Simulations in Support of the Salt Defense Disposal Initiative (SDDI): Water and Salt Transport Driven by Heat Generating Nuclear Waste in Bedded Salt

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Los Alamos Team Members

- Dylan Harp – Simulation Expert
- Amy Jordan – PhD Student
- George Zyvoloski – Code Development
- Terry Miller – Mesh Generation
- Hakim Boukhalfa – Chemistry
- Florie Caporuscio – Chemistry
- Jim Ten Cate - Physics
- Yassin Labyed - Physics
- Bruce Robinson – Project Coordination

Outline

1) Background

2) Research objectives

3) Coupled <u>T</u>hermo/<u>H</u>ydro/<u>C</u>hem processes

4) Simulation results

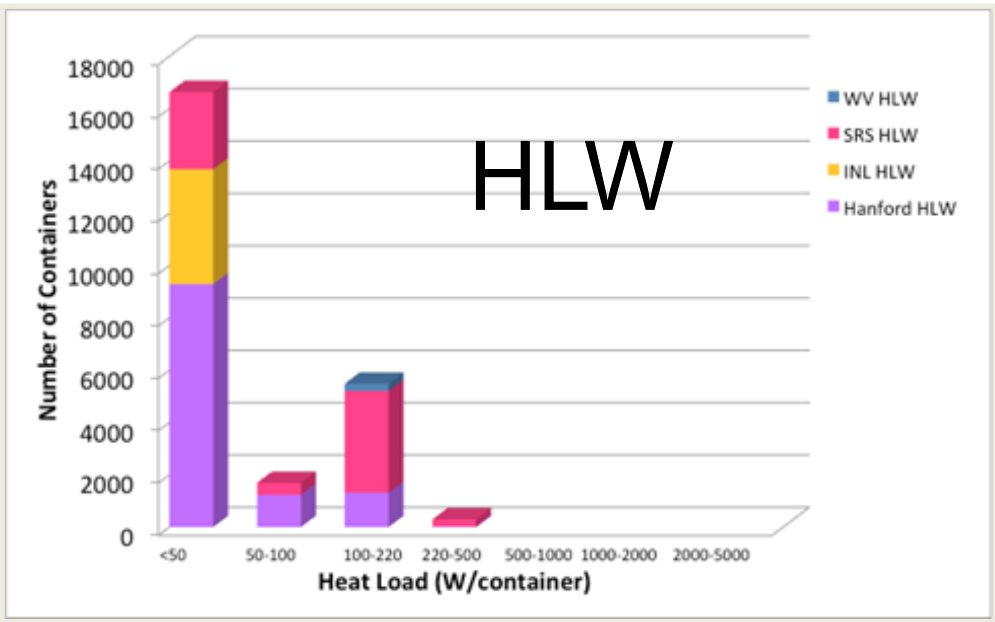
Background

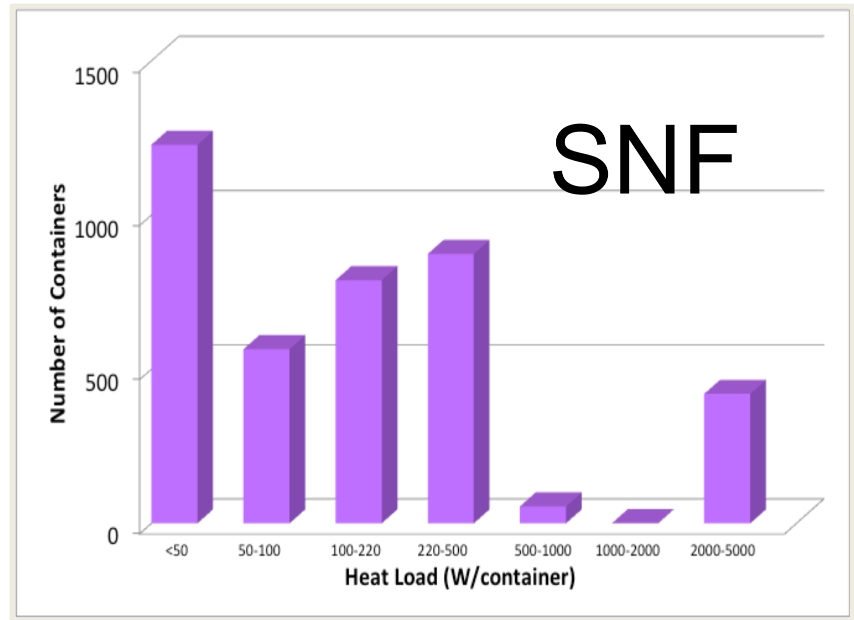
- Can we make a safety case for storing DOE managed high-level nuclear waste (HLW) and Spent Nuclear Fuel (SNF) in bedded salt?

Image: DOE-CBFO

Background

More than 90% of DOE managed waste is less than 220W



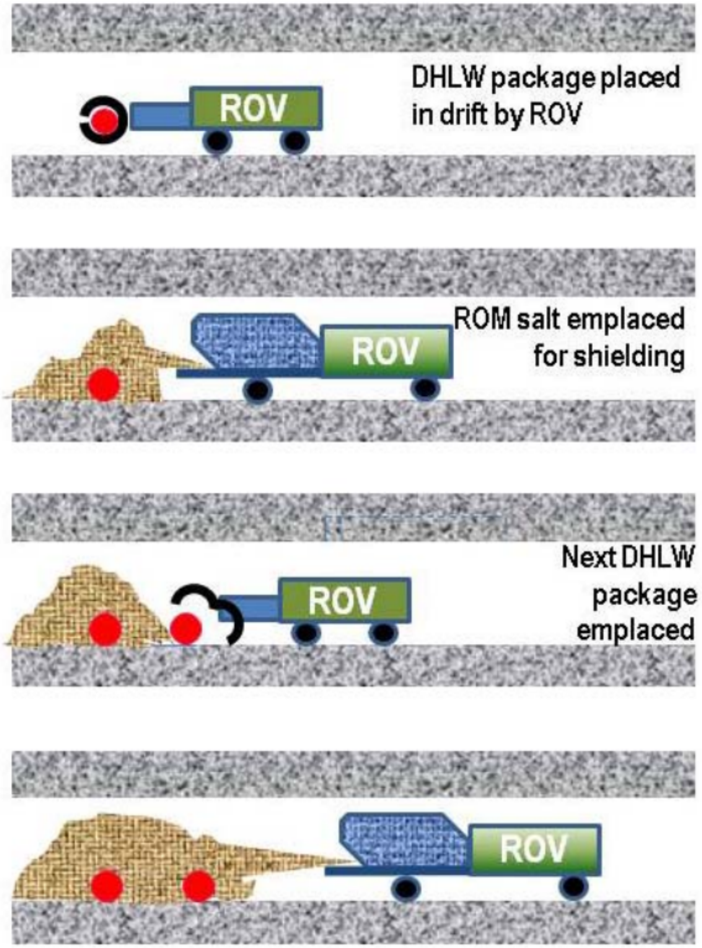


Carter, J.T., A.J. Luptak, J. Gastelum, C. Stockman, A. Miller. 2012. *Fuel Cycle Potential Waste Inventory for Disposition*. DOE Office of Nuclear Energy Report FCR&D-USED-2010-000031, Rev 5.

Background

In-Drift Disposal Concept

- Lower cost
- Easier logistics
- Tighter spacing



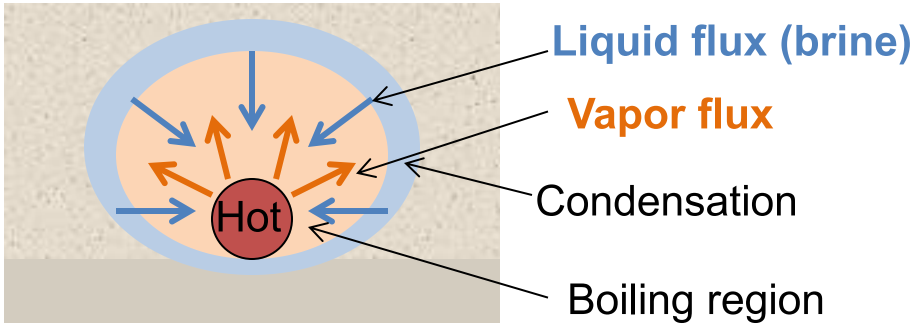
Hardin et al., FCRD-UFD-2012-000219

DOE/CBFO-12-3485

Background

- Bedded salt has favorable characteristics for heat-generating waste disposal:
  - Self-sealing plastic deformation
  - Very low permeability (intact/final)
  - High thermal conductivity
- Past heater tests in salt provide data for model validation
  - Possible evidence of **heat pipe** activity around a 130^{o}C heater

