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Coupled Model for Thermal-Hydrological-Chemical Processes in a High-Level Radioactive Waste Repository in Salt

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Outline

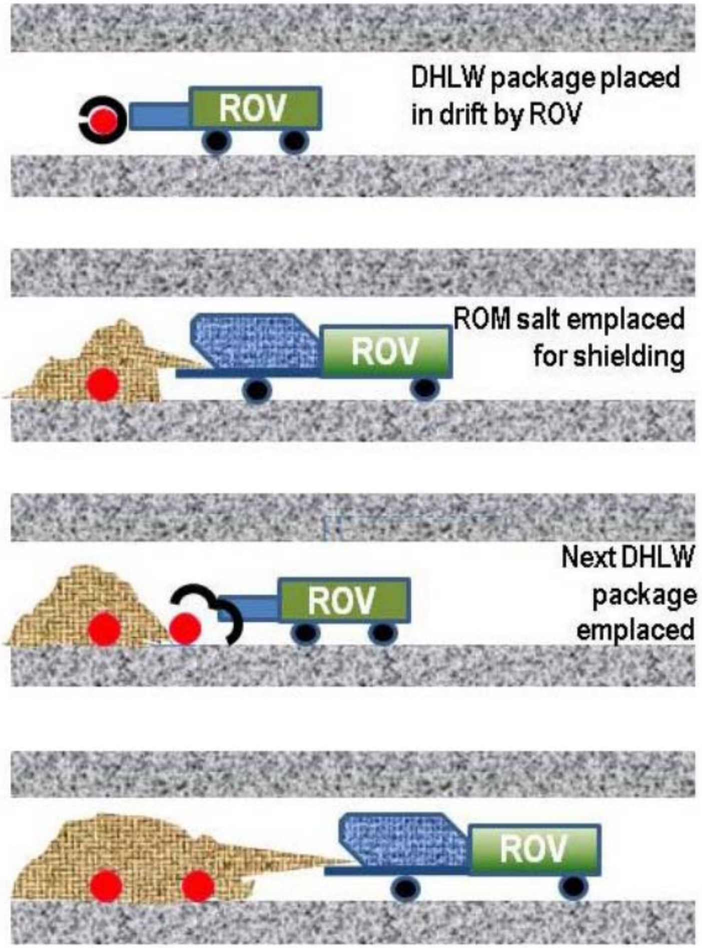
1) In-drift concept for Defense High Level Waste
2) Waste composition by thermal load
3) Background on salt and heat pipes
4) Simulator description : FEHM developed at LANL
5) Code validation example
6) Simulations with heat only
7) Addition of water and water vapor transport
8) Processes added to couple water and chemistry
9) Results of fully coupled Thermo/Hydro/Chem simulations

In-drift waste emplacement strategy

Simple lower cost method.

Backfill is readily available in salt formations

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



DOE/CBFO-12-3485

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**
- **Bruce Robinson – Project Coordination**

Distribution of Heat Loads: DOE-Managed Waste

More than 90% of is less than 220W

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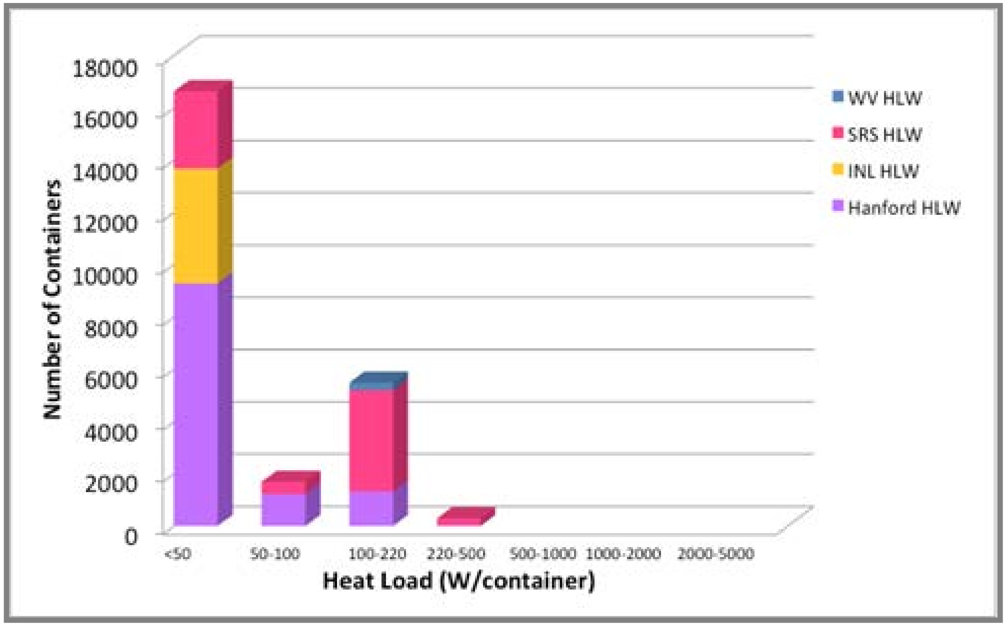
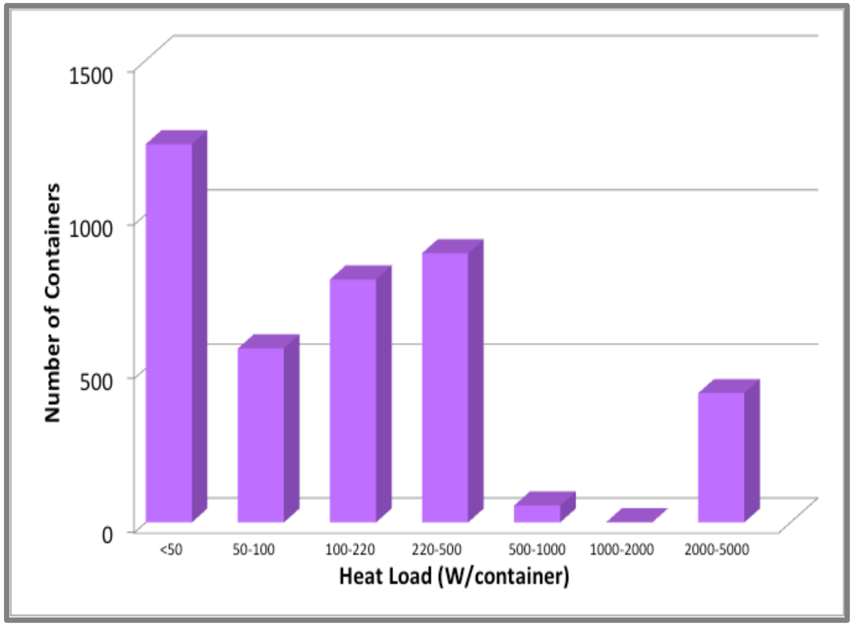
Defense waste heat loads are much lower than commercial SNF heat loads planned for Yucca Mountain (6200 – 8800W/canister)

High-Level Waste



DOE Spent Nuclear Fuel



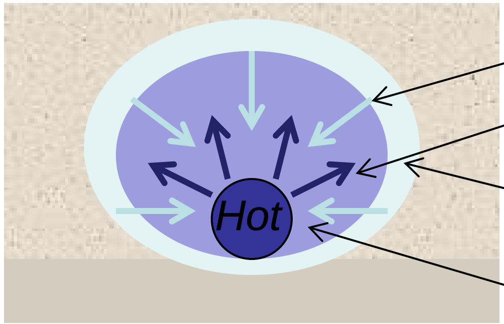
Carter, J.T., A.J. Luptak, J. Gastelum, C. Stockman, A. Miller. 2012. Fuel Cycle Potential Waste Inventory for Disposition. DOE Office of Nuclear Energy Report FCR&D-USED-2010-000031, Rev 5.

Background

- **Bedded salt has favorable characteristics for heat-generating waste disposal:**
  - Self-sealing rheology
  - Very low permeability in its intact/final states
  - High thermal conductivity
- **Past heater tests in salt provide data for basic model validation and salt material properties**
  - Evidence of **heat pipe** activity around a 130°C heater

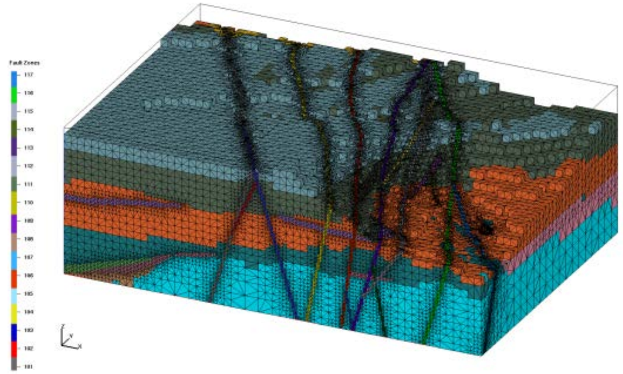
From Brady et al. (2013).

