

THM Model Validation: Integrated Assessment of Measured and Predicted Behavior

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THM Model Validation: Integrated Assessment of Measured and Predicted Behavior

**Stephen C. Blair, Steven R. Carlson, Jeff Wagoner,
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This paper presents results of coupled thermal-hydrological-mechanical (THM) simulations of two field-scale tests that are part of the thermal testing program being conducted by the Yucca Mountain Site Characterization Project. The two tests analyzed are the Drift-Scale Test (DST) which is sited in an alcove of the Exploratory Studies Facility at Yucca Mountain, Nevada, and the Large Block Test (LBT) which is sited at Fran Ridge, near Yucca Mountain, Nevada. Both of these tests were designed to investigate coupled thermal-mechanical-hydrological-chemical (TMHC) behavior in a fractured, densely welded ash-flow tuff.

The geomechanical response of the rock mass forming the DST and the LBT is analyzed using a coupled THM model. A coupled model for analysis of the DST and LBT has been formulated by linking the 3DEC distinct element code for thermal-mechanical analysis and the NUFT finite element code for thermal-hydrologic analysis. The TH model (NUFT) computes temperatures at preselected times using a model that extends from the surface to the water table. The temperatures computed by NUFT are input to 3DEC, which then computes stresses and deformations. The distinct element method was chosen to permit the inclusion of discrete fractures and explicit modeling of fracture deformations. Shear deformations and normal mode opening of fractures are expected to increase fracture permeability and thereby alter thermal-hydrologic behavior in these tests. We have collected fracture data for both the DST and the LBT and have used these data in the formulation of the model of the test. This paper presents a brief discussion of the model formulation, along with comparison of simulated and observed deformations at selected locations within the tests.

Drift-Scale Test

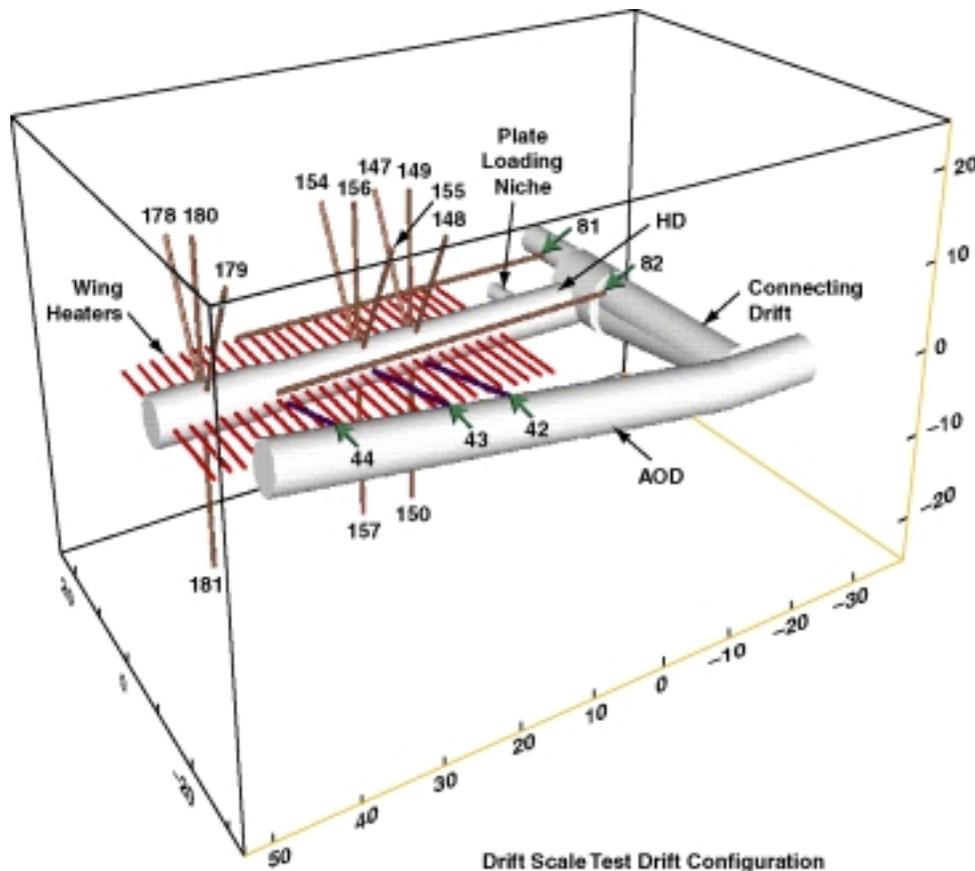
Test Description and Model Development

The drift-scale heater test, the DST, is being conducted in an alcove of the Exploratory Studies Facility (ESF) at Yucca Mountain, Nevada. The DST is a large-scale, long-term thermal test designed to investigate coupled thermal-mechanical-hydrological-chemical behavior in a fractured, welded tuff rock mass.

