Thermohydrological Model Uncertainty Reduction Using Physical Analog Models

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by
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Thermohydrological Model Uncertainty Reduction Using Physical Analog Models

Objective

Evaluate the ability to numerically simulate thermohydrological processes in experiments at two scales:

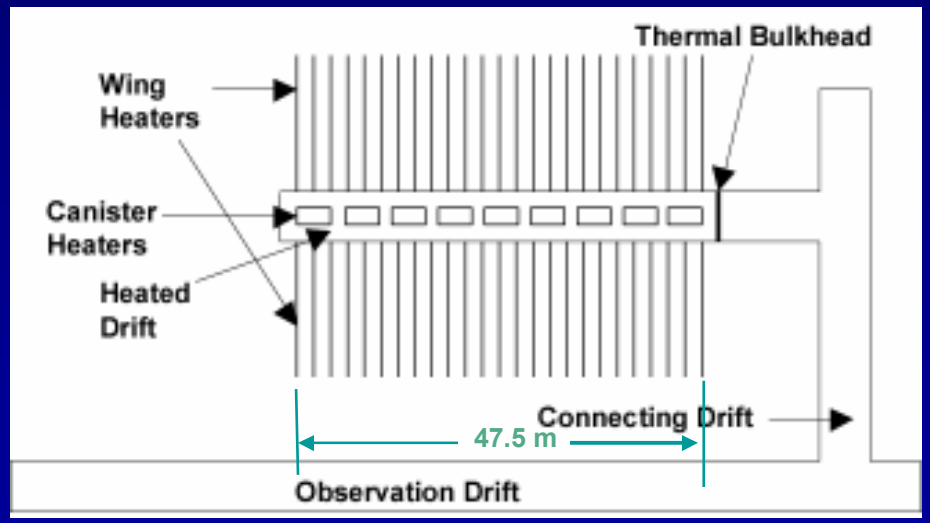
- laboratory
- field

to replicate thermohydrological conditions at the potential repository at Yucca Mountain

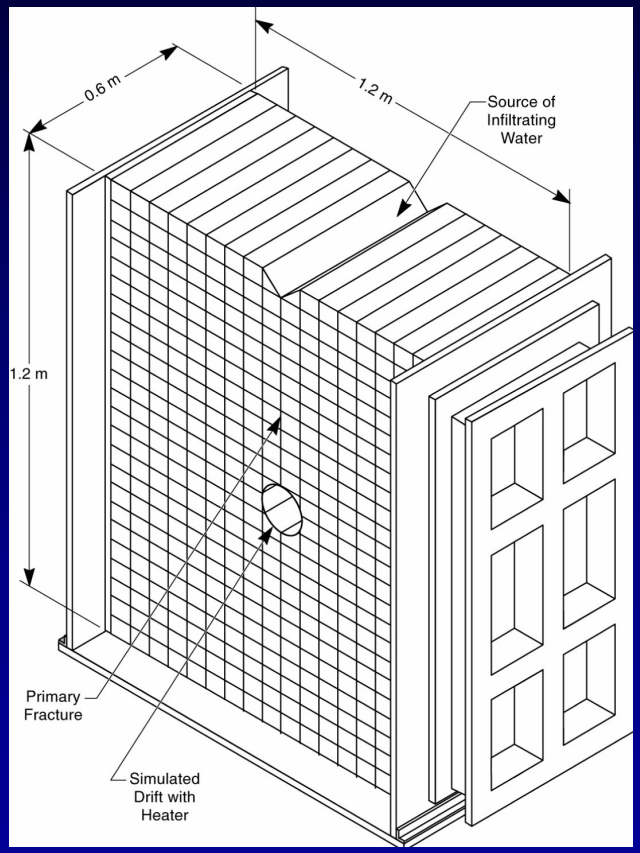
→ Increased confidence in multiphase simulators used to predict repository performance

Thermohydrological Model Uncertainty Reduction Using Physical Analog Models

The results from two experiments were used to evaluate the ability of MULTIFLO to replicate thermohydrological processes active in heated fractured porous media



DOE Drift-Scale Heater Test



CNWRA Laboratory-Scale Heater Test

Comparative Advantages of Scale

Laboratory-scale experiment

- Better characterized medium — Removes natural heterogeneity
- Controlled boundary fluxes — Controlled boundary conditions required
- State variables more easily monitored

Field-scale experiment

- Capture natural heterogeneity — Natural heterogeneity difficult to characterize
- Larger size establishes boundary conditions — Larger size difficult to monitor
- Spatial scale closer to actual application