Heat pipe

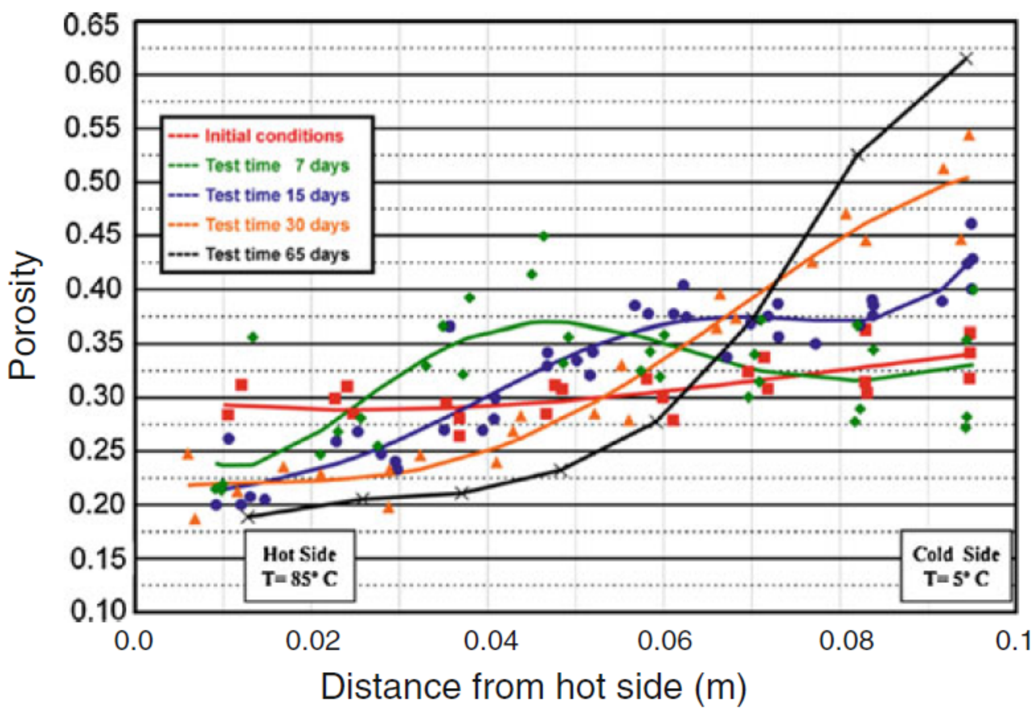


From Brady et al. (2013).

Background

Laboratory evidence for a heat pipe in salt

- Olivella et al. (2011 Transport in Porous Media)
  - Small experiment
  - Porosity change due to thermal gradient in granular salt



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

Background

- Water sources in bedded salt:
  - **Intracrystalline** (brine inclusions)
  - **Intercrystalline** (e.g., mobile "pore fluid")
  - Water associated with **clay minerals** and polyhalite
- Water may be liberated from brine inclusion migration and clay dehydration (above 65ºC)

Photo: H. Boukhalfa

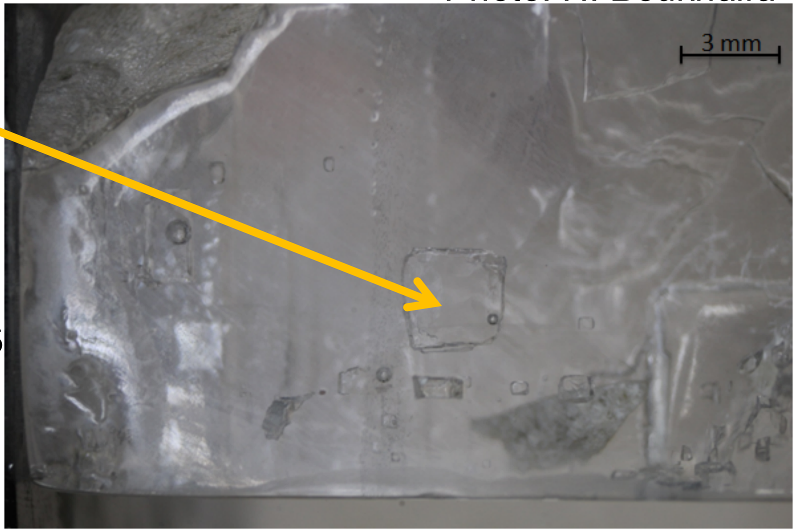
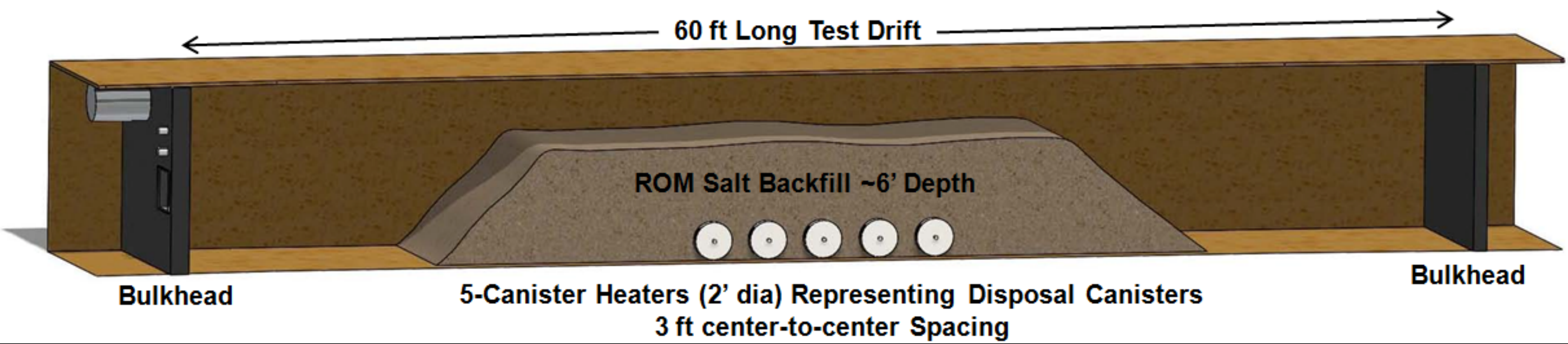


Photo: D. Weaver

Research Objectives

- Use modeling to help **design and instrument** a field-scale experiment for the Salt Defense Disposal Investigations (SDDI).
- Predict **moisture**, **mass redistribution**, and **temperature** following In-Drift waste disposal in bedded salt.
  - New code development required

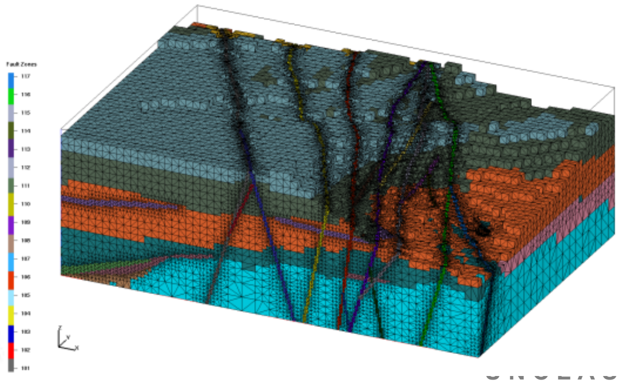
SDDI Test Drift #1

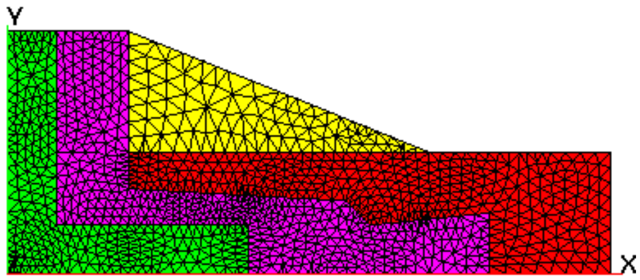


D. Weaver

Simulator Description

- FEHM developed at Los Alamos 30+ years
  fehm.lanl.gov
- Used for 150+ peer reviewed articles
  fehm.lanl.gov/pdfs/FEHM_references_list.pdf
- Fully coupled thermal, mechanical, chemical, multiphase (gas, water vapor, water, rock)
- Uses LaGriT: Powerful 3-D grid generation tool