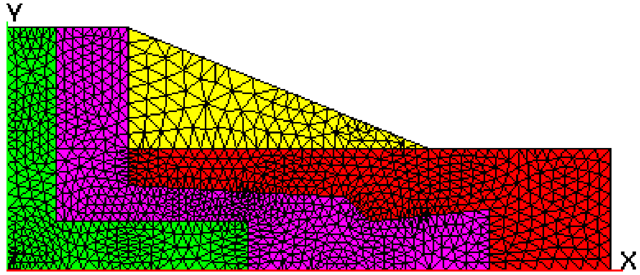
Heat pipe:



Simulator Description

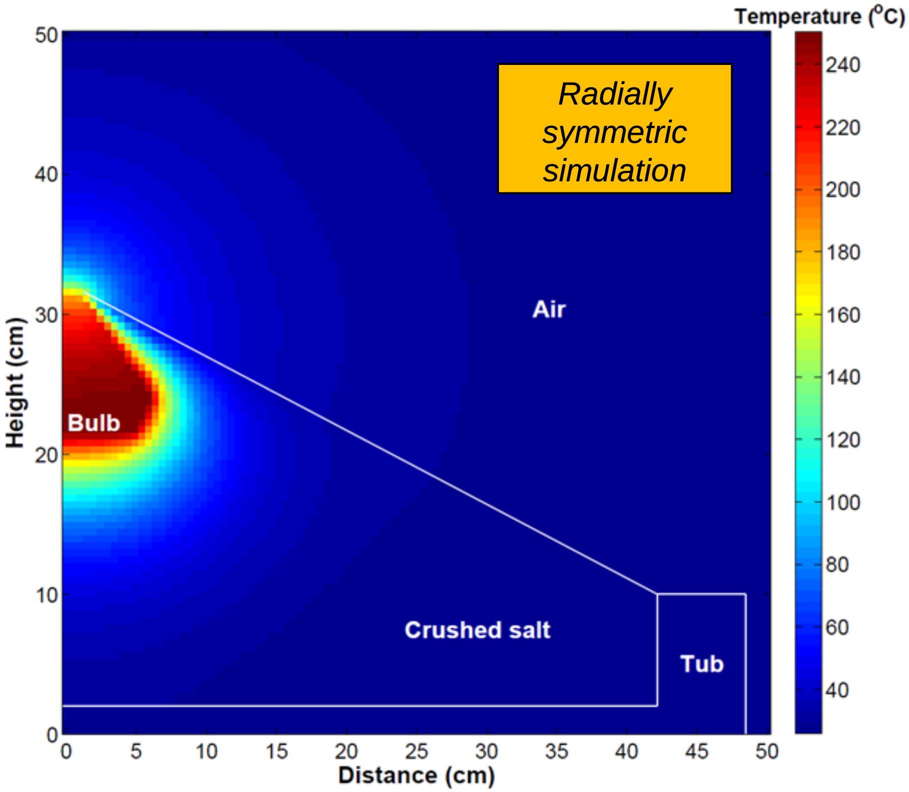
- **FEHM developed at Los Alamos 30+ years** **fehm.lanl.gov**
- **Used for 150+ peer reviewed articles**
  fehm.lanl.gov/pdfs/FEHM_references_list.pdf
- **Fully coupled thermal, mechanical, chemical, multiphase (gas, water vapor, water, rock)**
- **Uses LaGriT: Powerful 3-D grid generation tool**

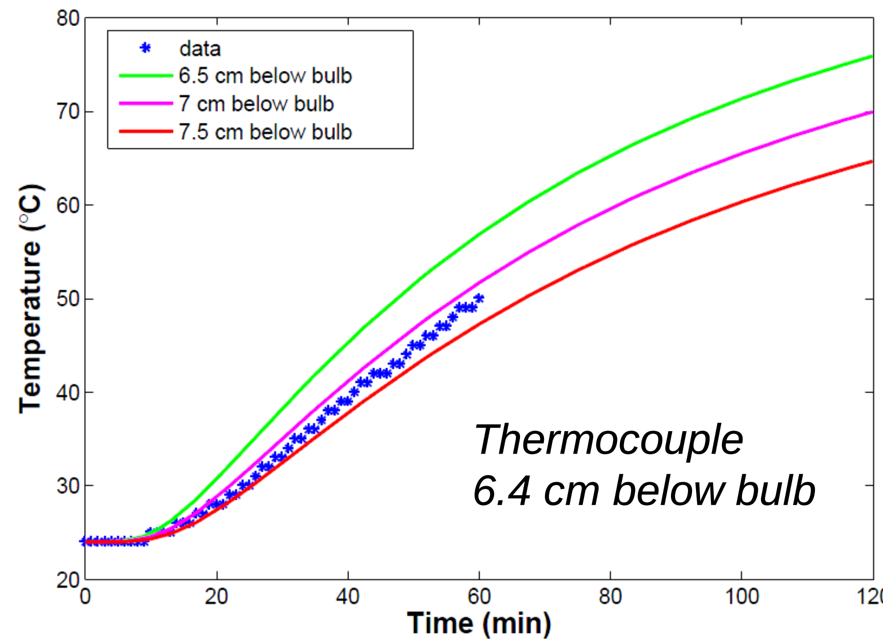




Code Validation Sample

- **Pile of crushed salt:**





- *Purpose:*
  - Test crushed salt (RoM) thermal model:

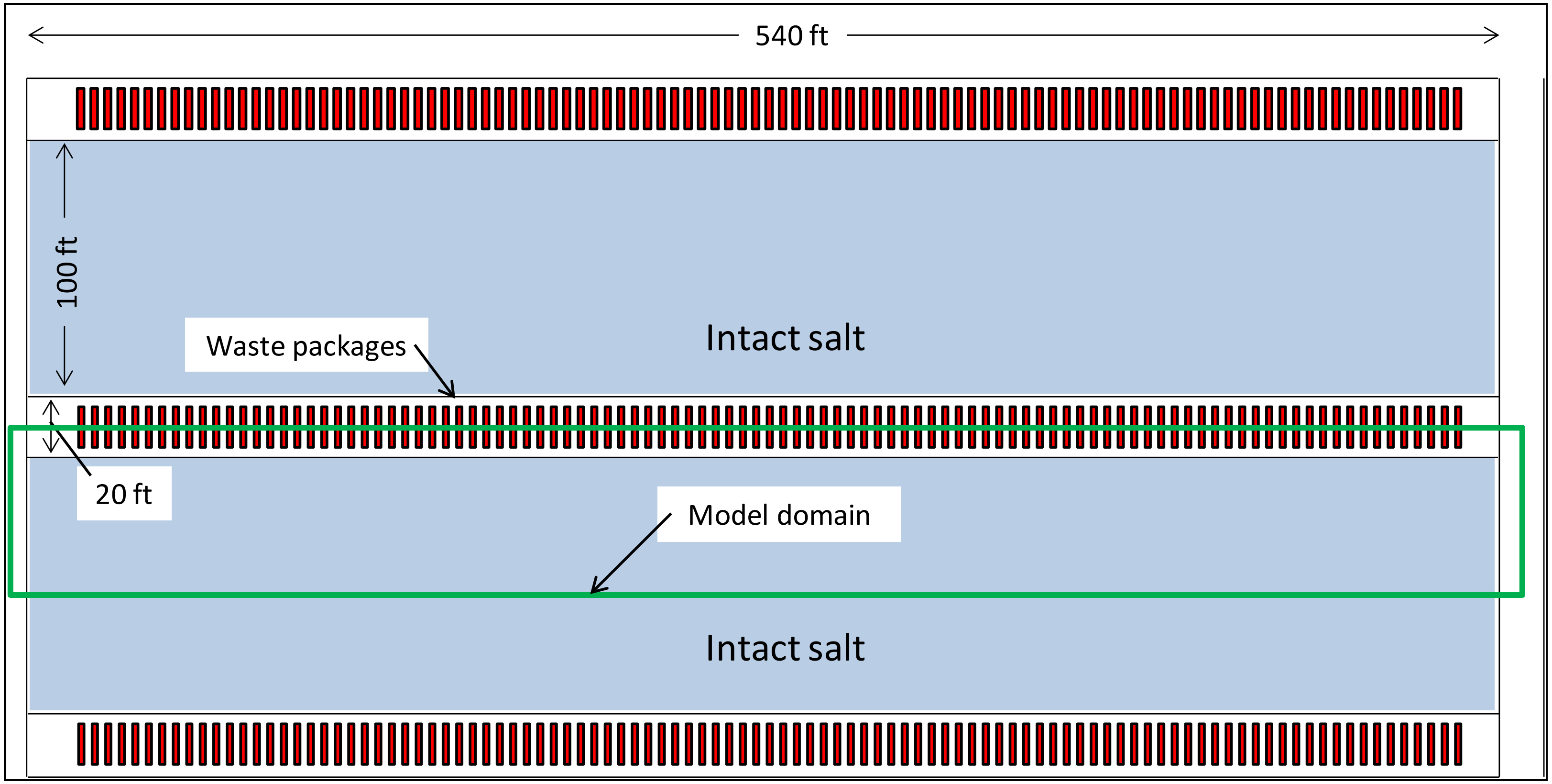
□= porosity

$$k_{T-WIPP}(\phi) = 1.08(-270\phi^4 + 370\phi^3 - 136\phi^2 + 1.5\phi + 5)$$

Stauffer et al., 2013

Thermal only simulation examples

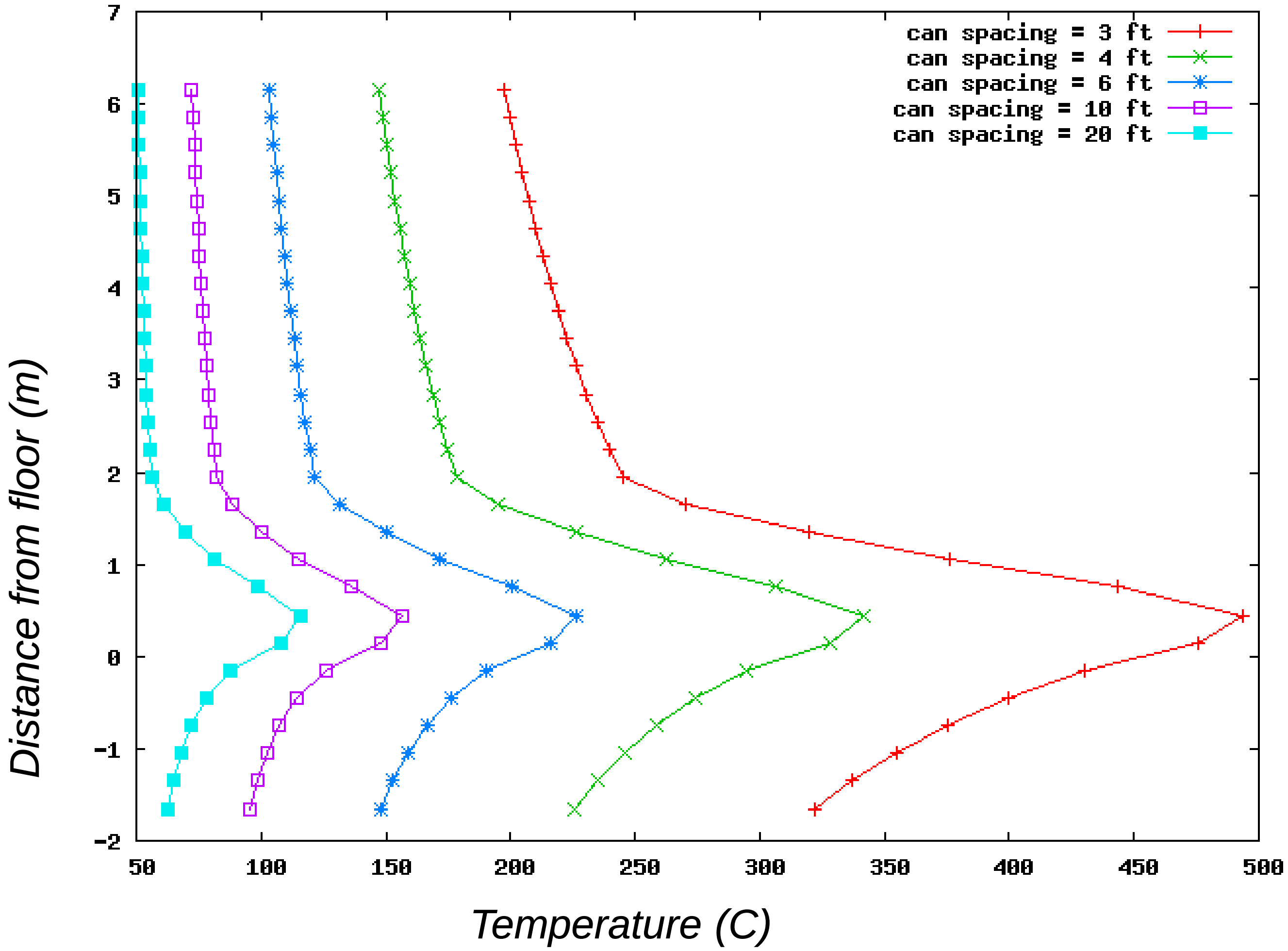
Map view of a potential salt repository : in-drift style



Reflection boundaries are used to reduce model domain

Thermal only simulation examples

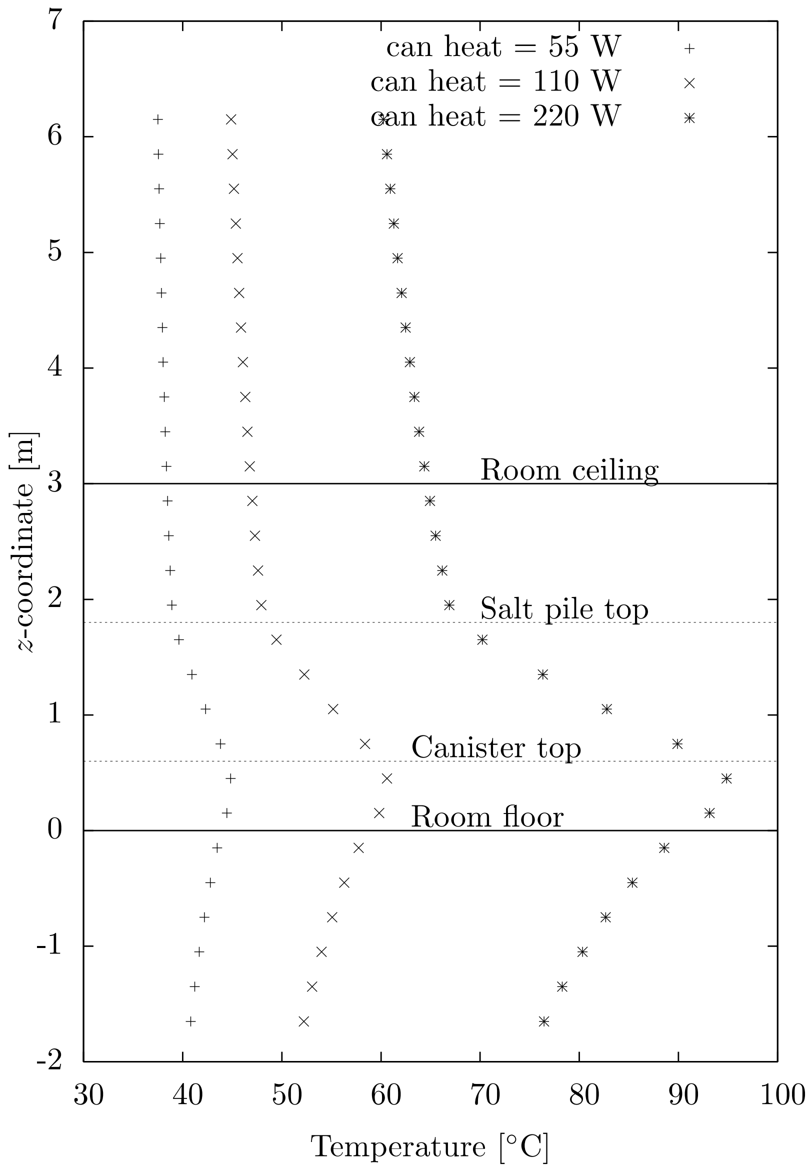
Vertical temperature for different 1000W canister spacing



2014 Harp et al., Modeling of High-Level Nuclear Waste Disposal in a Salt Repository, accepted, Nuclear Technology.

Thermal only simulation examples

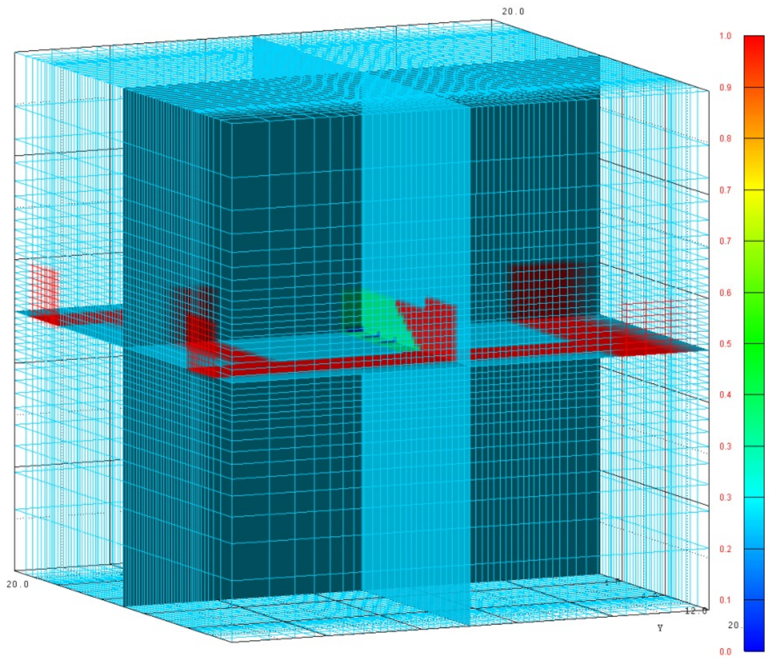
Vertical temperature for canisters spaced 0.9 m apart



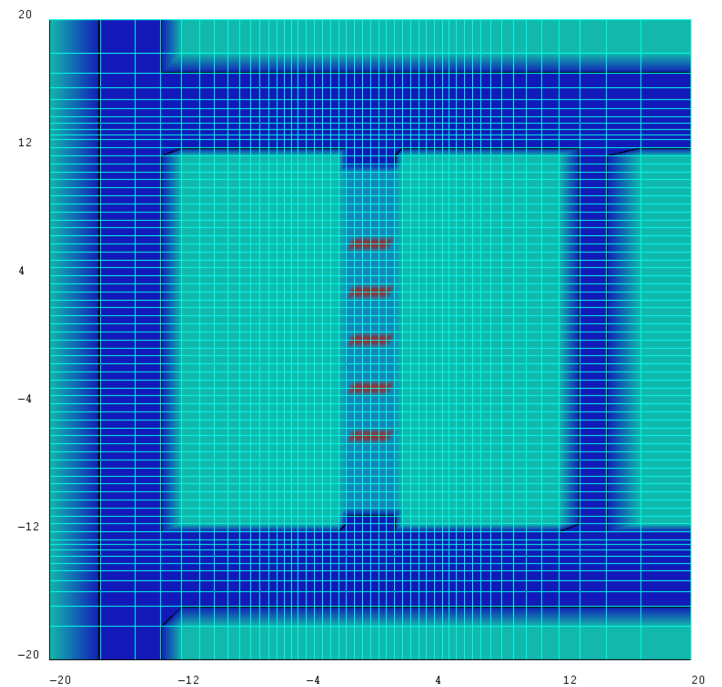
220W Canisters reach 95C

2014 Harp, D.R., P.H. Stauffer, P.K. Mishra, D.G. Levitt, B.A. Robinson, Modeling of High-Level Nuclear Waste Disposal in a Salt Repository, accepted, Nuclear Technology.

Many of the remaining simulations are for a set of 5 canisters lying in-drift on the floor



3-D model domain with red access tunnels and green backfill. Intact salt is cyan.