Combined scales provide an opportunity to capture strengths of both scales

Thermohydrological Model Uncertainty Reduction Using Physical Analog Models

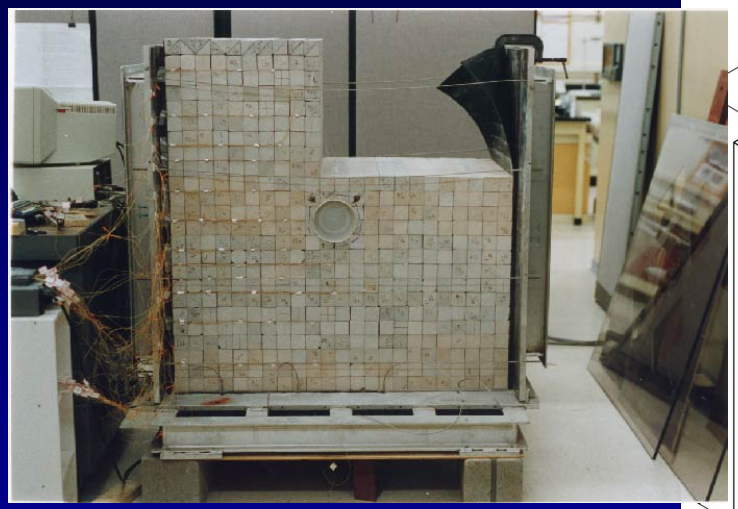
CNWRA Laboratory-Scale Heater Test

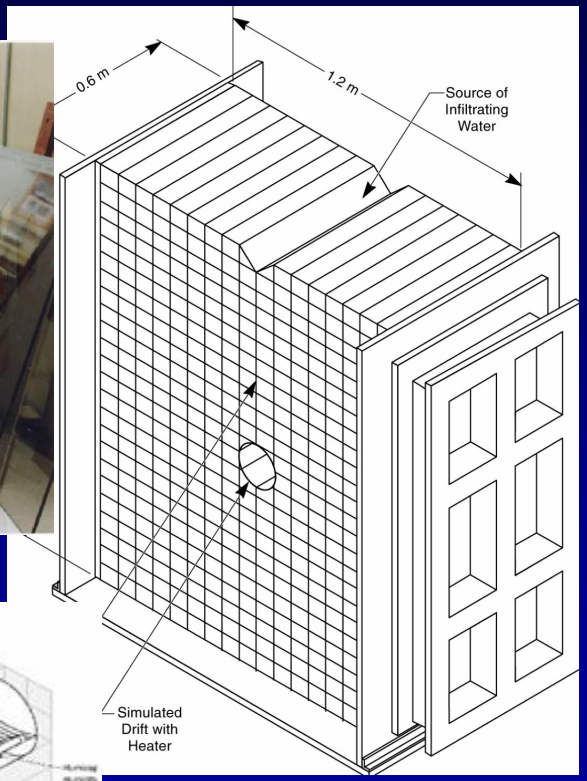
7-month duration

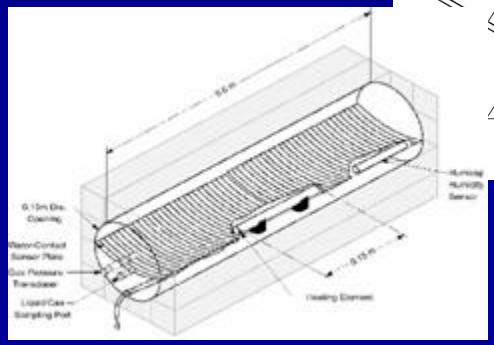
Temperature, saturation, and chemistry were monitored during the conduct of a laboratory-scale experiment