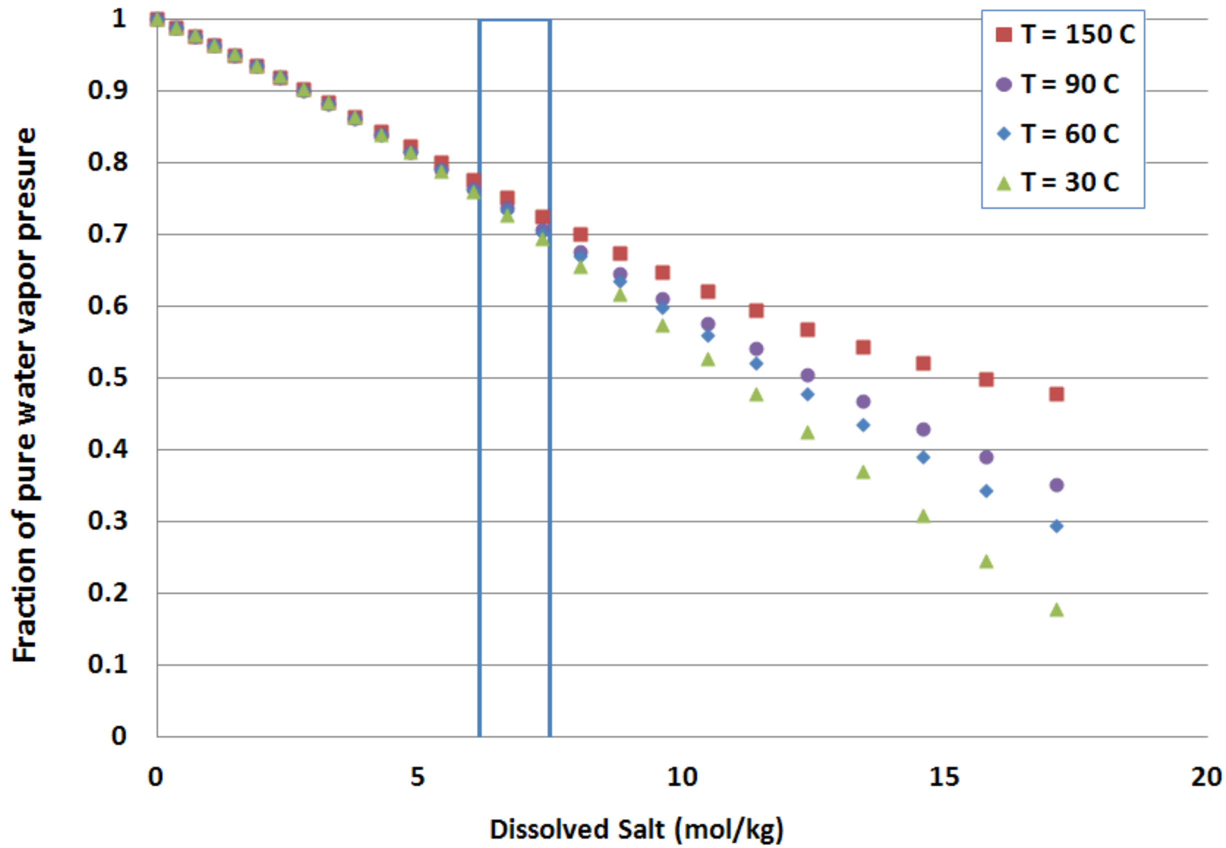
Thermo Hydrological Chemical Simulations Require Coupled Processes with Feedbacks

- Changes in porosity lead to changes in:
  - permeability
  - thermal conductivity and heat capacity
  - vapor diffusion coefficient
- Changes in temperature lead to changes in:
  - thermal conductivity
  - salt solubility
  - water vapor pressure
  - brine viscosity

Salt Specific Algorithms in FEHM for Thermo Hydrological Chemical Simulations

Water vapor pressure as a function of dissolved salt concentration and temperature

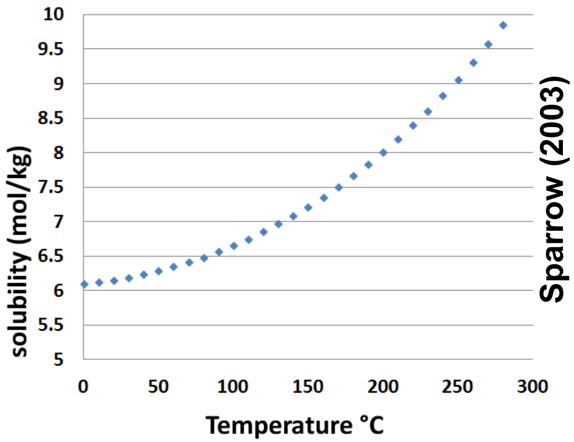
The blue vertical lines span the region of interest for most of our simulations

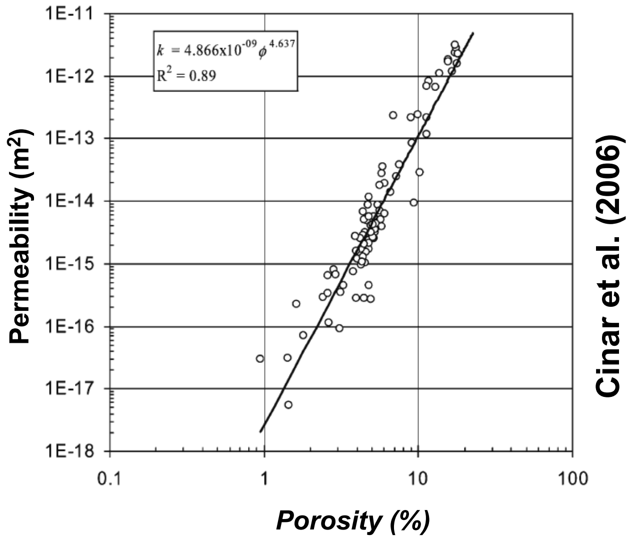


Sparrow (2003)

Salt Specific Algorithms in FEHM for Thermo Hydrological Chemical Simulations

- Thermal conductivity of salt as a function of porosity and temperature
- Salt solubility as a function of temperature
- Precipitation/dissolution of salt
- Water vapor diffusion coefficient as a function of pressure, temperature, and porosity
- Permeability-porosity relationship for RoM salt

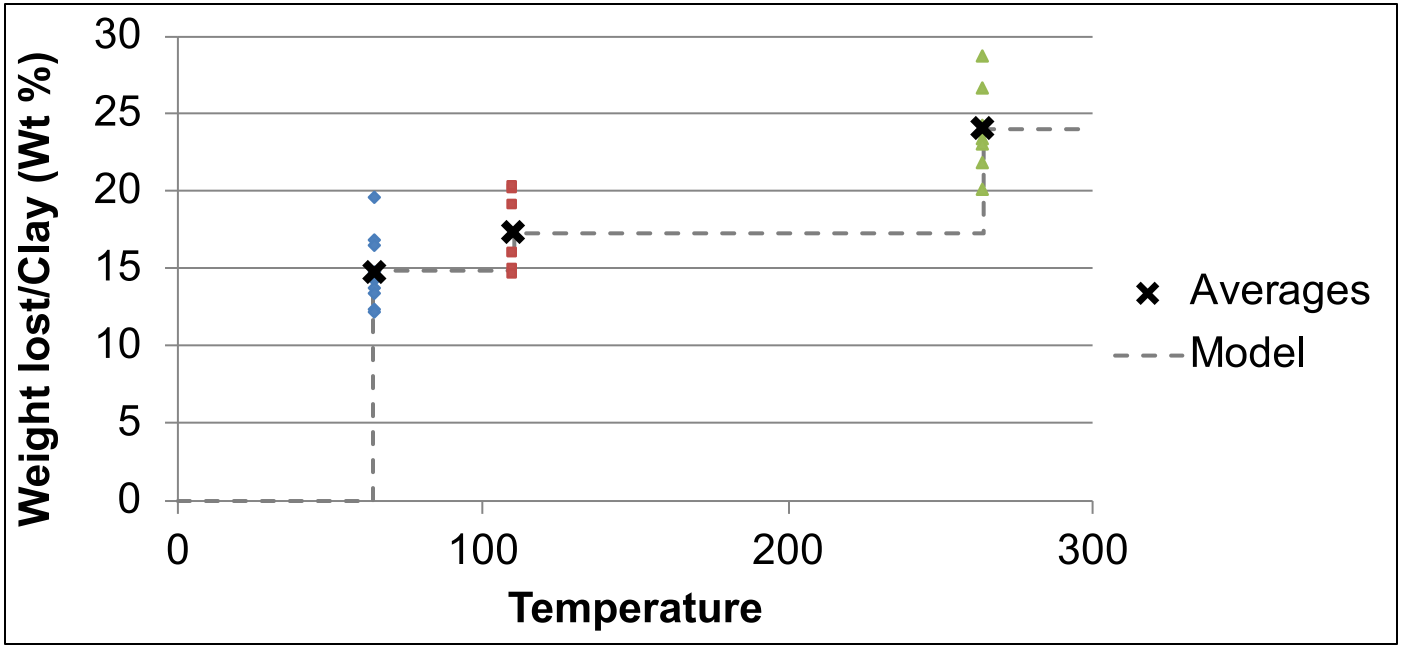




2013 Stauffer, P.H., et al., Coupled model for heat and water transport in a high level waste repository in salt, FCRD-UFD- 2013-000206 Los Alamos National Laboratory Document LA-UR 13-27584