The general layout of the DST is shown in Figure 1. The heated drift (HD) is a 5-m-diameter drift approximately 60 m long. Access to the HD from the ESF is gained through the Access Observation Drift (AOD) and a connecting drift. Heat is being supplied to the rock mass forming the DST via nine electric canister heaters located in the HD, and wing heaters placed in 50 boreholes oriented perpendicular to the HD. These wing heater holes are spaced at 2-m intervals along each rib of the HD. The wing heaters extend into the rock approximately 11 m from the rib. Together, these heaters are providing approximately 180 kW of power to heat an approximately planar region of rock that is approximately 50 m long and 27 m wide. The test plan (CRWMS M&O 1997) calls for 4 years of heating followed by a 4-year cool-down period.

The heating portion of the DST was started in December 1997, and the target drift wall temperature of 200°C was reached in summer 2000. Deformation of the rock mass is being monitored with an array of multiple-point borehole extensometer (MPBX) systems. Locations of the MPBX holes are shown in Figure 1. These boreholes represent only a small fraction of the boreholes drilled into the DST for emplacement of various types of instrumentation that enable temperature, geophysical, hydrological, and chemical measurements.

The THM model for the DST incorporates the actual geometry of excavations forming the DST. The model was run in two different modes; a “basecase” model that included fractures, and a simple “continuum” model. For the continuum case, no fractures were included and 3DEC was used to simulate the DST as one large, uniform isotropic block of rock. Fractures included in the basecase model are derived from a data set of fractures mapped in the DST block. Temperatures are from TH simulations of the DST. The drift dimensions and the sensor and borehole locations were taken from CRWMS M&O 1998. Specifics of the model formulation are discussed below. DTN information for temperatures, MPBX data, fractures, and other information is listed in Table 1. The input and output files for the Drift-Scale Test model validation simulations have been submitted to the TDMS (DTN: LL010700123123.013).



Source: Borehole locations are from *Drift-Scale Test As-Built Report* (CRWMS M&O 1998).

Figure 1. Layout of the Drift-Scale Test. Numbered boreholes are those containing MPBX instrumentation.

Table 1. DTNs for Model Validation

Description	Start Date	End Date	Data Tracking Number
Large Block Test Data			
Fracture Sets	02/97	02/98	LL981004604243.024
Temperatures	02/97	09/98	LL980918904244.074
MPBX Displacements	02/97	09/98	LL980919404244.076
	02/97	02/98	LL981004604243.024
Single Heater Test Data			
Temperatures	08/96	11/97	SNF35110695001.008
	12/97	01/98	SNF35110695001.009
MPBX Displacements	08/96	11/97	SNF35110695001.008
	12/97	01/98	SNF35110695001.009
Drift-Scale Test Data			
Temperatures	01/97	03/98	LL981105604243.025
	12/97	02/98	LL980601704244.062
	11/97	05/98	MO9807DSTSET01.000
	06/98	08/98	MO9810DSTSET02.000
	09/98	05/99	MO9906DSTSET03.000
	06/99	10/99	MO0001SEPDSTPC.000
	11/99	05/00	MO0007SEPDSTPC.001
Smoothed MPBX Displacements	12/97	07/00	SN0106F3912298.028
Fracture Data	NA	04/00	LL000116204243.035

Temperatures. Temperature inputs for the model validation simulations were taken from the NUFT simulations of the DST described in the *Thermal Tests Thermal-Hydrological Analyses/Model Report* (CRWMS M&O 2000, Section 6.2.3, p. 63). Temperatures from these simulations were regridded using the EarthVision program as follows. A three-dimensional temperature field for the region simulated by the large-scale mechanical model was produced from the two-dimensional NUFT temperature field in two steps: the NUFT temperature field was first reflected across a vertical plane through the center of the drift, then the temperatures were repeatedly replicated in the direction along the drift axis to form a 3D array.