The test medium consisted of concrete blocks to replicate fractured rock

Matrix saturation was measured at the end of the test

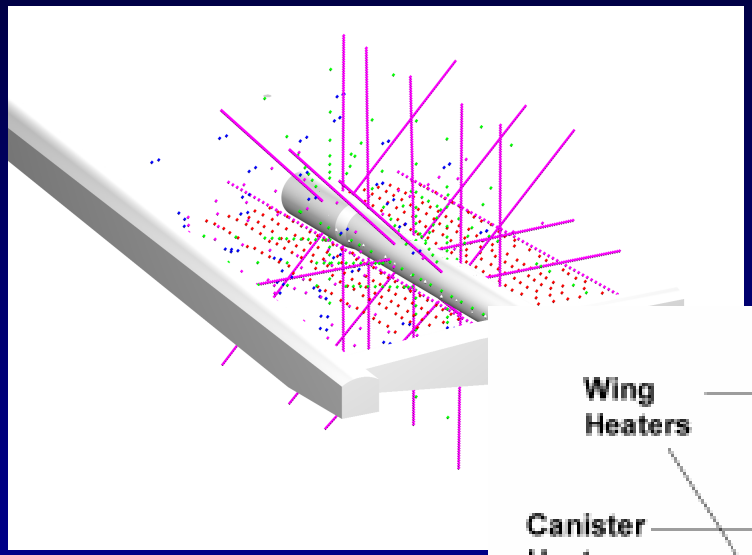






Thermohydrological Model Uncertainty Reduction Using Physical Analog Models

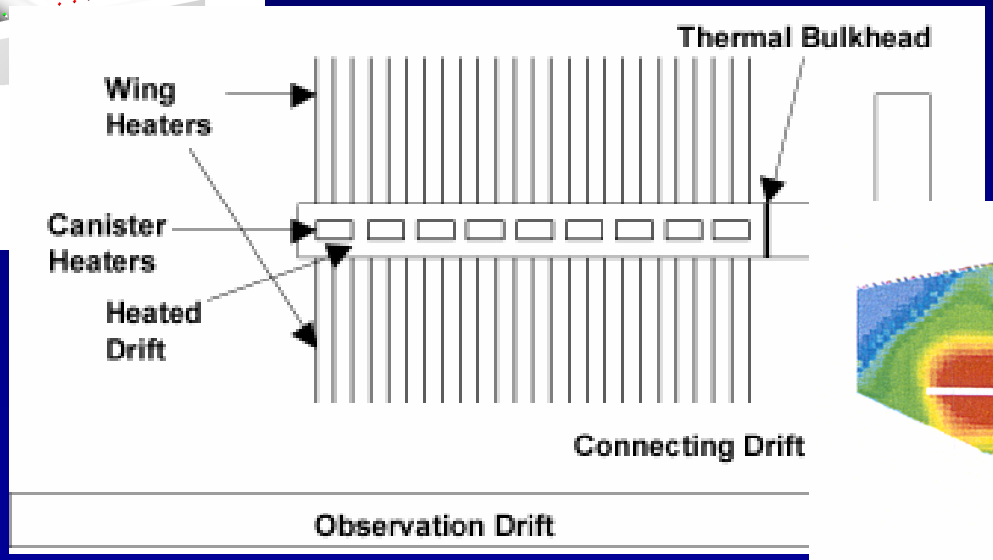
DOE Drift-Scale Heater Test

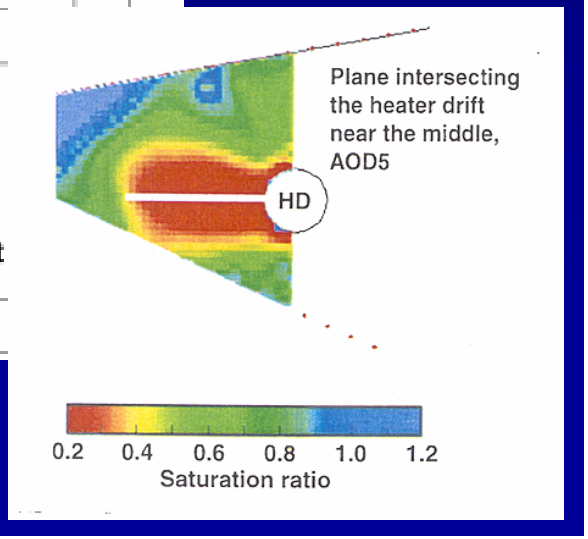


8-yr duration: 4-yr heating & 4-yr cooling

47.5-m-long heated drift, 25 inner & outer wing heaters on both sides of heated drift

Heated drift closed by thermal bulkhead





Temperature directly measured

Saturation inferred using several geophysical techniques

Test Results

Laboratory-Scale Heater Test	Drift-Scale Heater Test

Measured parameters

Laboratory-Scale Heater Test

- Temperature during test
- Post-test matrix saturation
- Post-test fracture flow staining
- Dripping into the analog emplacement drift

Drift-Scale Heater Test

- Temperature during test
- Matrix saturation indirectly measured using ERT, radar, and neutron-probe measurements
- Water chemistry

Compared model parameters

Laboratory-Scale Heater Test

- Matrix temperatures
- Matrix saturation
- Fracture flow pattern

Drift-Scale Heater Test

- Borehole temperatures
- Matrix saturation
- Fracture permeability (saturation)

MULTIFLO

- Non-isothermal, two-phase simulator
- Fully implicit formulation using a variable substitution approach
- Space discretization is based on a block-centered grid using an integral finite-volume difference scheme
- Unstructured grid with arbitrary interblock grid connectivity and any polygon block boundary
- Supports dual-continuum model with user-specified relative permeability for fracture-to-matrix flow

Property Assignments
Sensitivity Analyses

Two levels of sensitivity analyses:

- **Evaluation of property values and boundary conditions that affect temperature evolution (laboratory-scale) and initial matrix saturation (field-scale)**

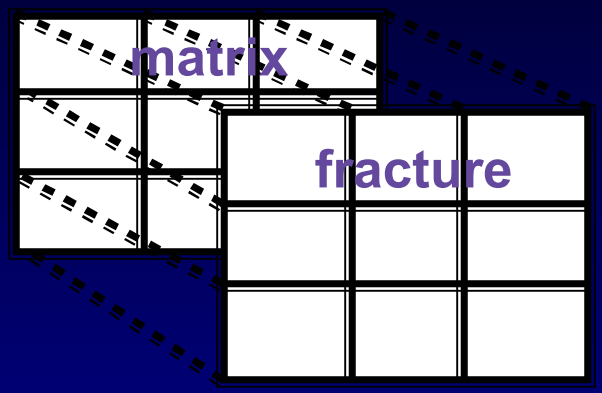
After the boundary conditions were determined, all subsequent analyses were performed relative to the same basecase conditions

- **Evaluation of property values and conceptual models that affect coupled thermohydrological processes**

Conceptual Model Evaluation: Fracture-Matrix Interaction Options

Dual continuum (matrix-fracture)

Generally accepted



1) Modified fracture relative permeability

$$k_{rl,f \rightarrow m} = \eta \, k_{rl,f} \qquad \eta < 1$$

2) Matrix/fracture area modifier:

Area modifier, A_{mod}, used to reduce matrix/fracture interfacial surface area, reduces both heat and mass transfer

3) Active-fracture model (Liu et al., 1998)

Modifies $k_{rl,f \rightarrow m}$, $k_{rl,f}$, and P_c

Active-Fracture Model
(van Genuchten-Mualem-Liu model)

van Genuchten relation (fracture system) modified to:

$$\alpha P_c = \left[S_{lf}^{(\gamma-1)/m} - 1 \right]^{1/n}$$

Relative liquid permeability function (fracture):

$$k_{rl,f} = s_{lf}^{(1+\gamma)/2} \left\{ 1 - \left[1 - s_{lf}^{(1-\gamma)/m} \right]^m \right\}^2$$

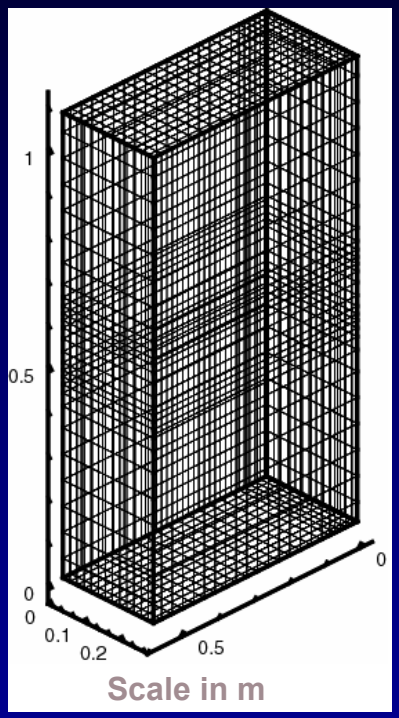
Relative liquid permeability function (fracture-to-matrix):

$$k_{rl,f \to m} = s_{lf}^{(1+\gamma)^2/2} \left\{ 1 - \left[1 - s_{lf}^{(1-\gamma)/m} \right]^m \right\}^2$$