Salt Specific Algorithms in FEHM for Thermo Hydrological Chemical Simulations

Clay dehydration algorithm based on laboratory data



Data from Hakim Boukhalfa

Mass of water produced at 64°C at node *i* based on the fraction of clay (f_c), porosity, density of rock, and volume of the cell:

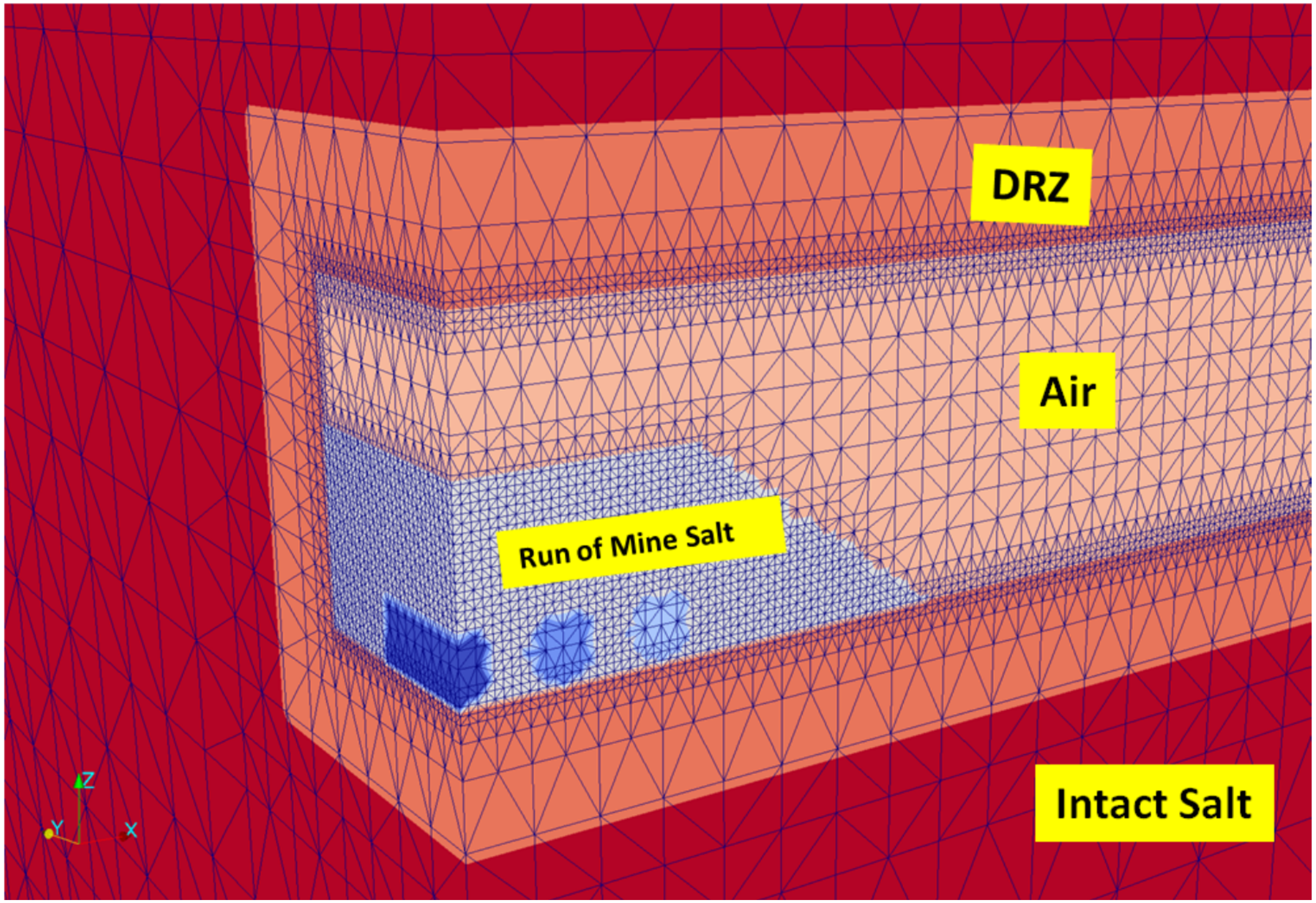
$$M_w = 0.148\ f_c (1 - \phi_i)\ \rho_r\ V_{cell}$$

NNSA

Range of parameters used in the simulations

Parameter	Natural Range	Simulated Range
Backfill saturation	0.01 – 0.09	0.01 – 0.1
Backfill porosity	0.3 - 0.4	0.35
Clay content	0 – 0.15+	0 – 0.1
Drift air temperature	15 – 30 C	30 C

High Resolution Numerical Mesh



2 Reflection boundaries are used to reduce mesh size (1/4 space)

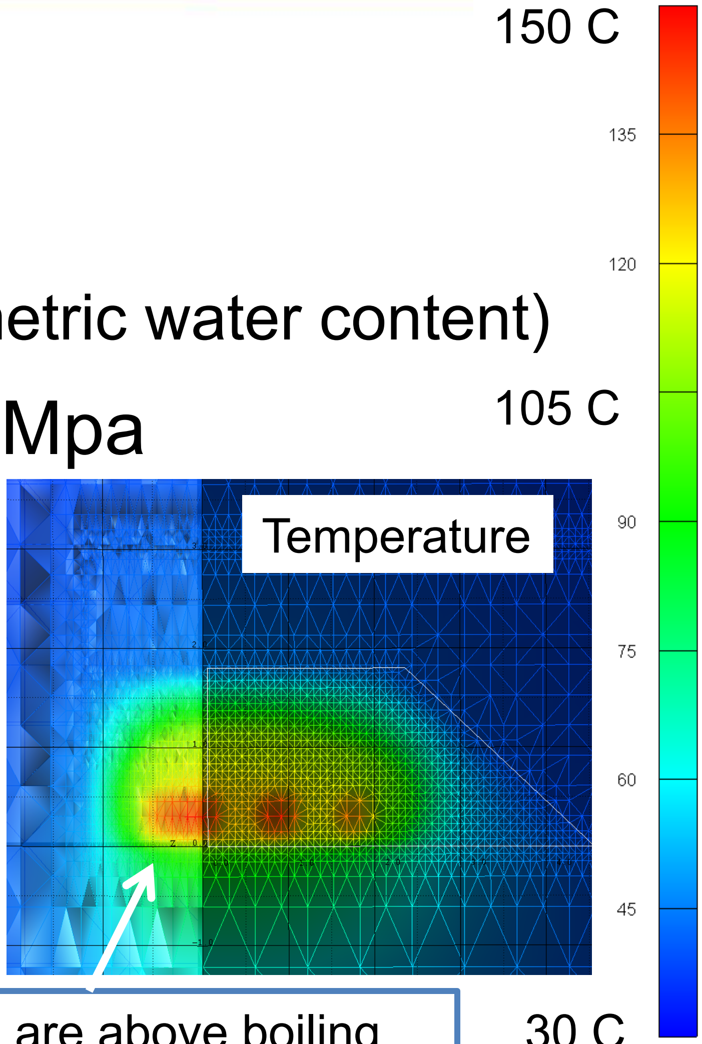
Results

Thermo Hydrological Chemical Simulations at the drift scale

- Time evolution of a hot case (5 x 750W)
- Impact of thermal load
- Impact of initial backfill saturation
- Impact of clay dehydration