Map view at the drift floor, canisters are red

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Comparison of Thermal only VS Thermal + water + water vapor

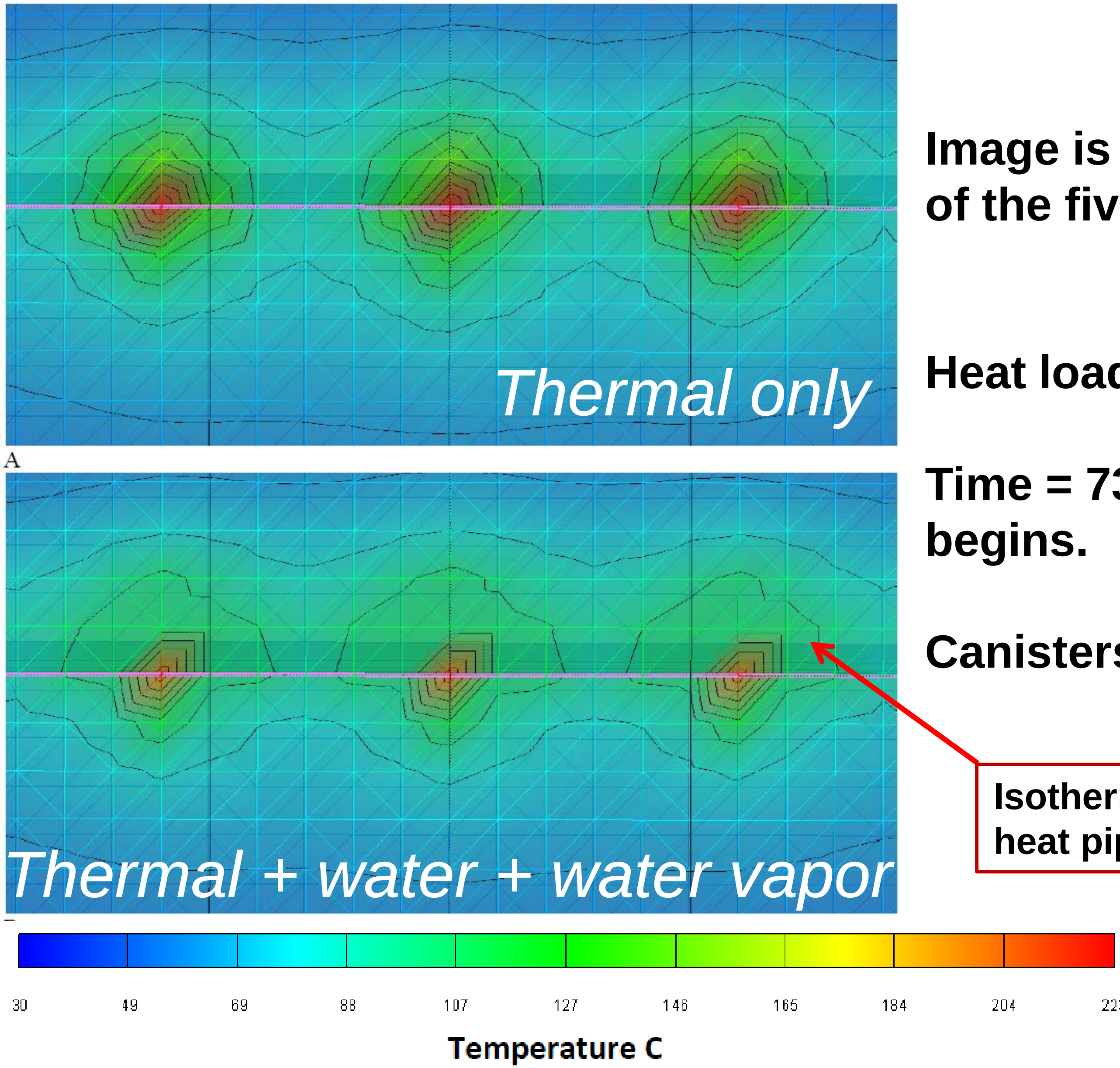


Image is zoomed in on three of the five heaters

Heat load = 1500W/canister

Time = 730 days after heating begins.

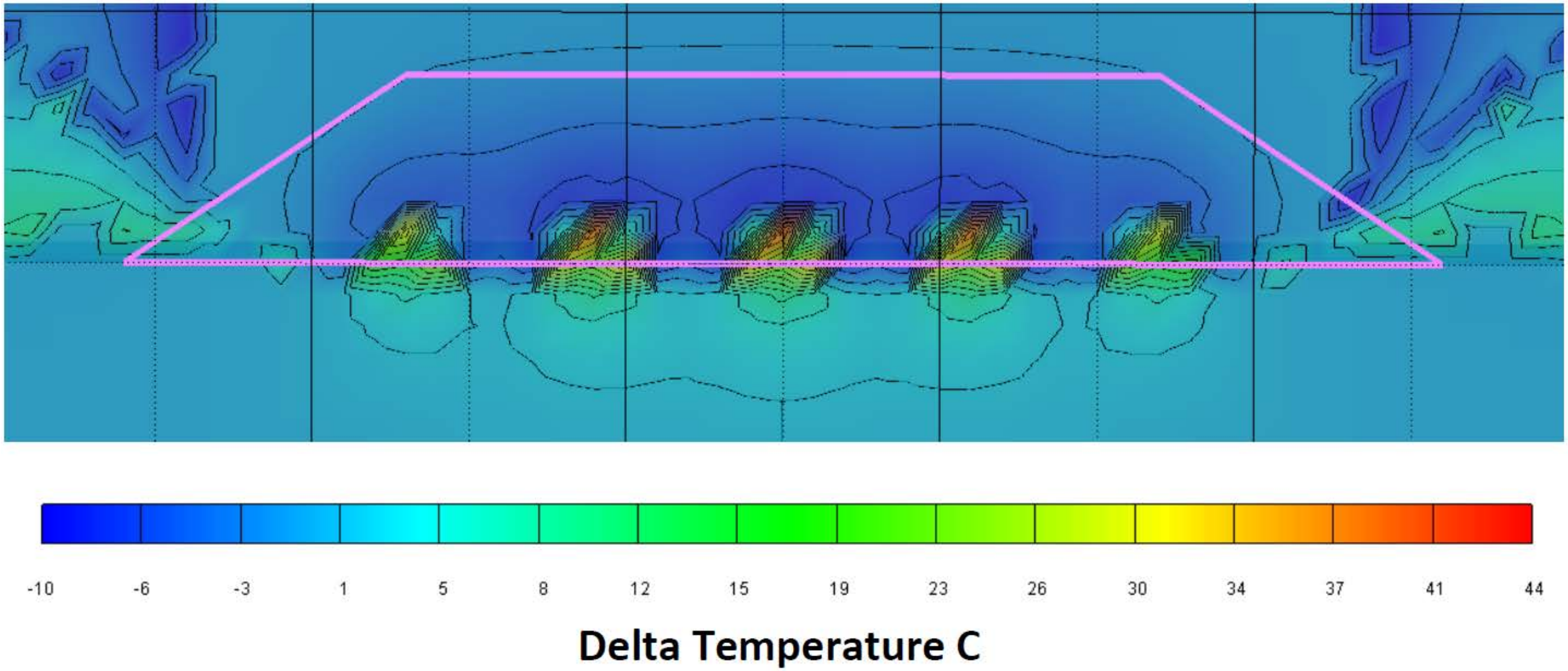
Canisters spacing = 1 m.

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>



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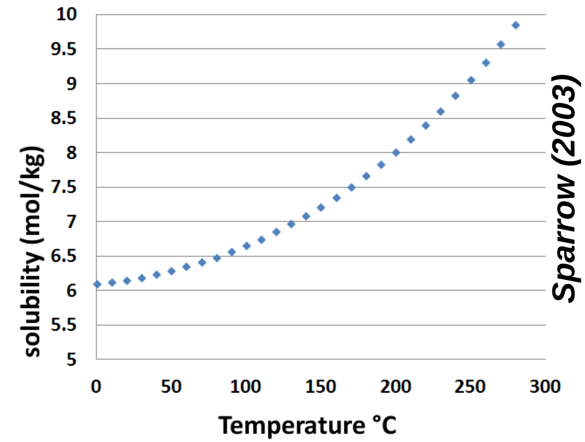
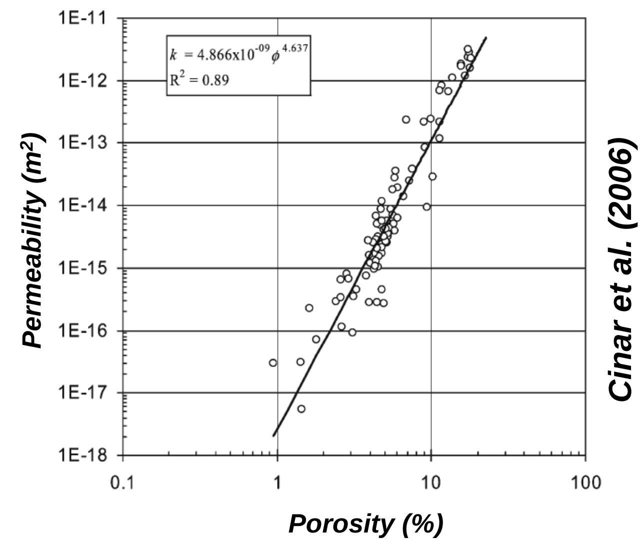
Thermo Hydrological Chemical Simulations require many coupled processes with feedbacks

- **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

- **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**
  - Capillary pressure relationships
  - Permeability-Porosity Relationship for RoM Salt