Temperatures from the LDTH model and their coordinates were input into EarthVision along with an array of gridpoints generated by 3DEC for both the inner and outer regions at each calculation time. EarthVision performed a three-dimensional interpolation of the 3D LDTH model temperatures to provide an interpolated temperature for each calculation time at each of the 3DEC model gridpoints. The gridpoint temperatures were then input into 3DEC as a separate input file for each calculation time.

Temperatures were input at times of 1, 5, 10, 20, 30, 40, 60, 100, 180, 365, and 545 days after the start of heating. These times were selected to capture the initial thermal response of the rock to heating as well as the longer-term steady evolution of the temperature field. Figure 2 shows perspective plots of the temperature field at times selected for simulations.

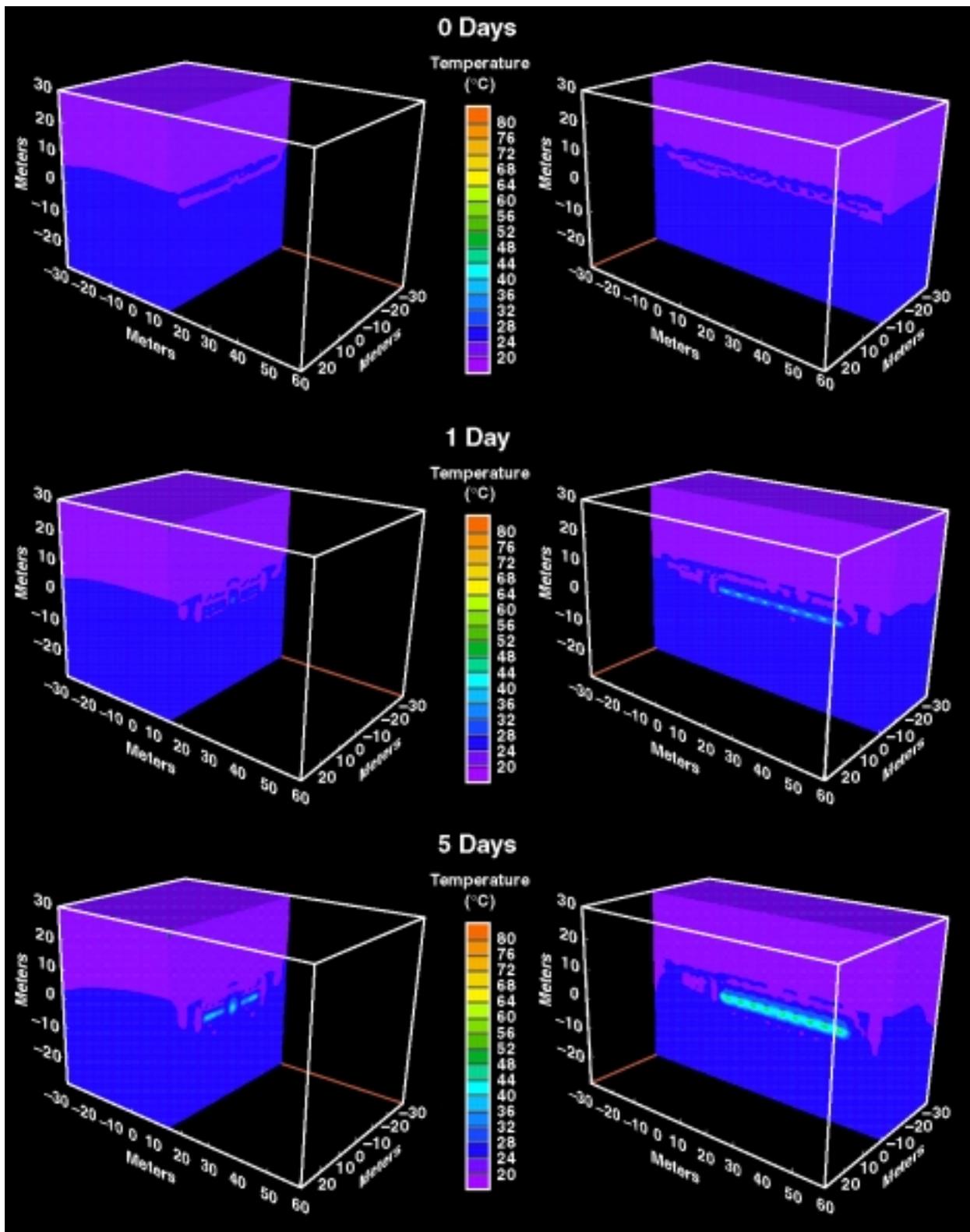


Figure 2. Perspective Plots of the Temperature Field at Times Selected for Simulations.