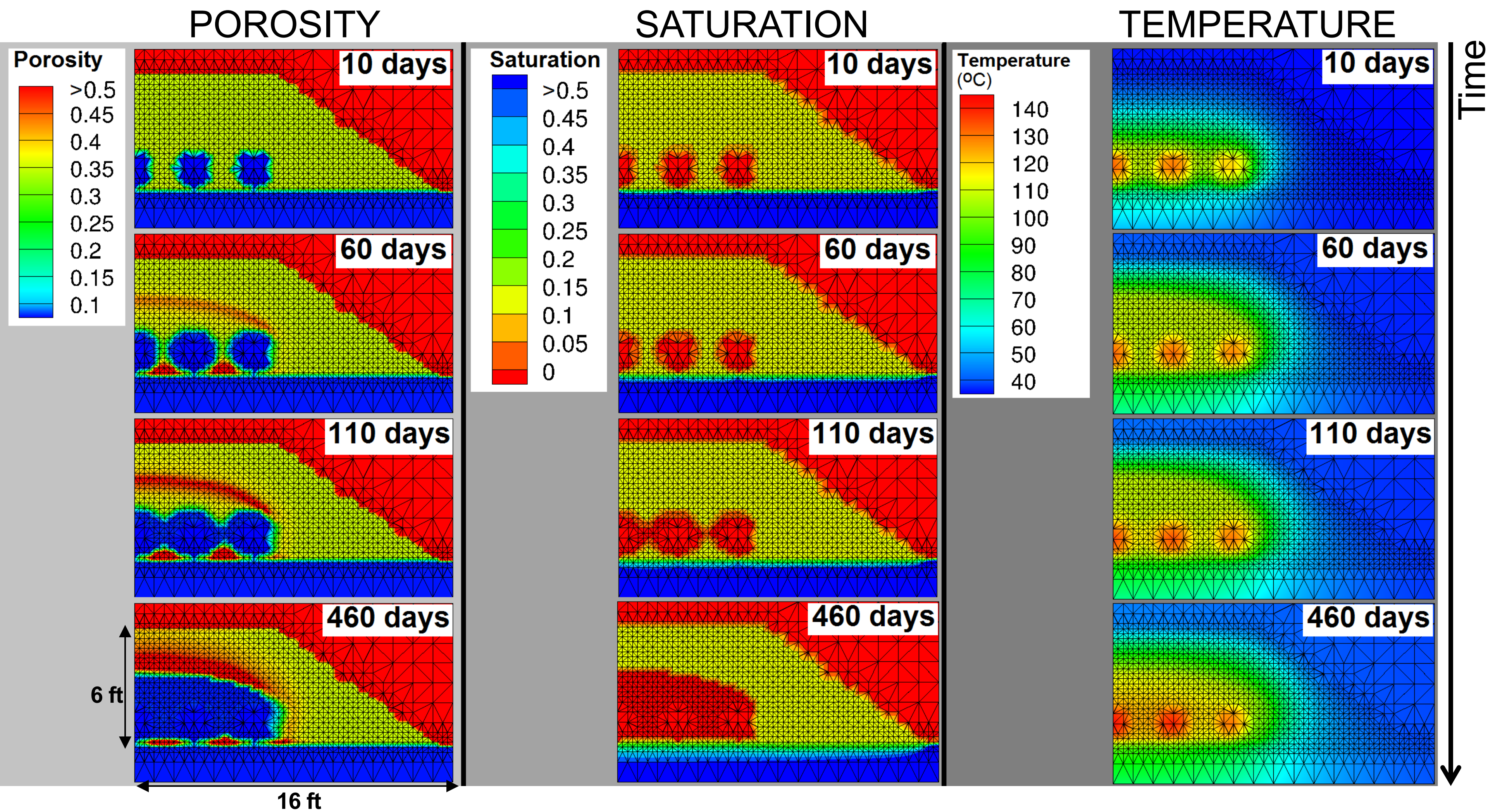
Results: Details of the hot case

- Heat load = 5 x 750W
- 2 year simulation
- Initial saturation 10% (2.5% gravimetric water content)
- Maximum capillary suction = 0.5 Mpa
- Clay fraction = 0.0
- Residual water saturation = 10%
- Initial temperature = 30 C
- Maximum temperature = 150 C