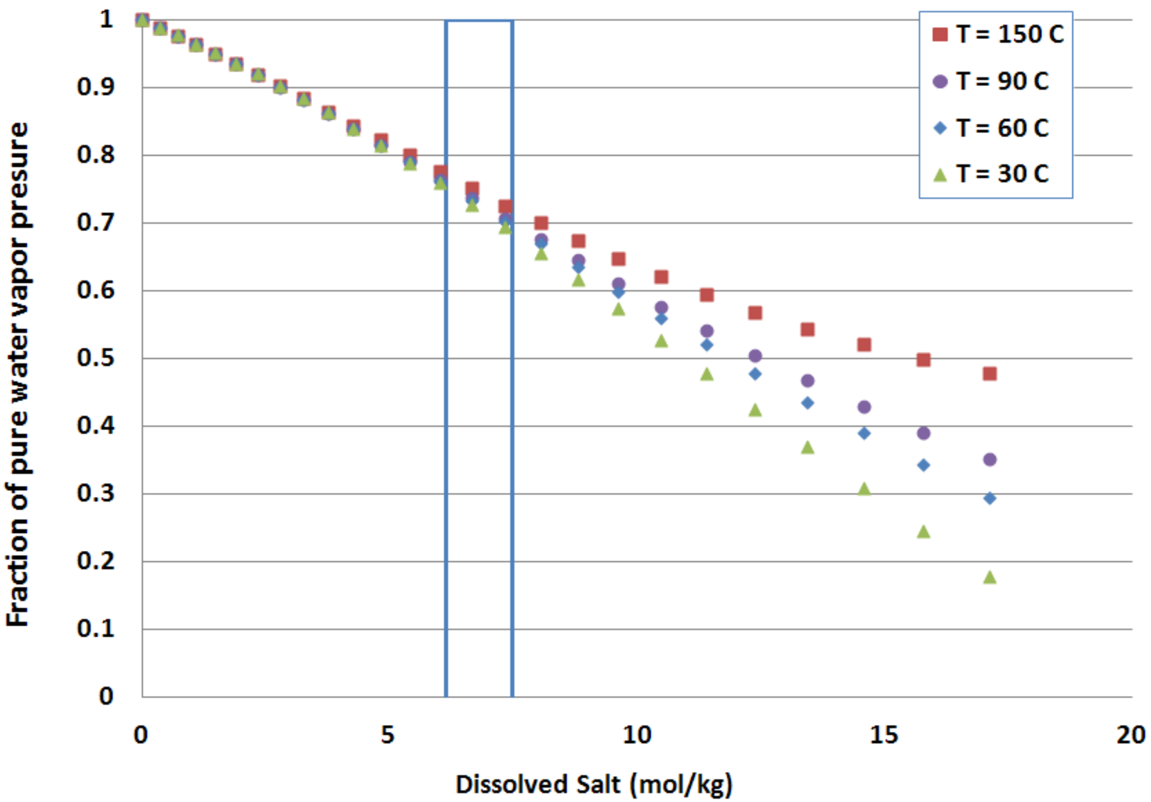




2013 Stauffer, P.H., et al., Coupled model for heat and water transport in a high level waste repository in salt, FCRD-UFD- 2013-000206 Los Alamos National Laboratory Document LA-UR 13-27584

Salt specific algorithms in FEHM for Thermo Hydrological Chemical Simulations

- **Vapor Pressure of Water as a function of Aqueous Sodium Chloride 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

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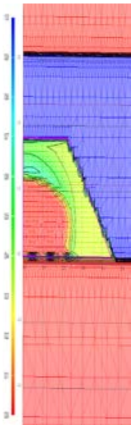
- Heat transfer across the air gap (radiation + convection)
- Clay Dehydration
- New diagnostic output (water vapor pressure, vapor diffusion coefficient, permeability, porosity, thermal conductivity)

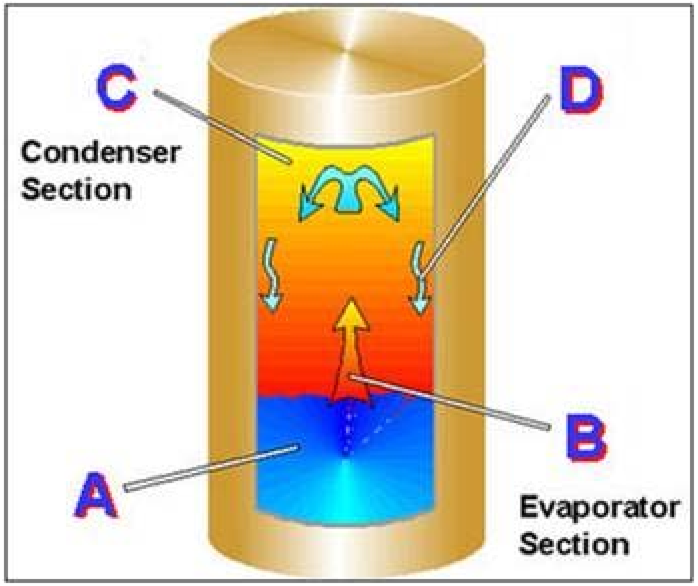
	Node	perm (m2)	porosity	Kx W/(m K)	Pwv (MPa)	D*wv (m2/s)	ps_delta_rxn	
Top	*117495*	*0.10000E-20*	*0.10000E-02*	*5.3361*	*0.31557E-02*	*0.10629E-12*	*0.0000*	*Intact Salt*
	102233	*0.10000E-18*	*0.10000E-01*	*5.0982*	*0.64491E-02*	*0.87686E-09*	*0.29872E-11*	*Intact Salt*
	85866	*0.10000E-10*	*0.99900*	*14.000*	*0.80089E-02*	*0.28997E-04*	*0.0000*	*AIR*
	70134	*0.27929E-11*	*0.48402*	*0.57114*	*0.19505E-01*	*0.19459E-04*	*0.39003E-05*	*Crushed Salt*
	54963	*0.15400E-17*	*0.89400E-02*	*4.0922*	*0.10769*	*0.79177E-05*	*0.0000*	*Crushed Salt*
	43160	*0.88841E-17*	*0.13046E-01*	*3.9657*	*0.10906*	*0.93052E-05*	*0.0000*	*Crushed Salt*
	39022	*0.10000E-20*	*0.10000E-04*	*1.1000*	*0.11204*	*0.88788E-06*	*0.0000*	*Waste Canister*
	34337	*0.10000E-20*	*0.10000E-04*	*1.1000*	*0.11307*	*0.90078E-06*	*0.0000*	*Waste Canister*
	15980	*0.10000E-20*	*0.10000E-04*	*1.1000*	*0.84381E-01*	*0.86175E-06*	*0.0000*	*Waste Canister*
	10667	*0.10000E-18*	*0.10000E-01*	*4.2656*	*0.64085E-01*	*0.39347E-05*	*-0.91248E-07*	*Intact Salt*
	3612	*0.10000E-18*	*0.10000E-01*	*4.3988*	*0.44300E-01*	*0.23626E-05*	*0.11403E-07*	*Intact Salt*
	2639	*0.10000E-20*	*0.10000E-02*	*4.8613*	*0.12512E-01*	*0.56724E-08*	*0.0000*	*Intact Salt*
Bottom	*21*	*0.10000E-20*	*0.10000E-02*	*5.3361*	*0.31560E-02*	*0.24695E-13*	*0.0000*	*Intact Salt*



Example diagnostic output for a vertical line of nodes

Generic Heat Pipe Explanation

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



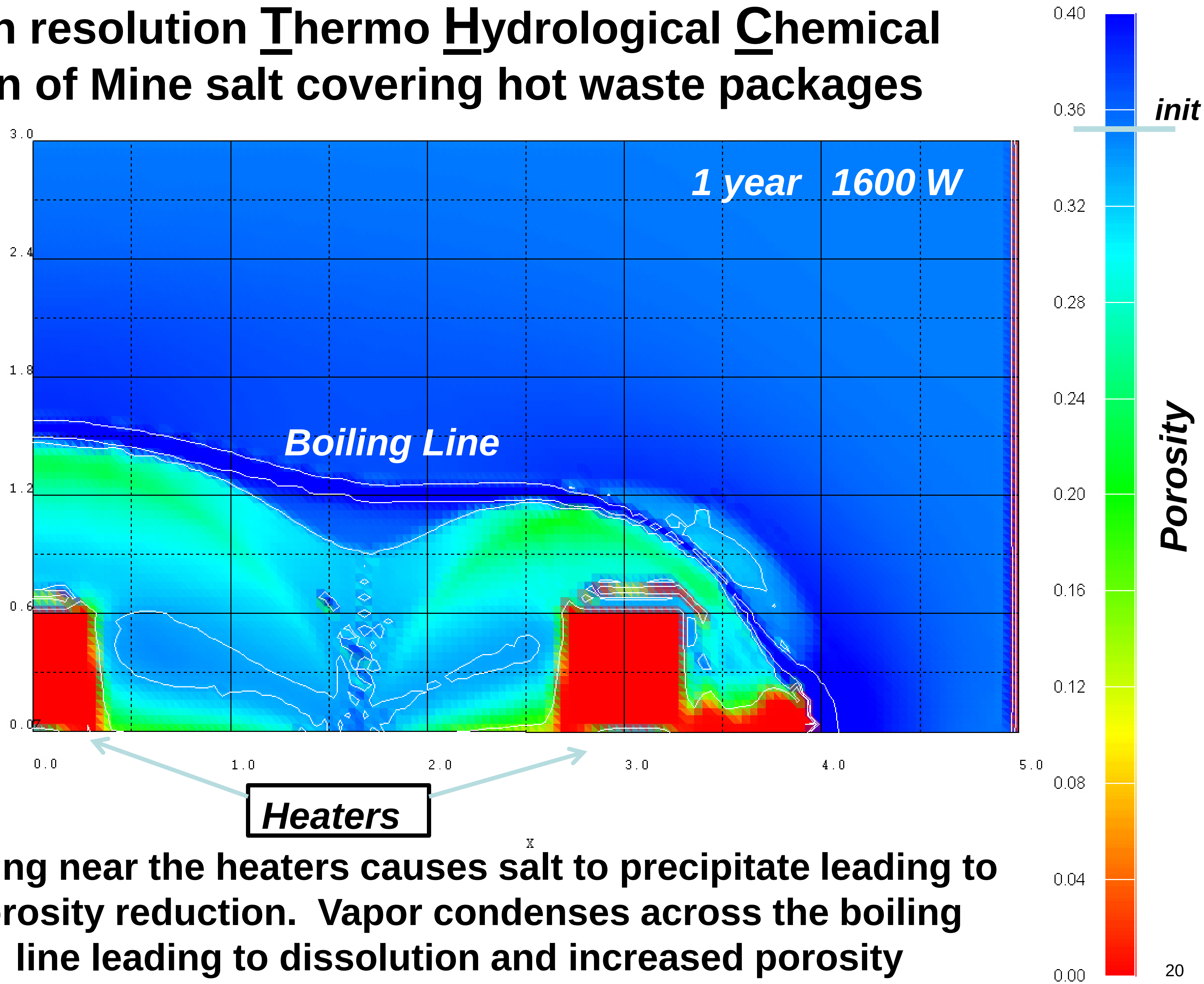
Heat pipes lead to isothermal regions where phase change is absorbing energy