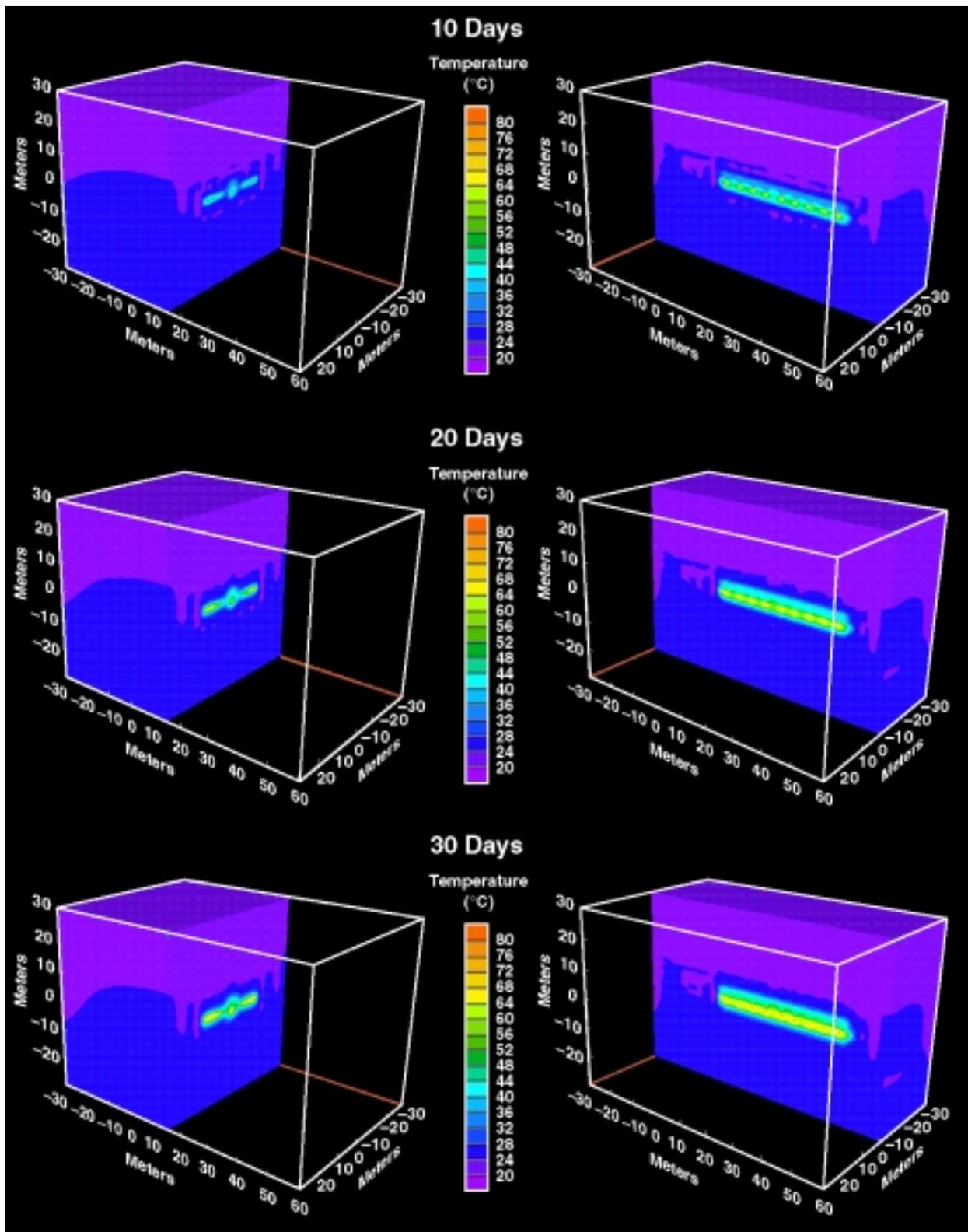


Figure 2 (Continued).