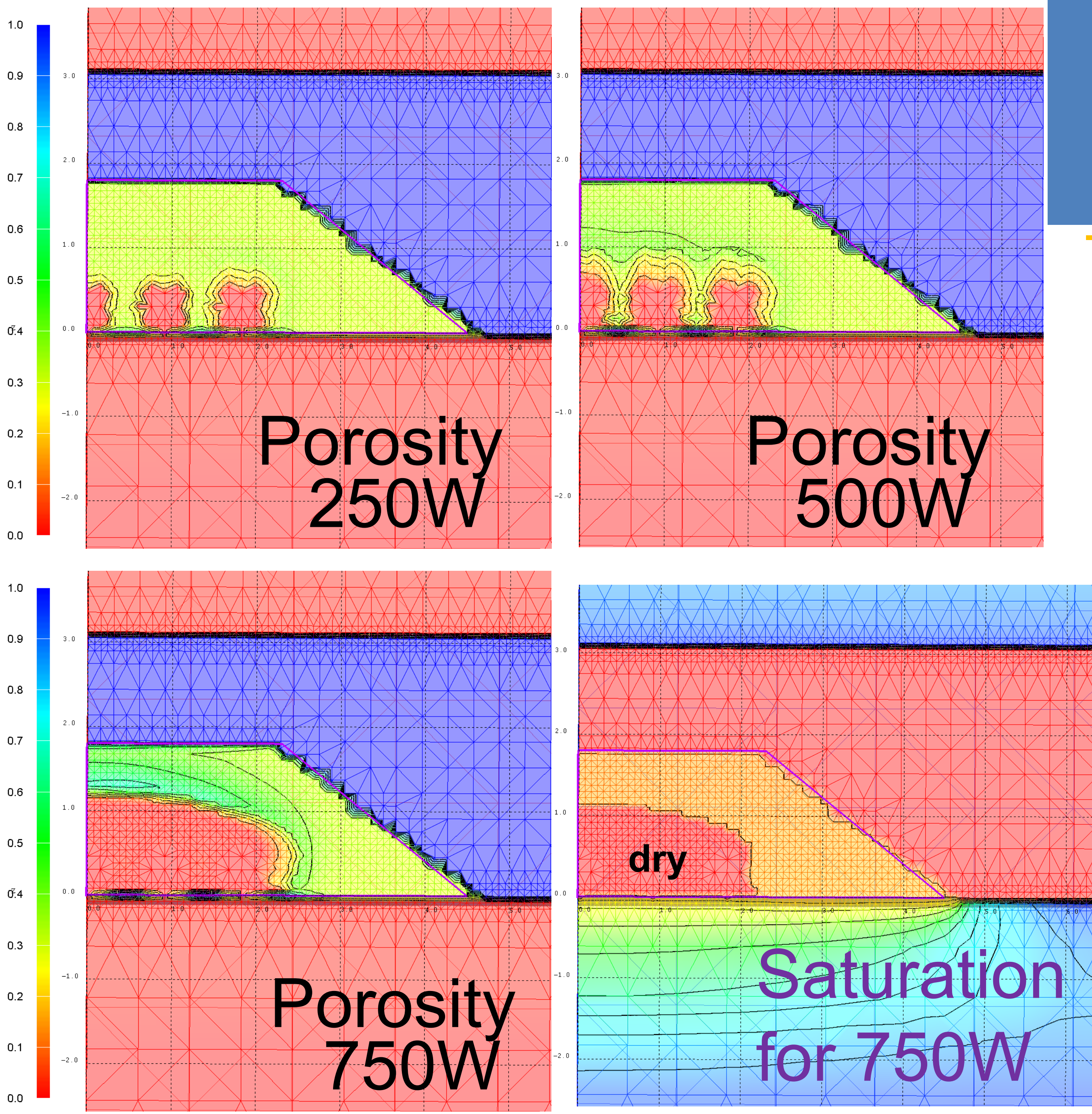


Red and yellow colors are above boiling

Results: Time Evolution of a hot case



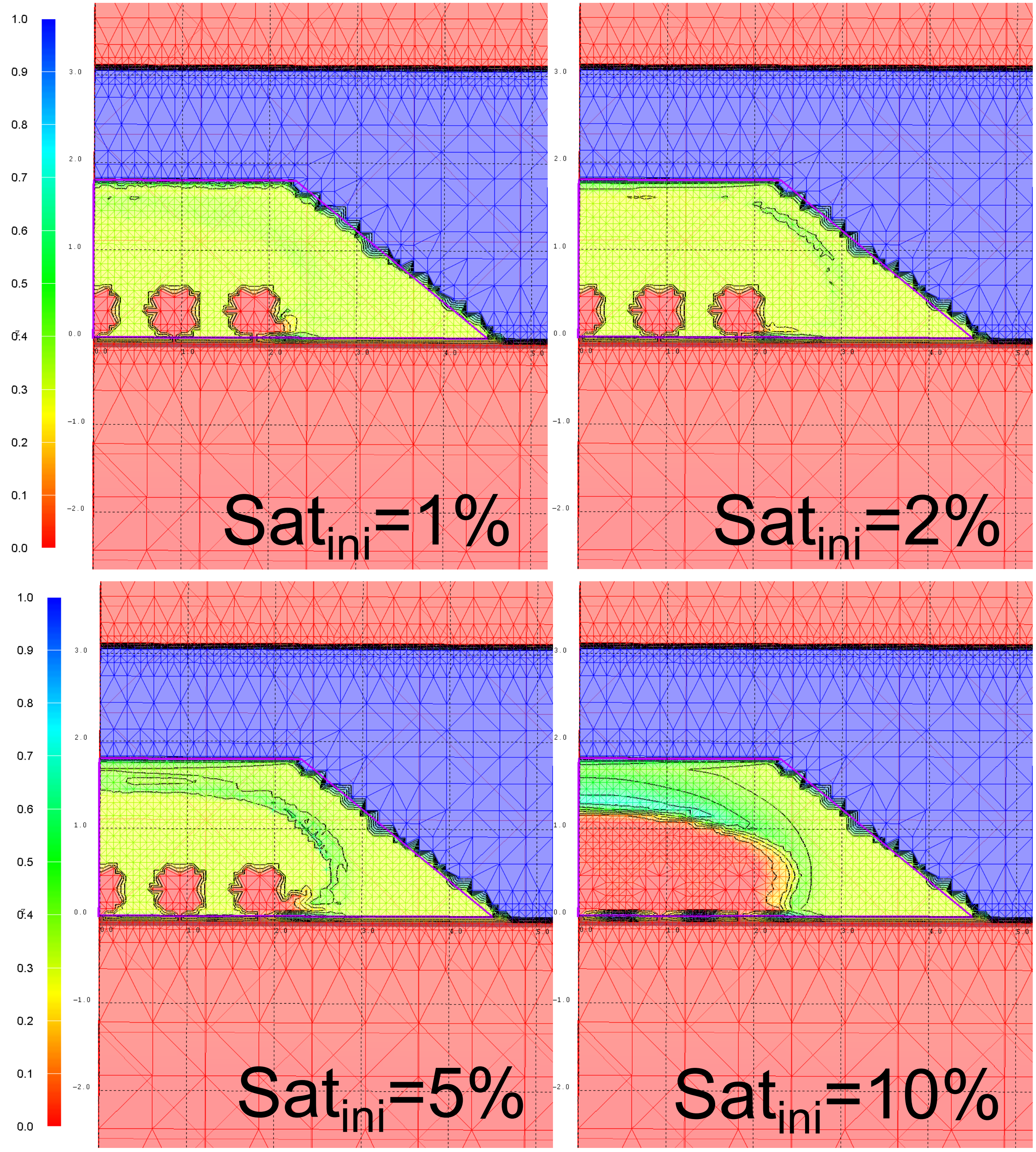
Results



Porosity changes more with higher heat loads

More heat pipe with higher heat loads

Time = 2 years
Sat_{ini} = 10%



Results

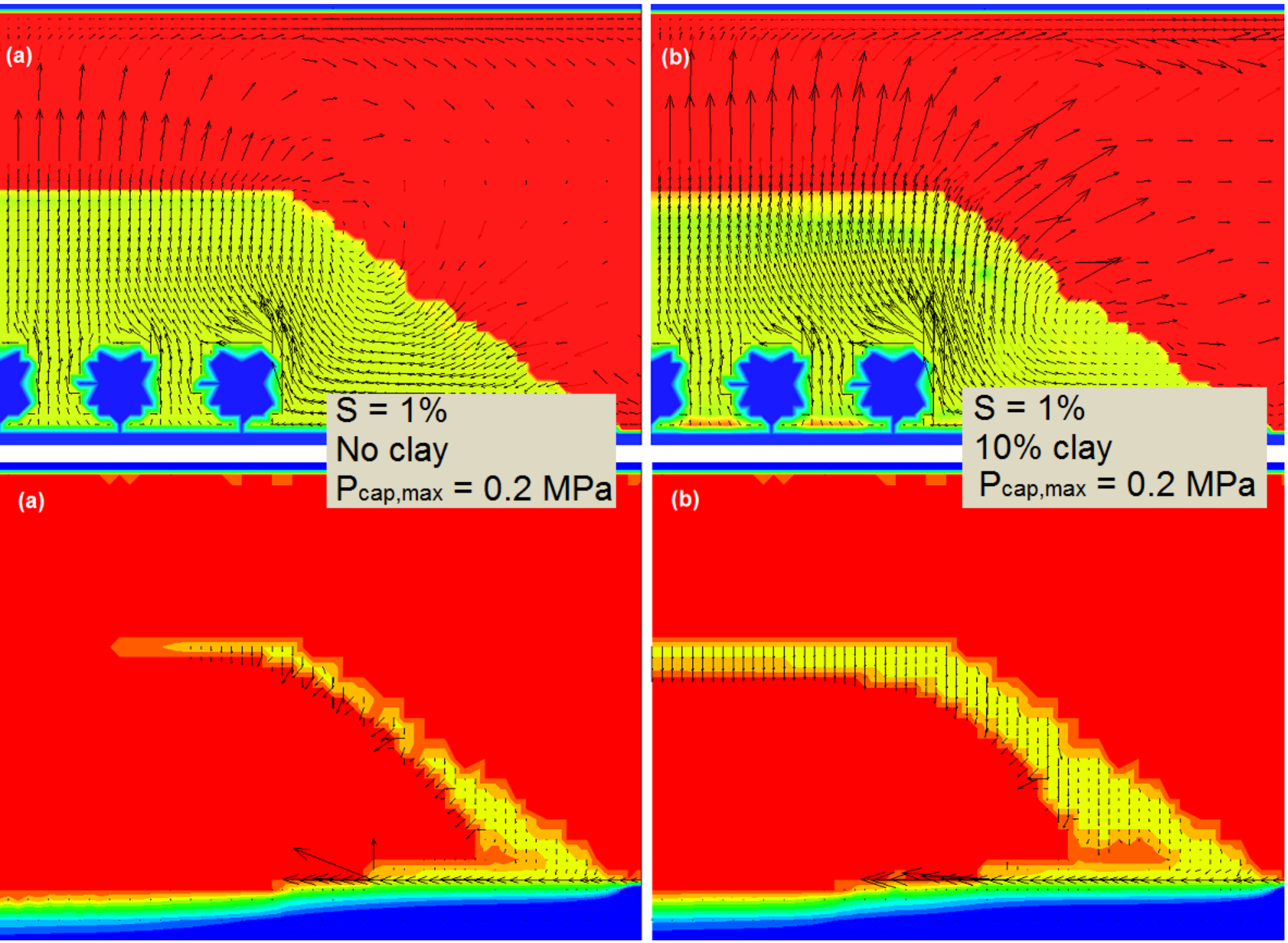
Porosity changes more with higher Initial saturation in the run of mine salt backfill

More heat pipe in a wetter system

All at 750W
Time = 2 years

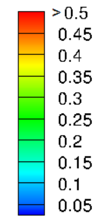
Results: Clay Dehydration

No clay | **10% clay**



Results at 460 days

Porosity

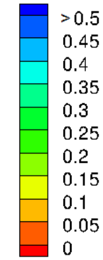


Vapor flux (m/s)

→ = 3.2e-7 m/s

2nd order impact

Saturation



Liquid Flux (m/s)

→ = 1e-8 m/s

NNSA

Conclusions

- Including water and water vapor in simulations leads to:
  - Not much change in low energy cases (less than 250W per canister)
  - Heat pipes in some higher energy cases (greater than 250W per canister)
    - Lowers temperatures near the canisters
    - Salt mass transfer toward the canisters
    - Increased thermal conductivity near the canisters