Thermohydrological Numerical Models

Field-scale model		Laboratory-scale model
Model Dimensions		
3D, ¼ modeled		3D, ¼ modeled
200 m	x-direction	1.2 m
64.5 m	y-direction	0.6 m
100 m	z-direction	1.2 m
Boundary Conditions		
closed	side	mixed
specified infiltration	top	specified infiltration
open	bottom	open
open	drift wall	no boundary
Initial Conditions		
~97%	matrix saturation	20%
5%	fracture saturation	10%
natural geothermal gradient	temperature	22 C
ambient gradient	air pressure	103,150 Pa

Numerical Grids



Laboratory-scale test

Structured grid

24 × 14 × 30 = 10,800 nodes

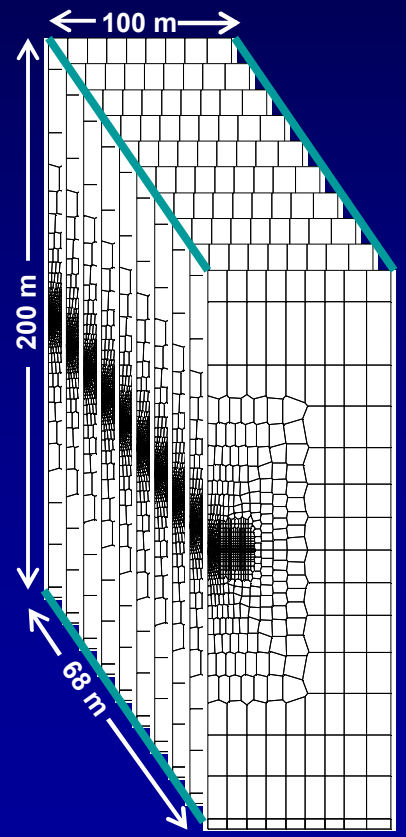
18,714 connections

Field-scale test

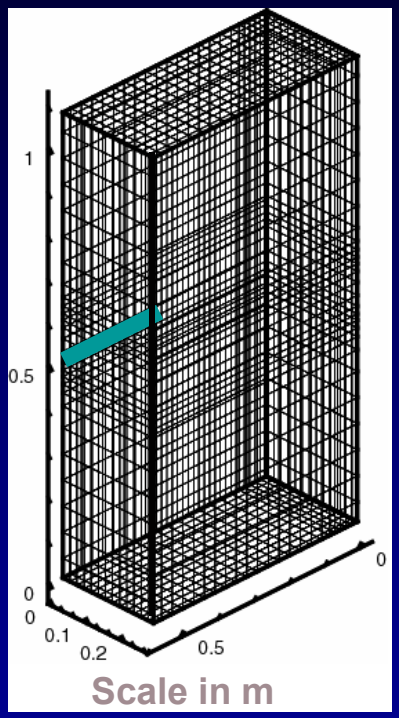
Unstructured grid

1,123 nodes per drift plane; 1,175 per rock plane

14 planes; 16,086 nodes; 51,248 connections



Numerical Grids With Heat Source



Drift explicitly included in model as a porous medium

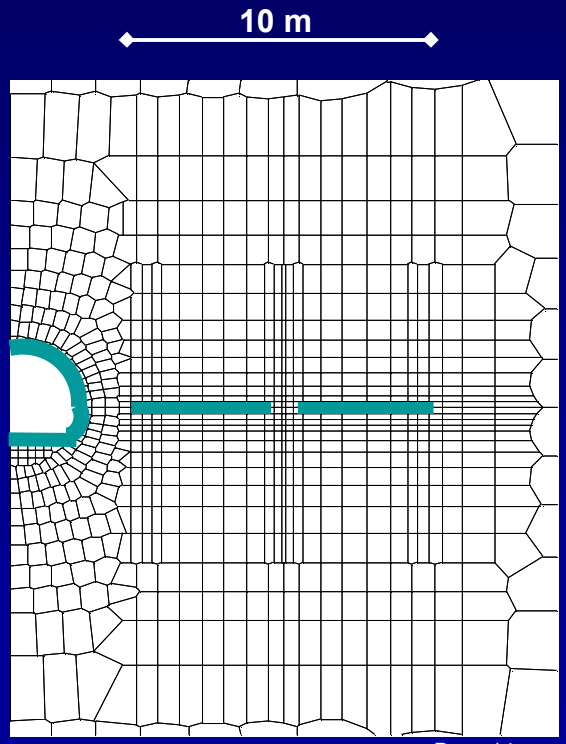
Physics of in-drift heat and mass transfer mechanisms not included

Heat sources continuous in drift

- canister heat applied to drift wall
- wing heaters represented by two planar heat sources

Drift not included in model

Drift wall set at atmospheric pressure



Property Values

Property	Laboratory Test	DST (Tptpmn)
Matrix permeability [m^2]	2.0×10^{-17}	4.07×10^{-18}
Matrix porosity [-]	0.5	0.11
Matrix van Genuchten α [Pa^{-1}]	6.36×10^{-7}	3.86×10^{-6}
Matrix van Genuchten m [-]	0.3717	0.291
Fracture permeability [m^2]	1.0×10^{-10}	2.76×10^{-13}
Fracture porosity [-]	0.01	0.01
Fracture van Genuchten α [Pa^{-1}]	1.00×10^{-3}	5.16×10^{-4}
Fracture van Genuchten m [-]	0.800	0.608
Thermal conductivity (dry) [W/m-K]	0.50	1.56
Thermal conductivity (wet) [W/m-K]	1.00	2.33
Area modifier A_{mod} [-]	1.0	1.0
Active fracture model γ [-]	0.4	0.41
Initial saturation [-]	0.3	0.82

Laboratory-Scale Ambient Model Analyses

Parameter Varied During the Laboratory-Scale Experiment Ambient Sensitivity Analyses	
Parameter Varied	**Parameter Values**
Matrix permeability, k_{mat}	± 10 times, +100 times
Block size (m)	0.2, 0.5, 1, 2, 5, 10
Infiltration (mm/yr)	0.3, 1, 3, 10

