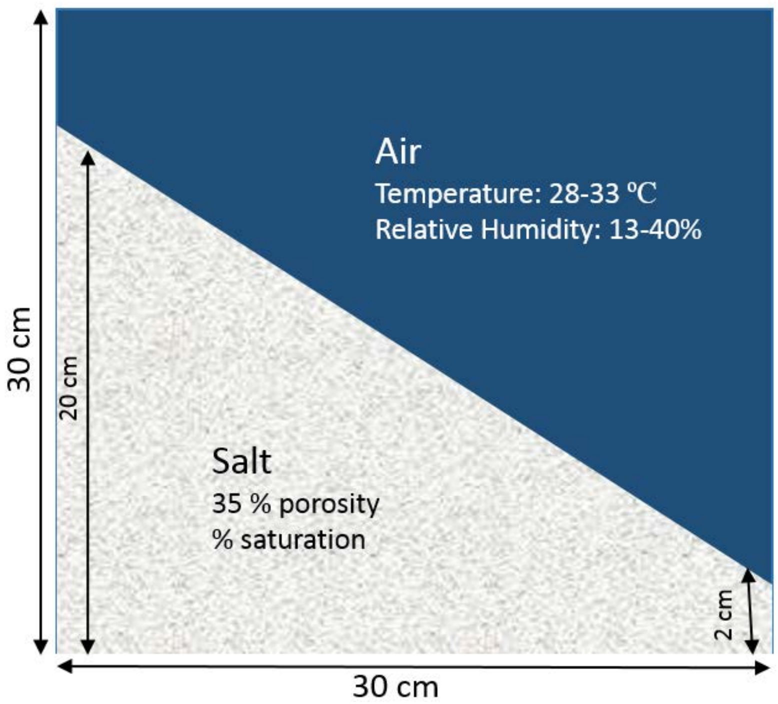
Pan Evaporation Experiment

- The boundary conditions for air-water-heat physics are now available within the boun control statement
  - New keyword 'fxa' for flowing ngas mass fraction added. This keyword apportions incoming flow when the flow arises from a fixed pressure condition
  - The boun control statement allows multiple time changes for all boundary values so that experimental time series input can be used
- Improved the stability in other ngas boundary conditions so that boundary cells can dry-out or become fully saturated without causing extra iterations





Pan Evaporation Experiment



- 2-D Radially symmetric model of mounded salt in a tray
- Time-variant boundary conditions of temperature and relative humidity (mass fraction of water in air)
- Water vapor pressure-lowering for pure salt water in use with FEHM salt capabilities

- Model domain of salt cone
- No-flow boundaries on all sides

Future Work

Tackle challenges in code to better represent physics in experiments:

- **Thermal conductivity experiment:**
  - Determine function of thermal conductivity for WIPP salt
  - Add gas migration to model for measure of temperature-dependent diffusivity
- **Olivella (2011) experiment with code comparison:**
  - Why does experiment and other codes show large porosity change on cold end?
  - Why doesn't FEHM reproduce this result?
- **Salt pan evaporation:**
  - Determine water vapor pressure lowering relationship for WIPP-site salt