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

3x5 m

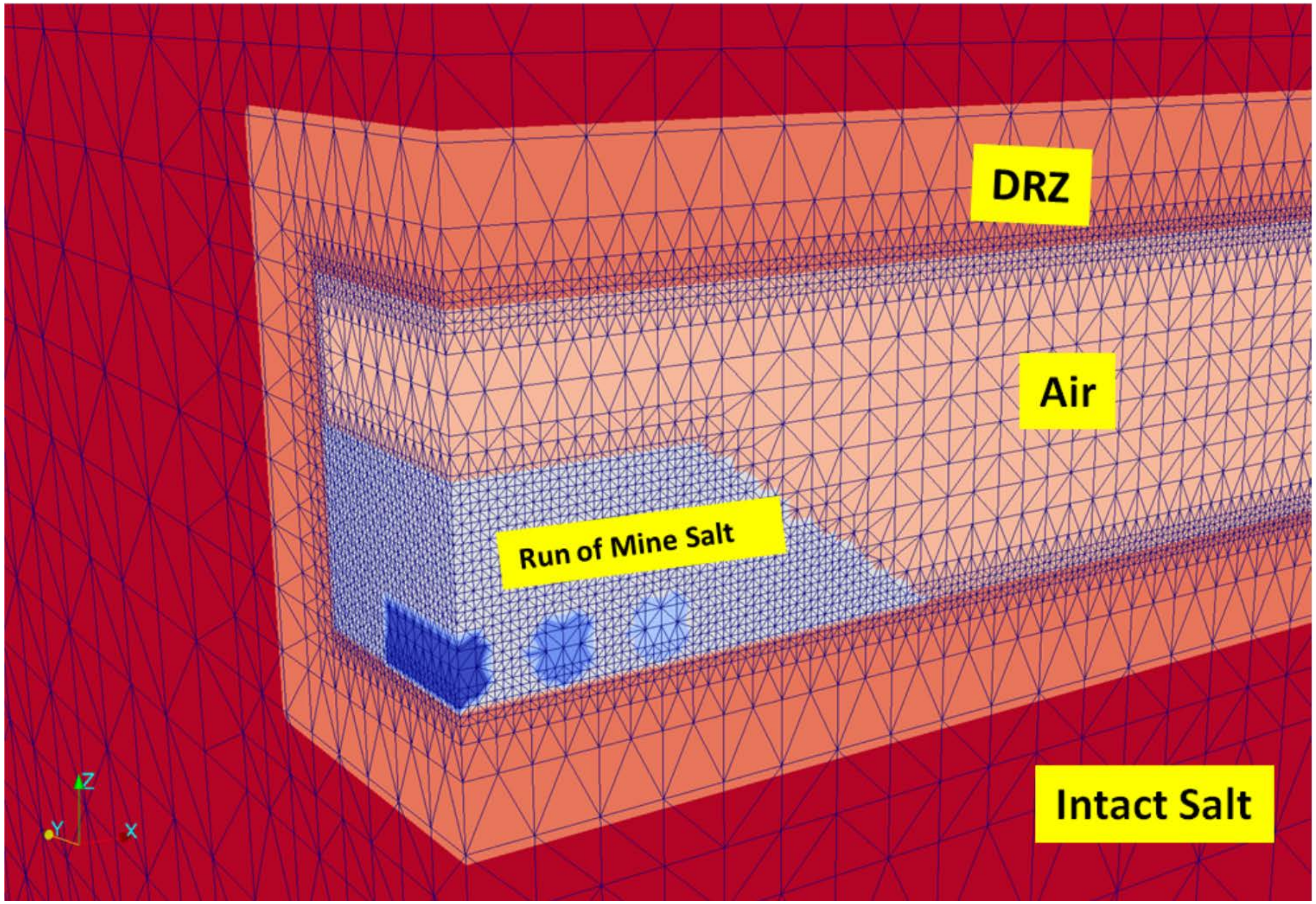
2-D slice

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

New mesh to get more resolution for coupled Thermal Hydrological Chemical Simulations



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

Range of parameters used in the simulations

Parameter	Natural Range	Simulated Range
Backfill saturation	0.01 – 0.05+	0.01 – 0.1
Backfill porosity	0.3 - 0.4	0.35
Clay content	0 – 15%+	0 – 10%
Background temperature	15 – 30 C	30 C