Laboratory-Scale Thermohydrological Model Analyses

Parameters Varied During the Laboratory-Scale Experiment Heating Phase Sensitivity Analyses	
Parameter Varied	**Parameter Values**
Matrix permeability, k_{mat}	± 10 times
Fracture permeability, k_{frac}	± 10 times, ± 100 times
Fracture van Genuchten α	1.0×10^{-5}, 1.0×10^{-4}, 1.0×10^{-3}
Area modifier, A_{mod}	0.1, 0.01, 0.001
Fracture-to-matrix relative permeability reduction, η	0.1, 0.01, 0.001
Active fracture model γ	0.2, 0.4, 0.6, 0.8

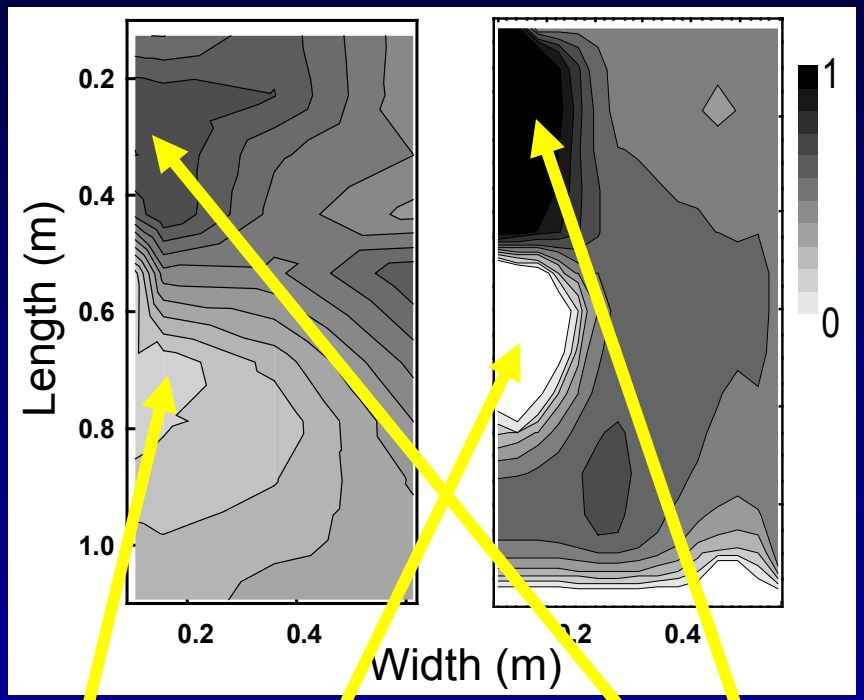
Laboratory-Scale Thermohydrological Model Analyses

Parameters Varied During the Field-Scale Experiment Heating Phase Sensitivity Analyses

Parameter varied	Parameter values
Matrix permeability	+10x
Fracture permeability, infiltration	k/100 at 0.3 mm/yr, k/10 at 1.0 mm/yr
Fracture van Genuchten α	+10x, -10x
Thermal conductivity	-20%
Drift wall heat load	-10%, -20%, -30%
Fracture-to-matrix relative permeability reduction, η	0.1, 0.01, 0.001
Fracture relative permeability	0.1, 0.01, 0.001
Active fracture model γ	0.2, 0.4, 0.6, 0.8

Lab-Scale Post-Test Matrix Saturation Measured versus Simulated

Measured **Simulated**



Low Saturation

High Saturation

Good agreement with test results:

Most important:

Reduced k_{mat} & large van Genuchten α

Least important:

Option 2: $A_{mod} < 1.0$

Poor agreement with test results using:

Option 1: $k_{rl,f} \rightarrow m = \eta k_{rl,f}$

Option 3: Active Fracture Model

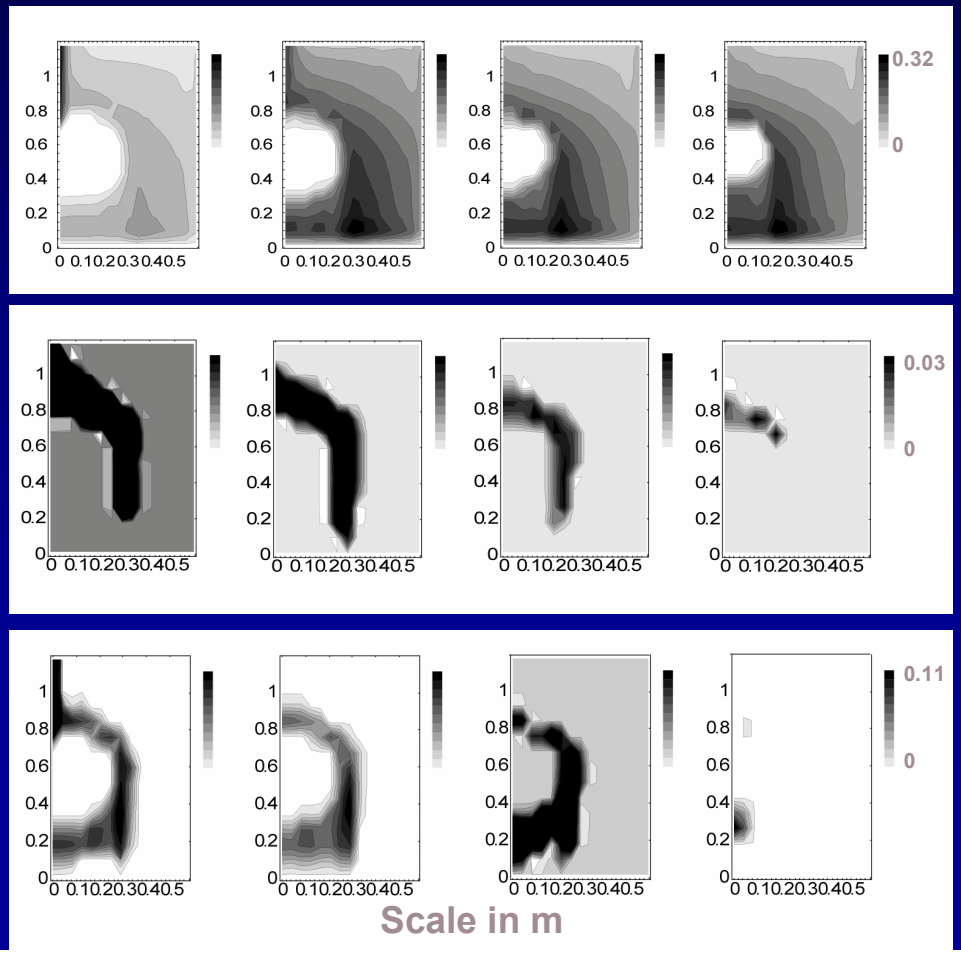
Alternative Models of Simulated Fracture Saturation in Laboratory-Scale Test