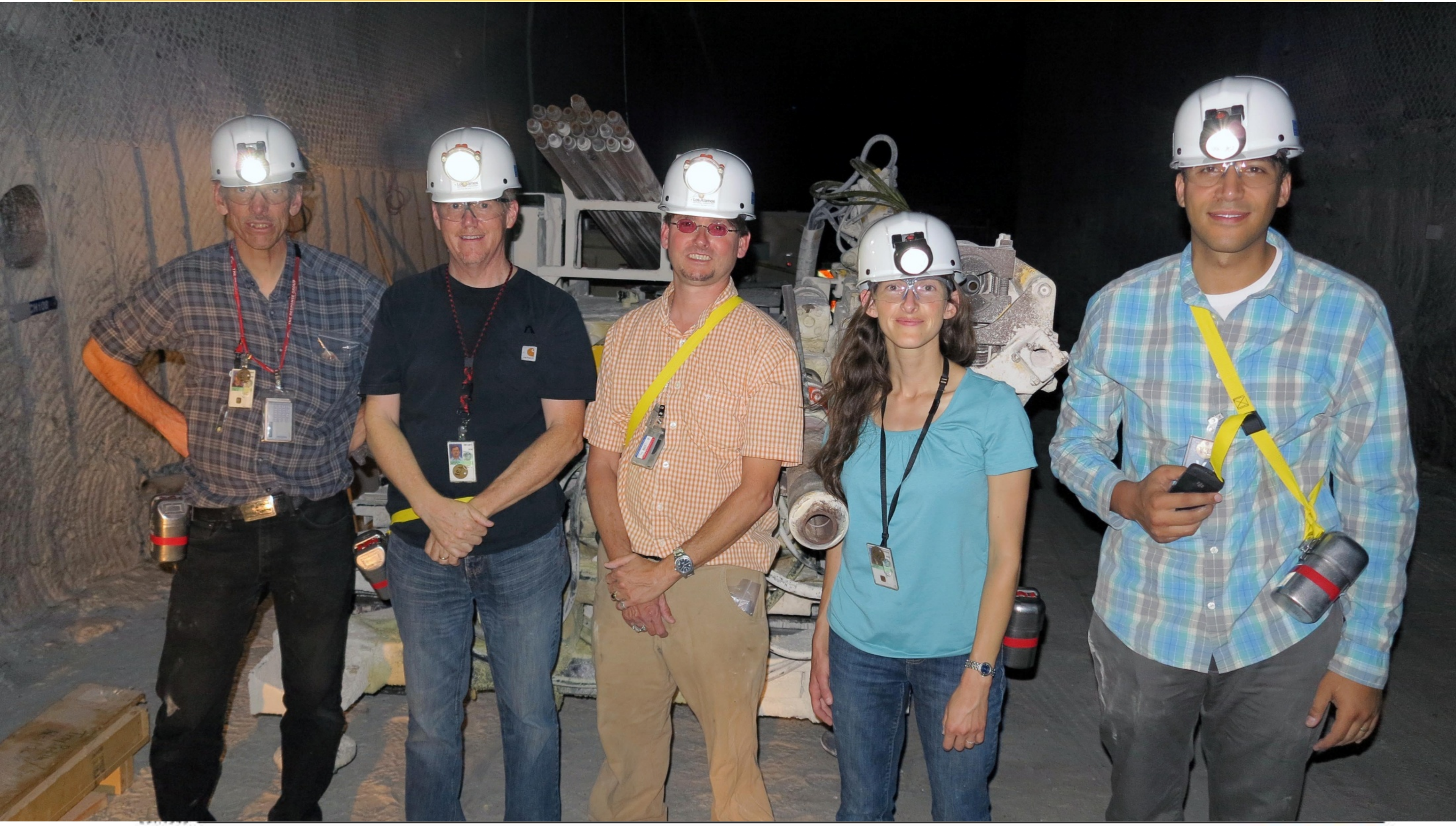
Conclusions

– Heat pipe development is positively correlated with:
  - Initial backfill saturation
  - Backfill capillary suction
  - Water mobility at low saturation
  - Clay content in the backfill
  - Water movement into the backfill from the damaged rock zone

Future Work

- Experimental validation
  - Heat pipe generation in Run of Mine salt backfill
  - Retention characteristics of Run of Mine salt backfill
  - Drift scale testing at WIPP
- Inclusion of isotopic tracers in the simulations
- Inclusion of evaporation
  - Barometric pumping
  - Pressure flow through the underground
    - Seasonal humidity and pressure differences
    - Bulkhead impacts
    - Damaged rock zone impacts

Questions?



Extra Slides if Time Permits

Comparison of Thermal only VS Thermal + water + water vapor

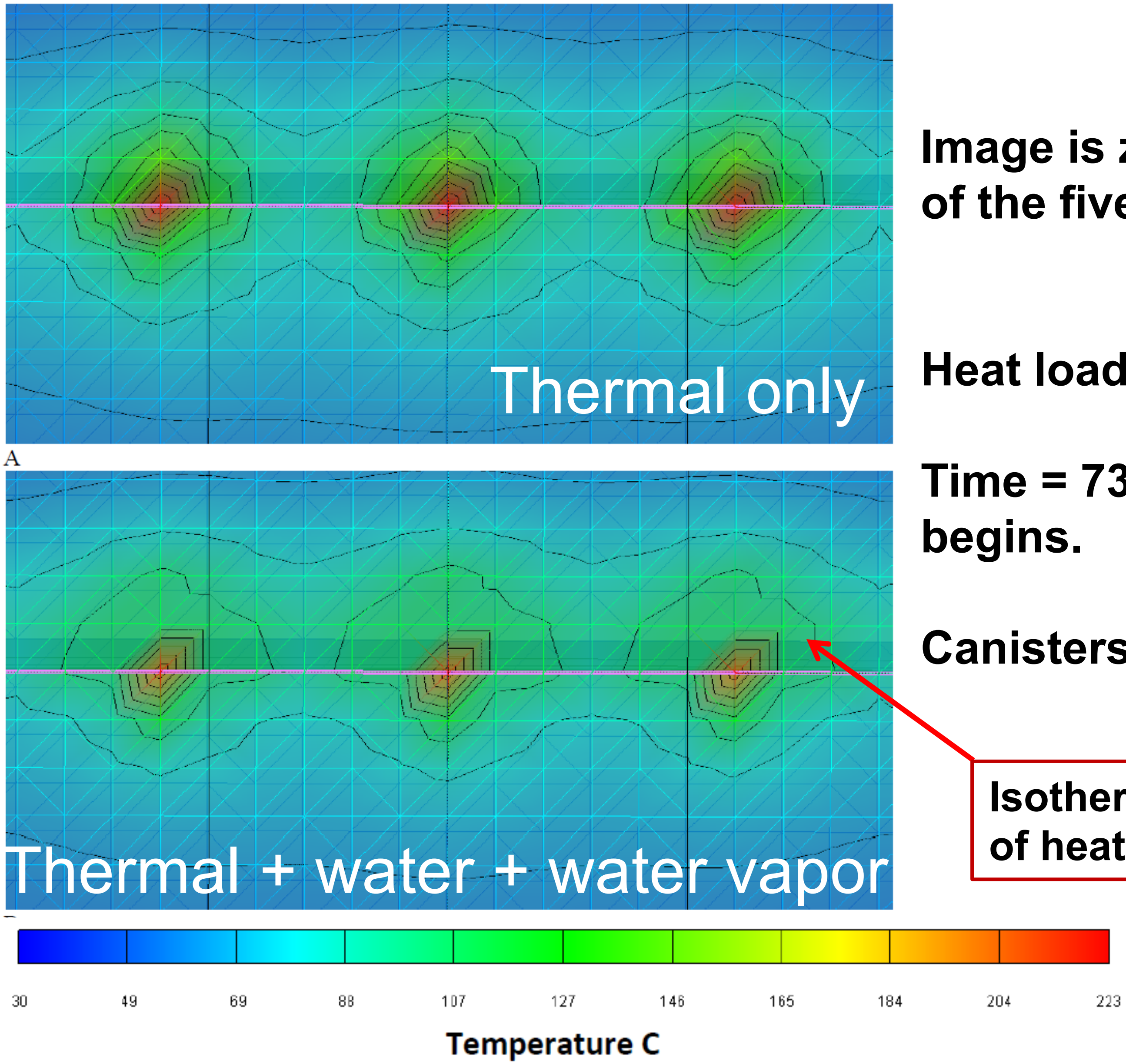


Image is zoomed in on three of the five heaters

Heat load = 1500W/canister

Time = 730 days after heating begins.