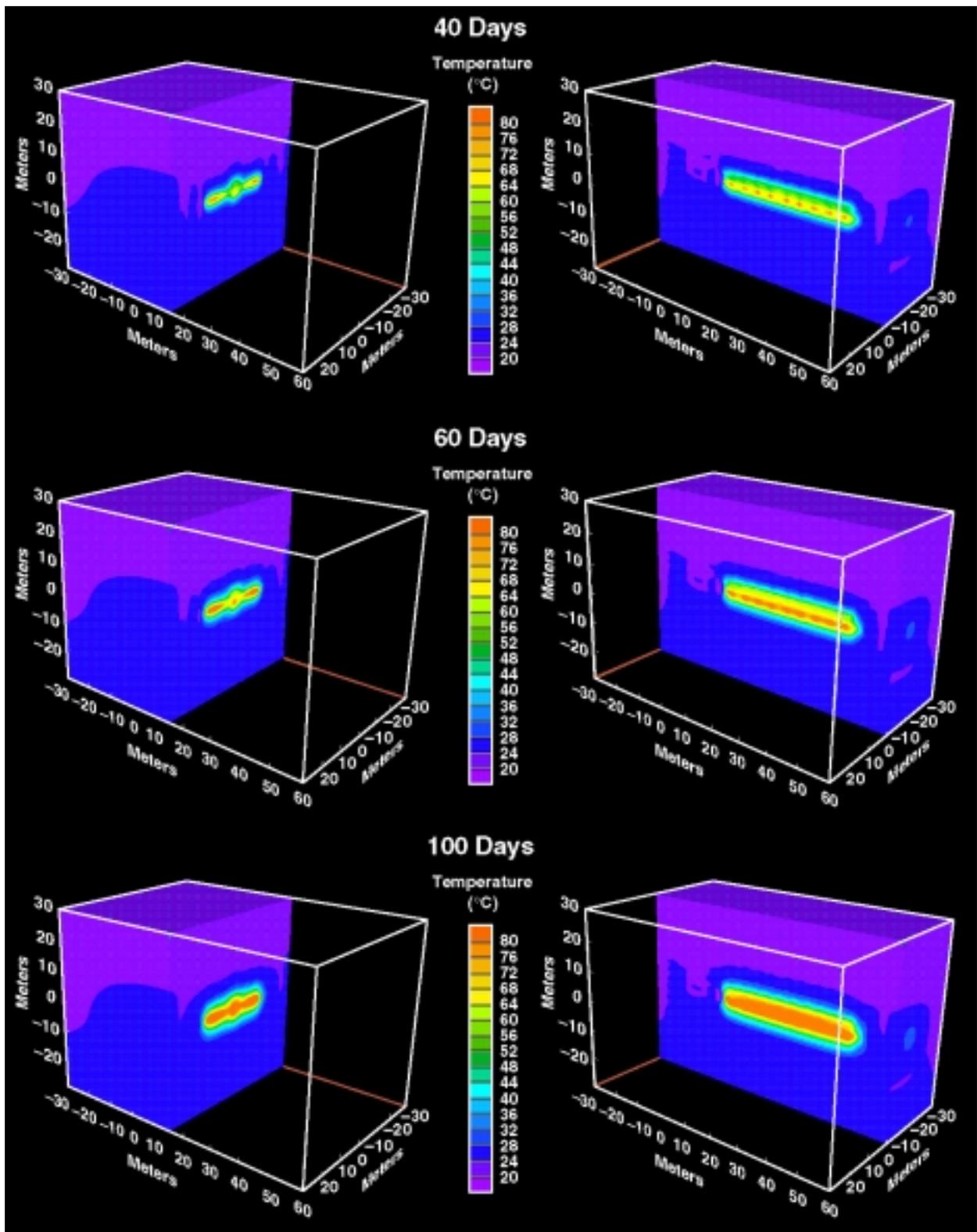


Figure 2 (Continued).