Results

Fully Coupled

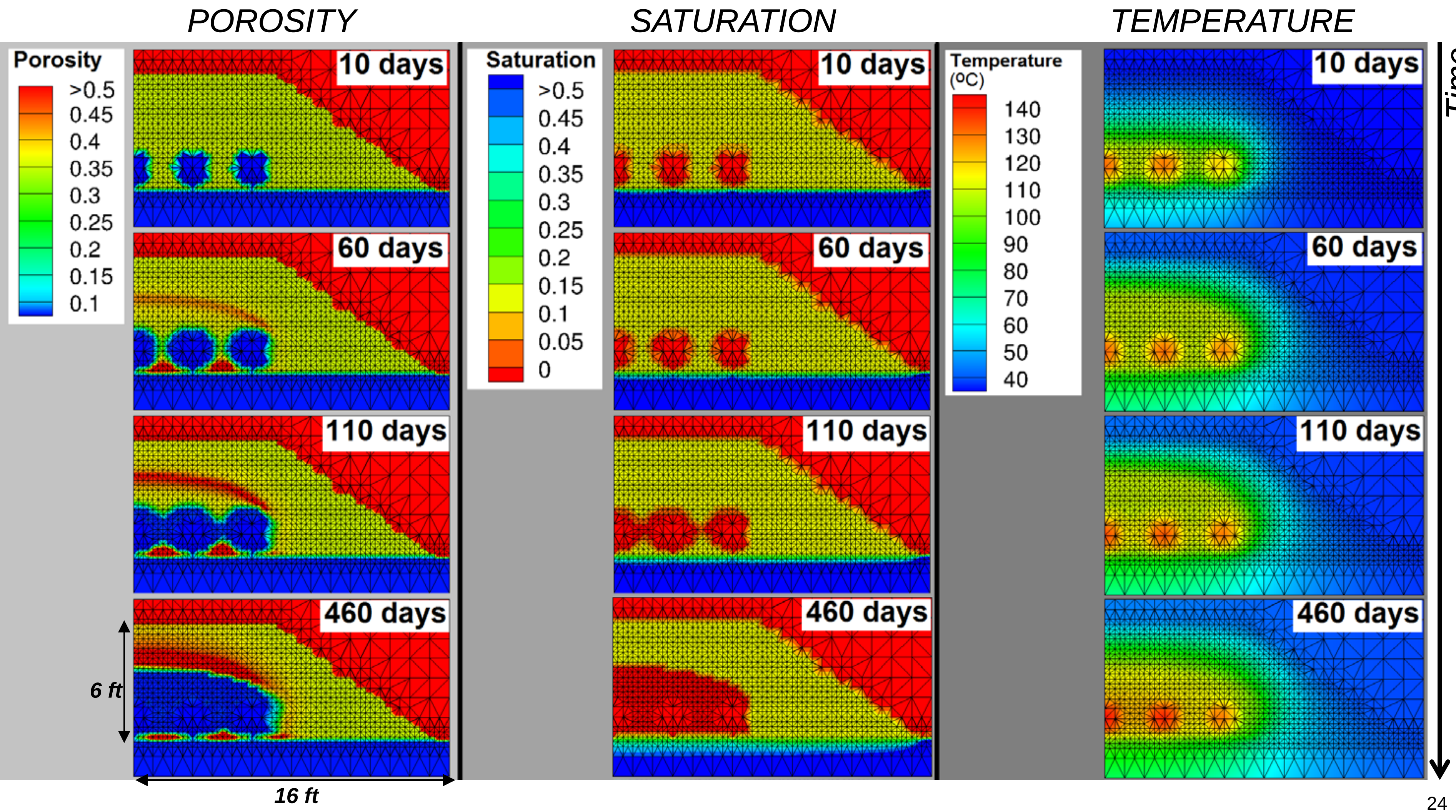
Thermo Hydrological Chemical

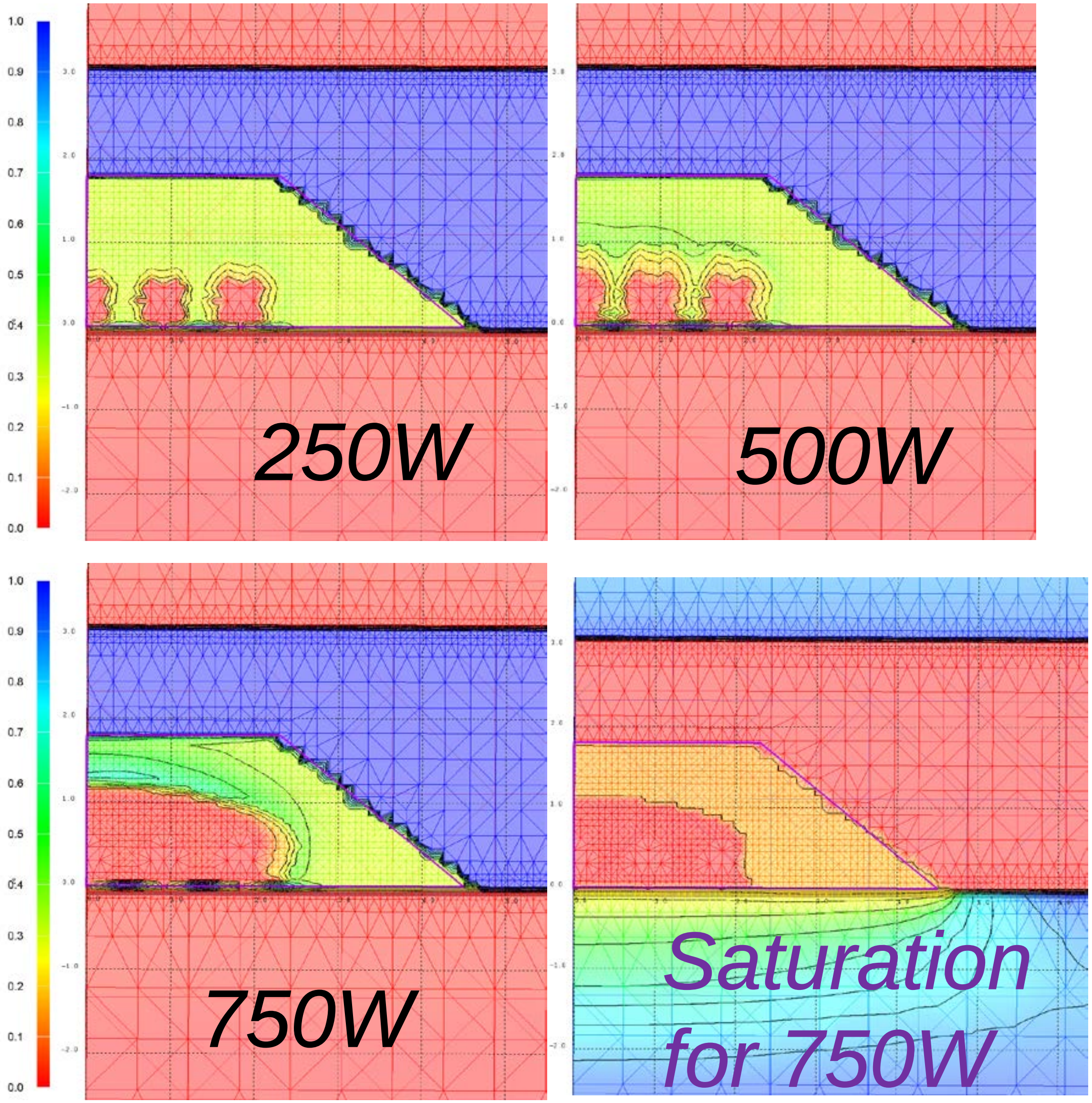
simulations

at the drift scale

Thermo/Hydro/Chem Modeling: Results

Simulation parameters: *Heater temperature (750 W), initial saturation in backfill (S = 10%), maximum capillary suction at zero saturation ($P_{cap,max}$ = 0.5 MPa), clay fraction (none), residual water saturation (S_r = 0.1)*

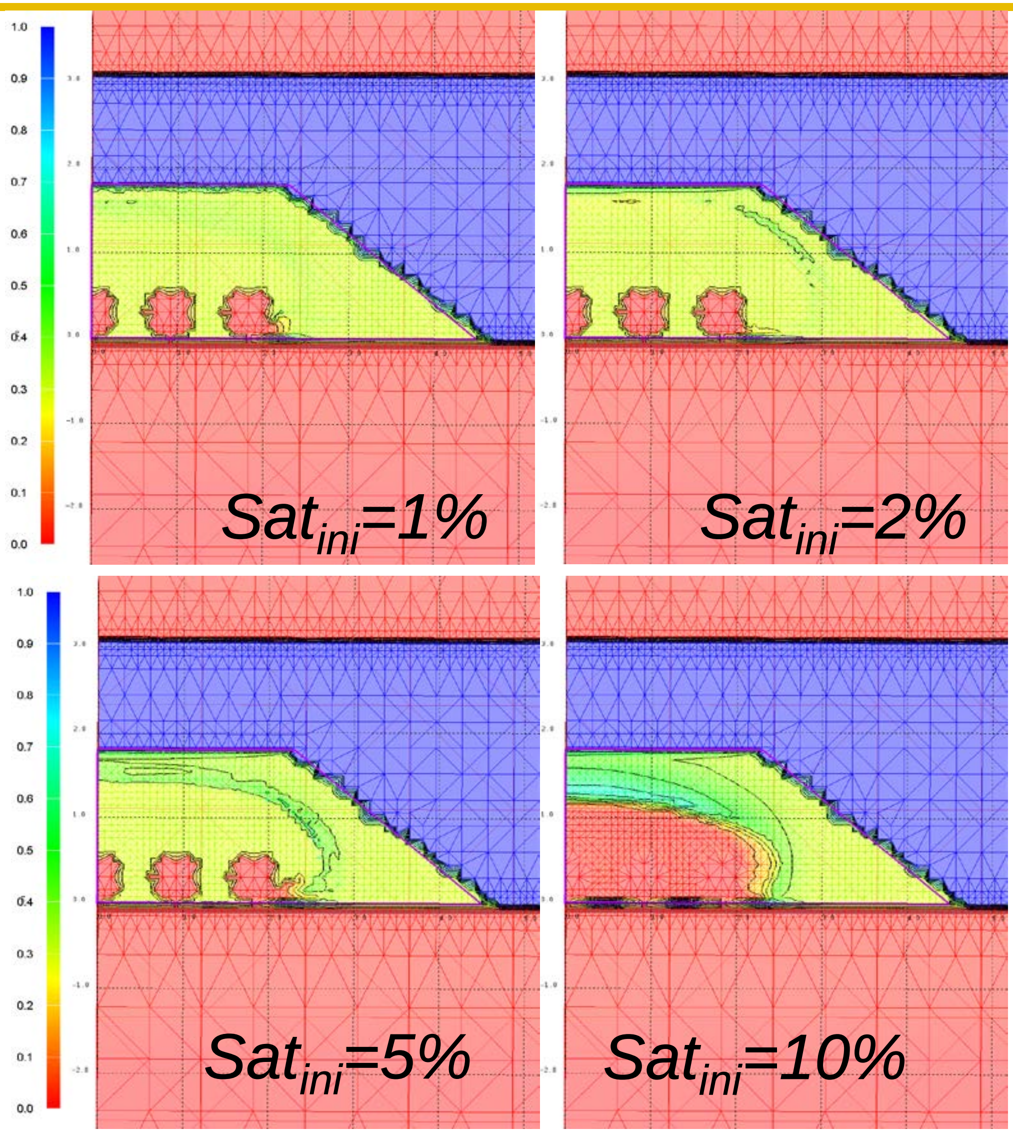




Porosity changes more with higher heat loads

More heat pipe at higher temperatures

Time = 2 years
Sat_{ini} = 10%



Porosity changes more with <u>higher</u> <u>Initial saturation</u> in the run of mine salt backfill

More heat pipe in a wetter system

All at 750W
Time = 2 years

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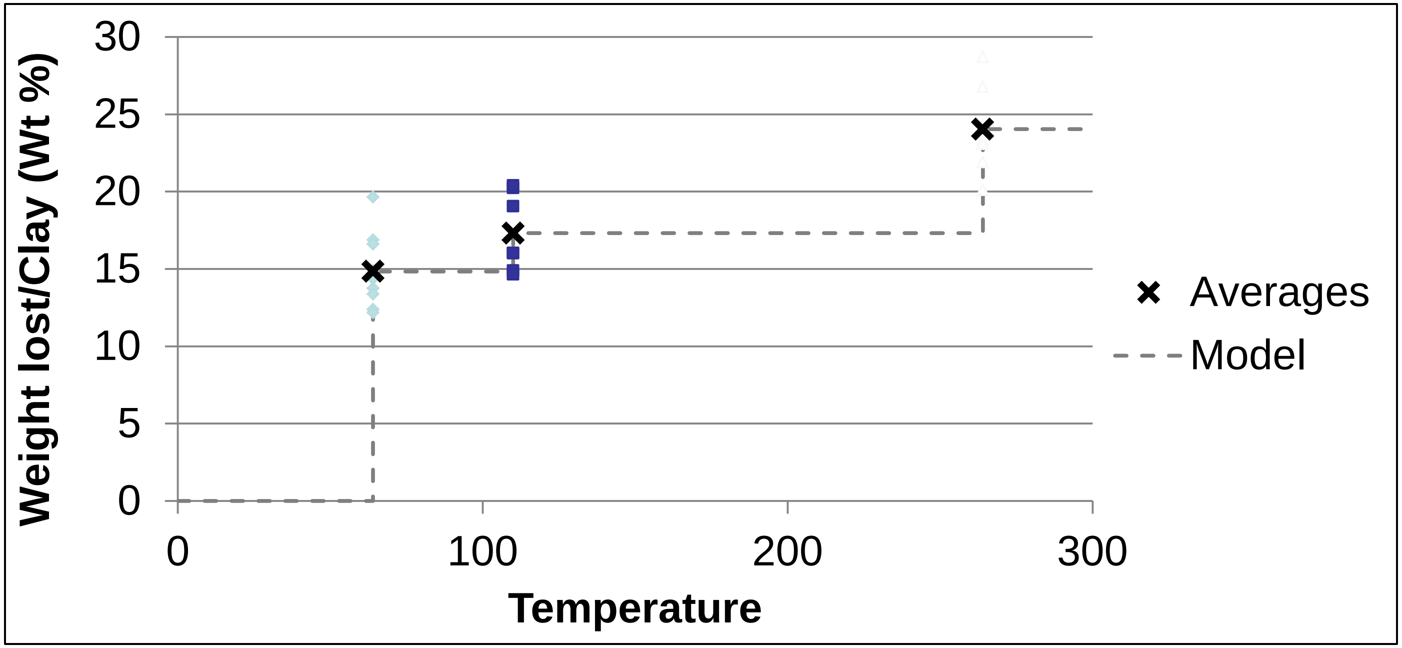
Clay Dehydration