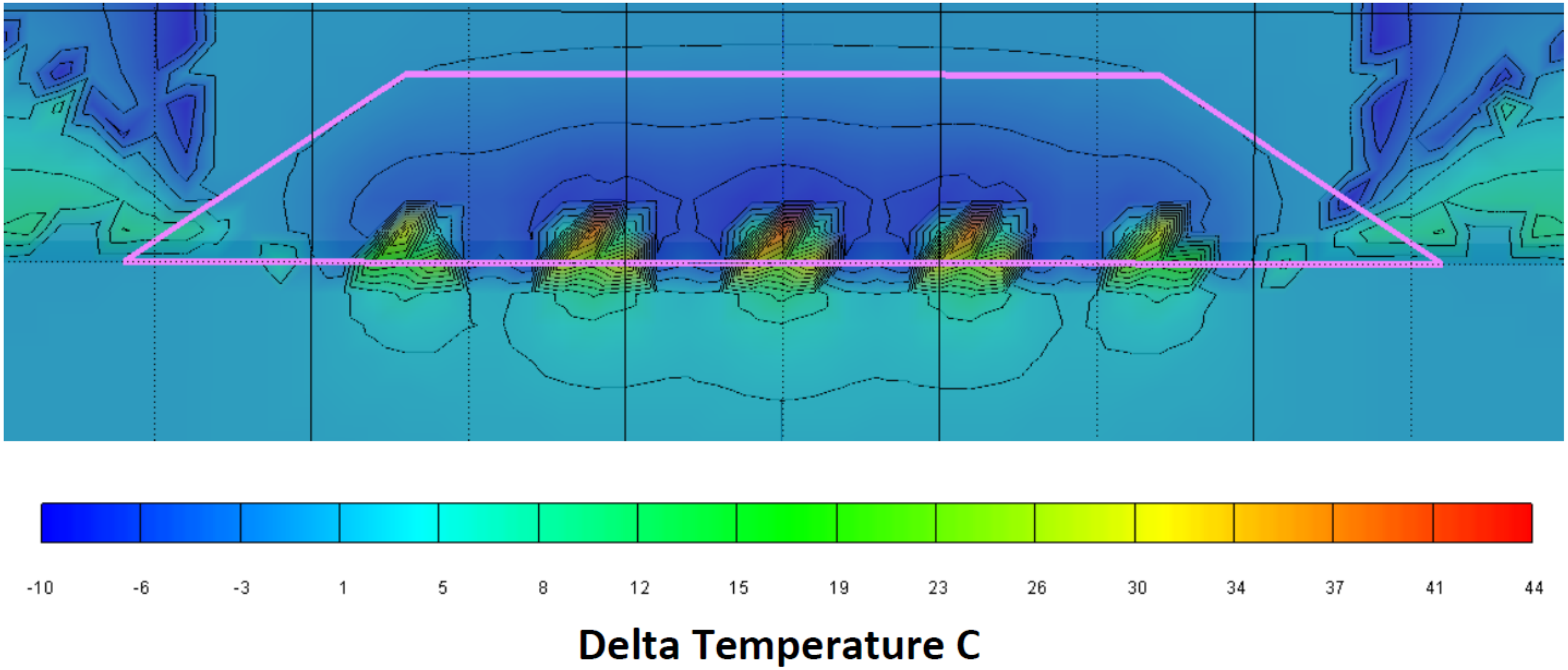
Canisters spacing = 1 m.

Isothermal region indicative of heat pipe

Temperature Difference Image
Thermal only – (Thermal + water + water vapor)

Heat load = 1500W/canister
Time = 730 days after heating begins.
Canisters spacing = 1 m.

<u>Vapor/liquid heat pipe is 44C cooler in the heaters</u>

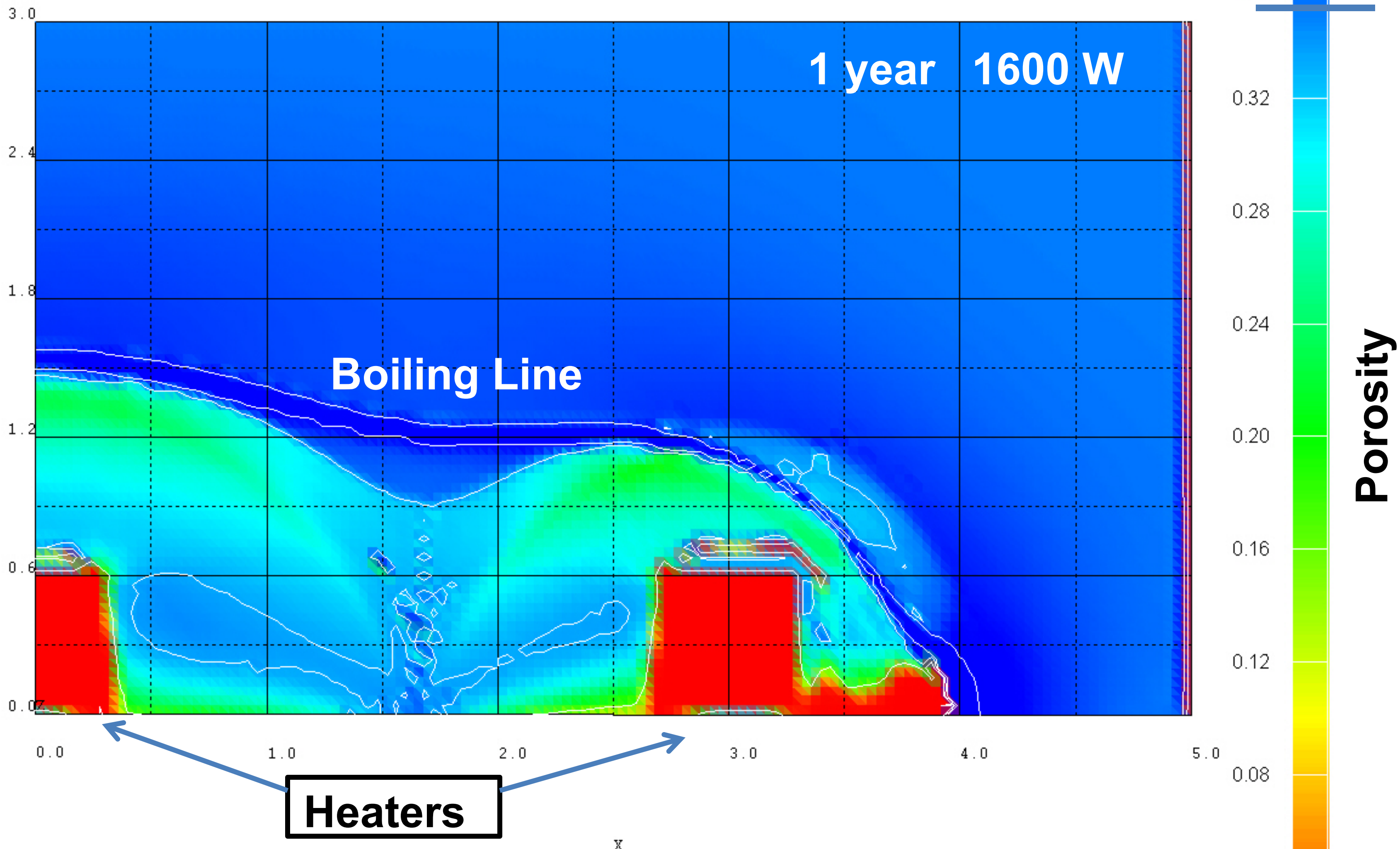


High resolution Thermo Hydrological Chemical Run of Mine salt covering hot waste packages

3x5 m

2-D slice

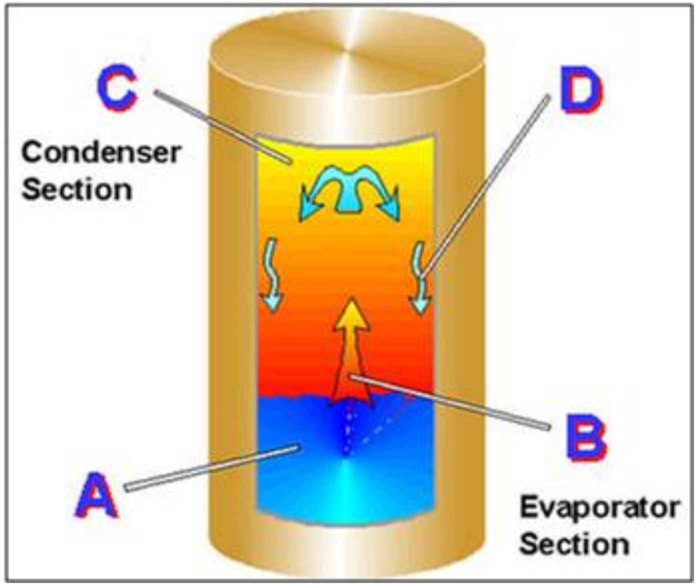
4 cm mesh



Boiling near the heaters causes salt to precipitate leading to porosity reduction. Vapor condenses across the boiling line leading to dissolution and increased porosity

Generic Heat Pipe Explanation

- Liquid at A
- Vaporizes at B
- Condenses at C
- And D, flows back as liquid to A.



Heat pipes lead to isothermal regions where phase change is absorbing energy