Test cell center ⟷ Test cell edge

Matrix-fracture interfacial area decreased using A_{mod} = 0.01

No active-fracture model and fracture permeability increased by 100x

Matrix-fracture interfacial area decreased using active-fracture model with γ_o = 0.6



Laboratory-Scale Heater Test Simulated Fracture Saturation

Good agreement with test results:

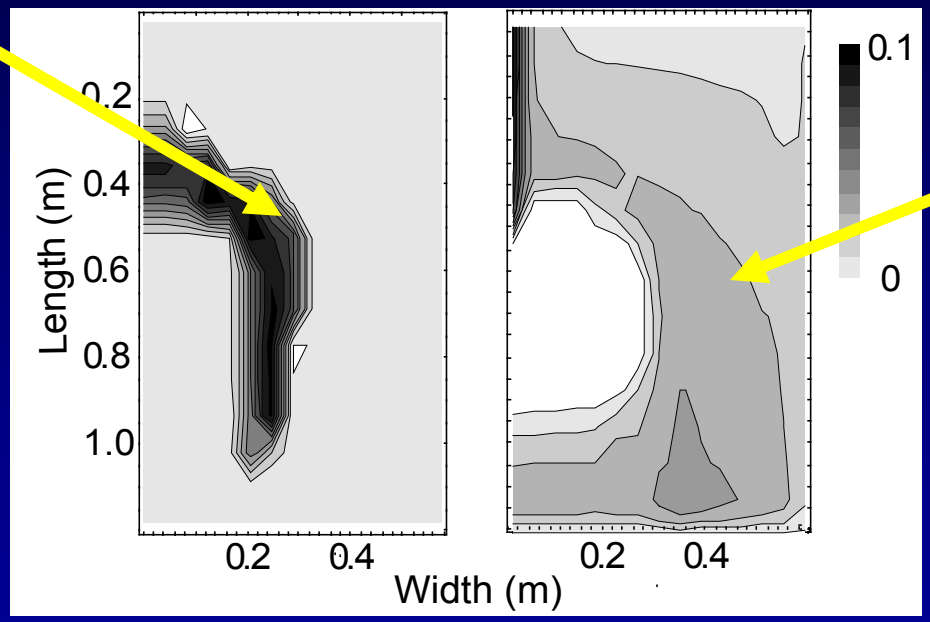
Most important: Small van Genuchten α or large k_f

Option 1
$k_{rl,f} \rightarrow m = \eta k_{rl,f}$

Option 3
Active Fracture Model

Focused Fracture Flow, Simulated

Diffuse Fracture Flow, Simulated

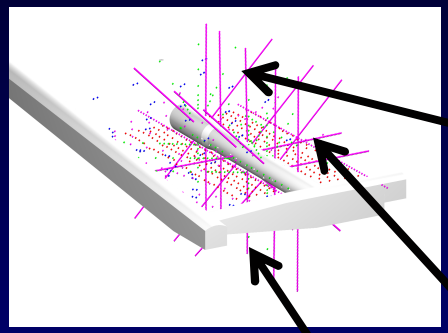


Poor agreement with test results:

Option 2
$A_{mod} < 1.0$
(Severe smearing)

Focused flow in fractures was indicated by staining on fracture surfaces when blocks were disassembled at end of test. Dripping into the drift (i.e., penetration of the boiling isotherm) was also observed