- **WIPP salt is impure – contains clays and other minerals**
- **In laboratory experiments with run-of-mine (RoM) salt, water release from clays was observed at discrete temperatures:**



Data from Hakim Boukhalfa

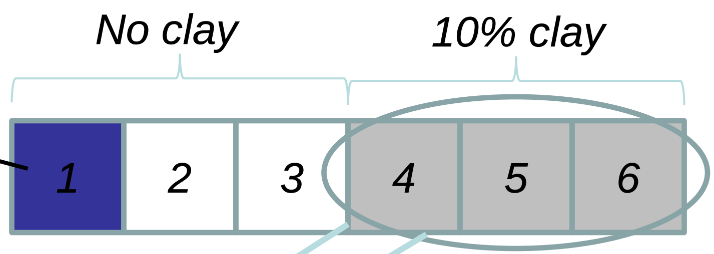
- **Mass of water produced at 64ºC at node *i* based on the fraction of clay (f_c), porosity, density of rock, and volume of the cell:**

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

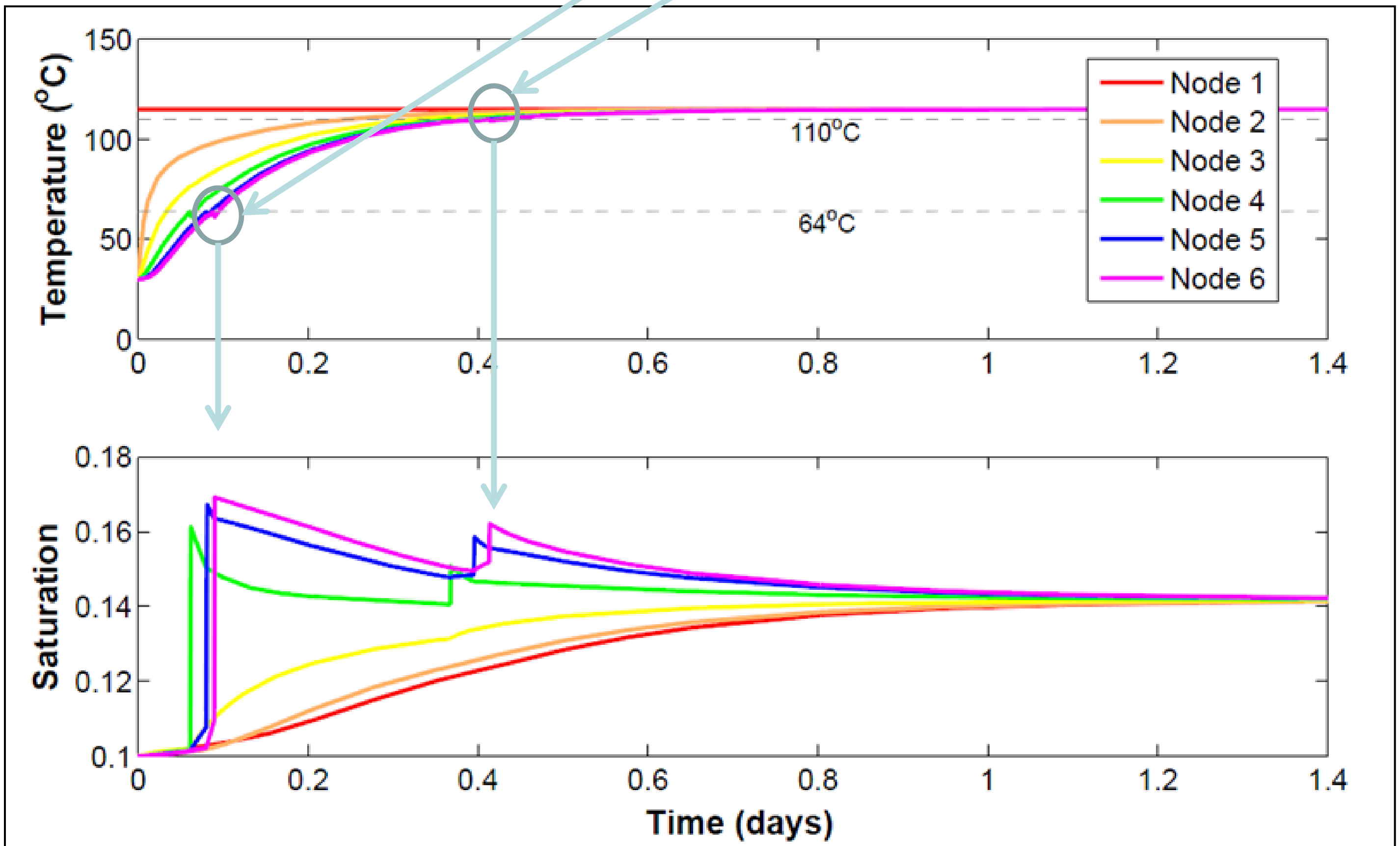
Clay Dehydration: Test Problem

6 nodes

Boundary condition: 115°C

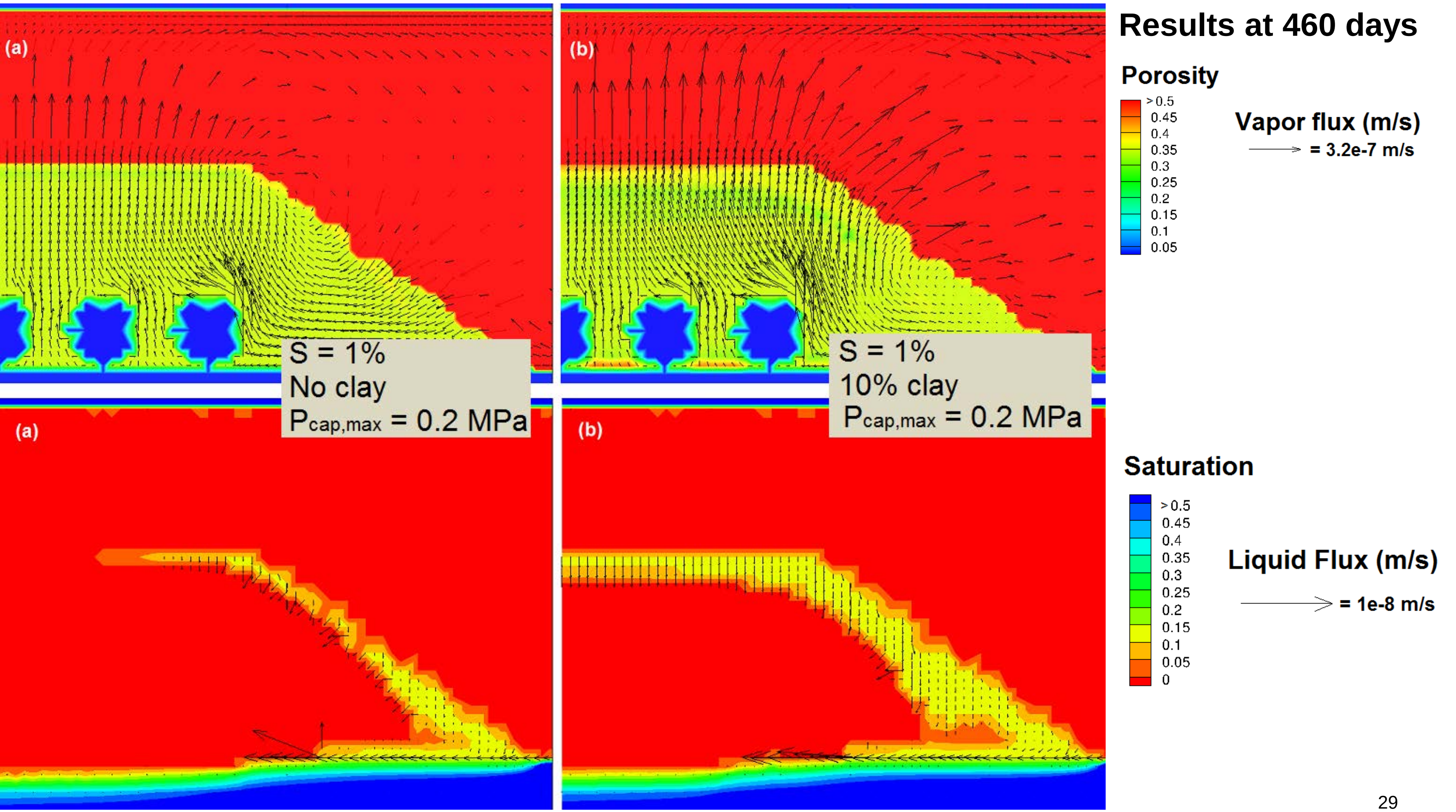


Initial condition: Node 1 = 115°C
Nodes 2 – 6 = 30°C



Clay Dehydration Modeling: Results

No clay | 10% clay



Conclusions

- **Including water and water vapor in simulations leads to**
  - Not much change in low energy cases (<250W per canister)
  - Heat pipes in some higher energy cases (>250W per canister)
    - Lower temperatures near the canisters
    - Salt mass transfer toward the canisters
    - Increased thermal conductivity near the canisters
  - Heat pipe development is positively correlated with:
    - Initial backfill saturation
    - Backfill capillary suction
    - Clay content in the backfill
    - Water mobility at low saturation
    - 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