Predicted versus Observed Temperature Histories Basecase

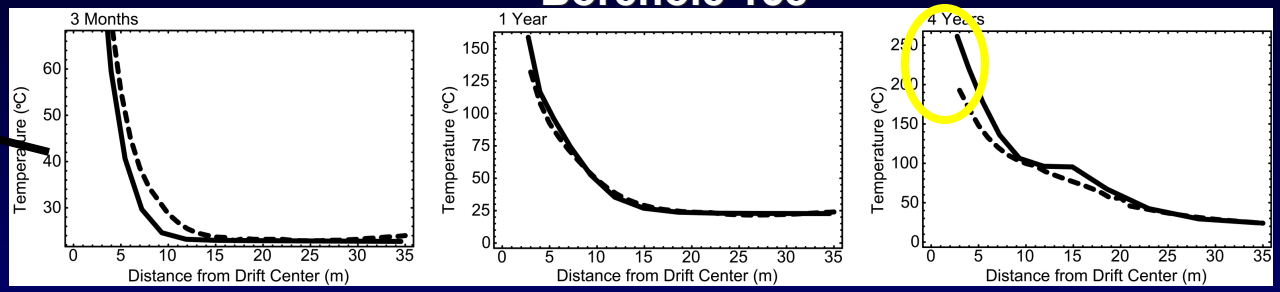


Observed -----

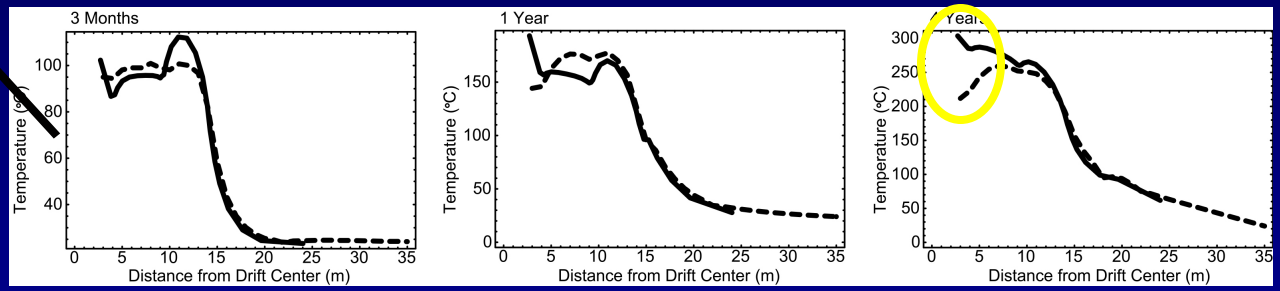
Predicted ___

Greatly over-predicts temperature, especially at later times

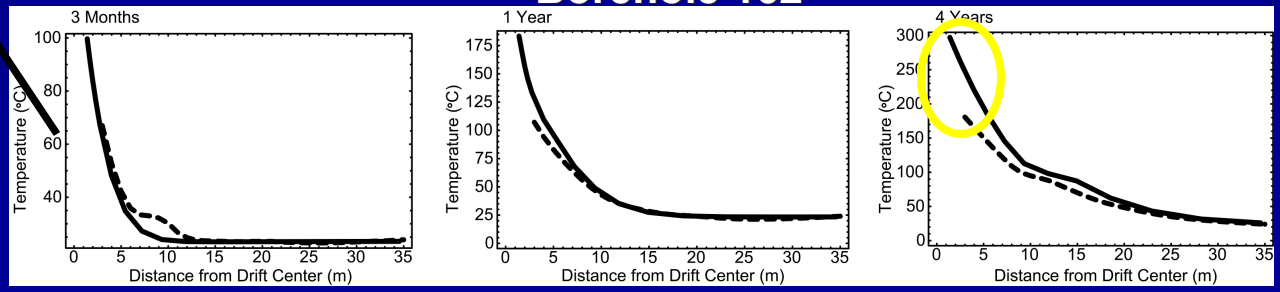
Borehole 158



Borehole 160

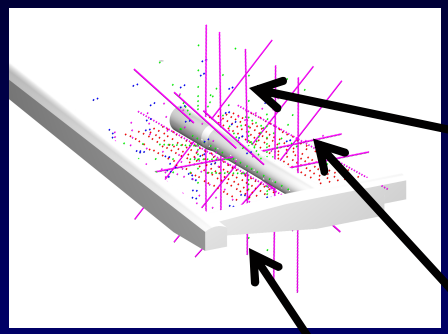


Borehole 162



3 months | 1 year | 4 years

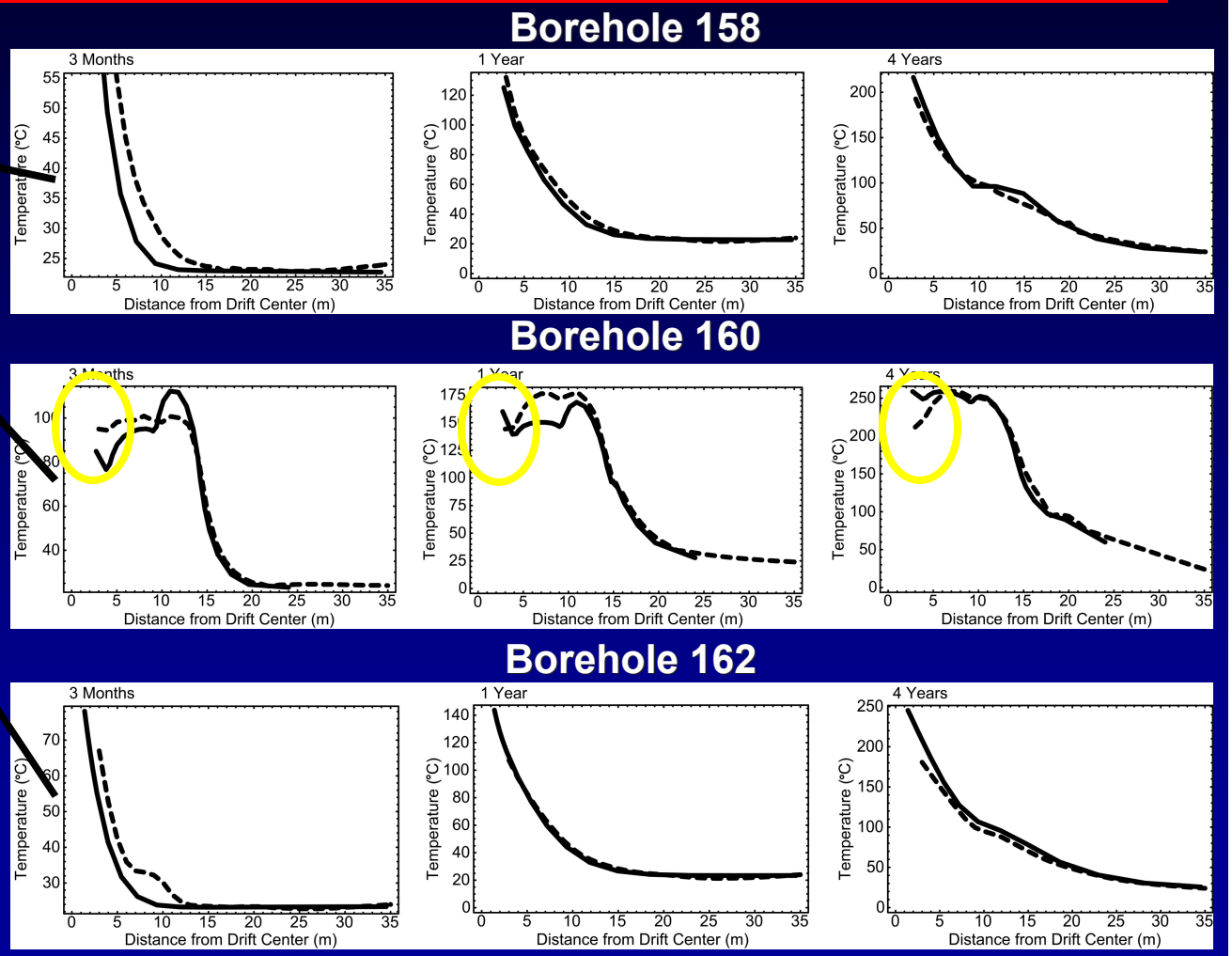
Predicted versus Observed Temperature 30% Reduction in Drift Wall Heat Load



Observed -----

Predicted ___

These results indicate time-variable heat loss by radiation and conduction through the thermal bulkhead



3 months 1 year 4 years

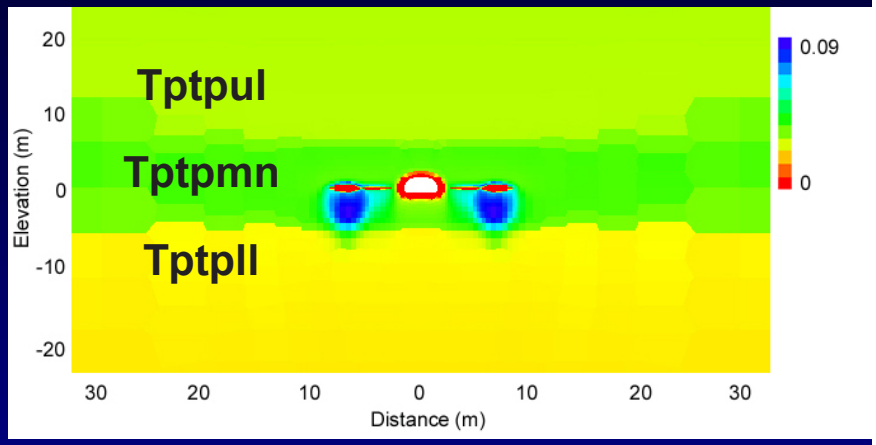
Drift-Scale Heater Test
Simulated Fracture Saturation

Selection of property values can have important effects on long-term repository simulations

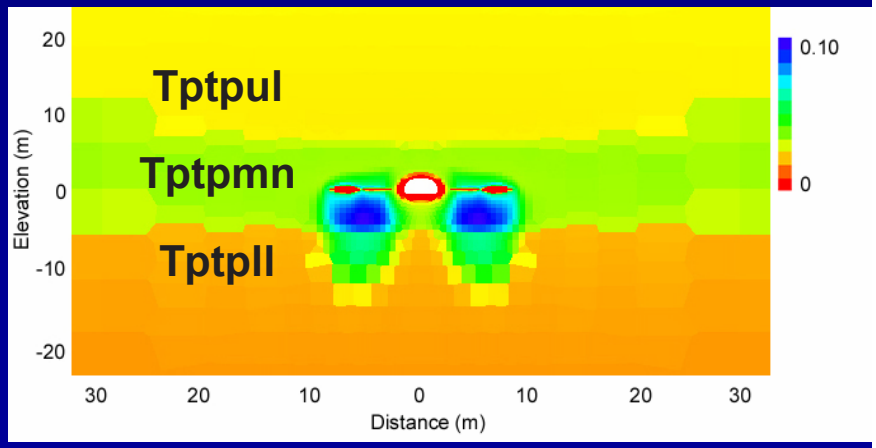
For example, increased fracture saturation (i.e., past the Tptpmn-Tptpll interface) is predicted when:

- High k_{mat},
- Active fracture model with γ=0.41,
- Low thermal conductivity, or
- Reduced van Genuchten α

Fracture saturation at 3 months



Basecase



Conclusions

- Results from two heater tests, one at lab scale and one at field scale, were used to evaluate MULTIFLO simulations of thermohydrological processes expected at the potential HLW repository

- Matrix permeability, fracture permeability & van Genuchten α, and matrix/fracture interaction model varied in simulations

- Temperature, matrix saturation, and fracture flow were compared

- Choice of matrix/fracture interaction model was of secondary importance to property value assignment, but that the reduction in interfacial area (i.e., A_{mod}) performed worse than the three options

- Simulations of DST indicate that ~30% of the canister heat was removed by conduction/radiation through the thermal bulkhead, but that the heat loss varied with time

Thermohydrological Model Uncertainty Reduction Using Physical Analog Models

This paper was prepared to document work performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA) and its contractors for the U.S. Nuclear Regulatory Commission (NRC) under Contract No. NRC–02–02–012. The activities reported here were performed on behalf of the NRC Office of Nuclear Material Safety and Safeguards, Division of High Level Waste Repository Safety. This paper is an independent product of the CNWRA and does not necessarily reflect the view or regulatory position of the NRC.

<u>Conversions</u>

1 m = 3.2 ft

10,000 Pa = 1 bar

9.87E-13 m^2 = 1 darcy

25.4 mm/yr = 1 in/yr

1 W/m-K = 0.5778 Btu/(ft-h-F)

deg C = (deg F - 32)/1.8