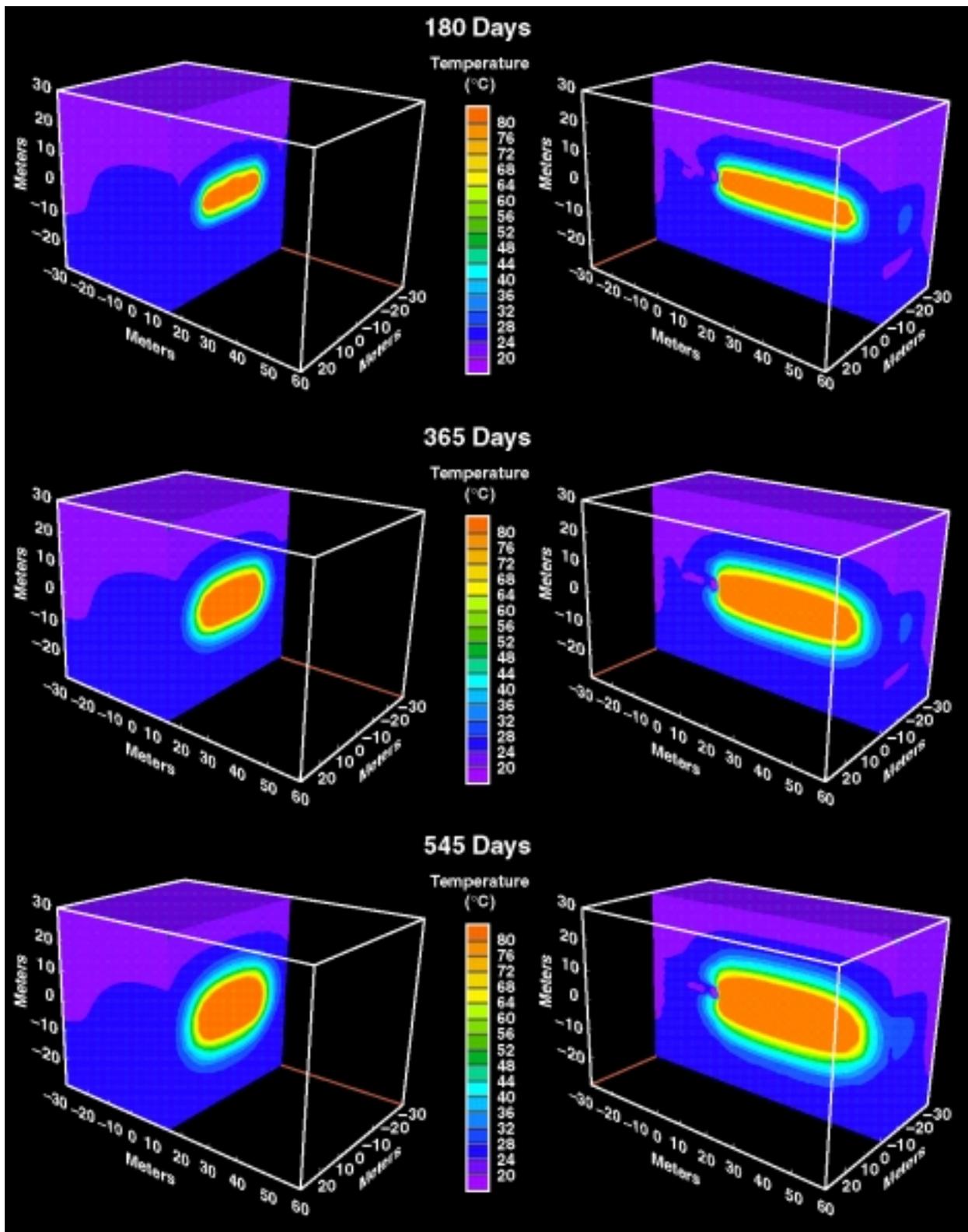


Figure 2 (Continued).

Fractures. Data on fractures in the rock mass forming the DST were obtained by analyzing video logs for approximately 30 of the boreholes drilled into the DST (DTN: LL000116204243.035). Individual fractures were identified from the logs and their locations and orientations were noted. Each fracture was assigned a qualitative designation of minor, moderate, or major. Major fractures were identified as those having significant aperture, secondary mineralization, alteration haloes, and local evidence of displacement. Fracture zones are also considered to be “major” fractures. The fractures used are listed in Table 2 and the spatial locations and orientations of the major fractures used in this study are shown in Figure 3. The figure shows a higher density of fractures in the region approximately 20 m from the bulkhead of the HD and between the HD and the AOD. The DTN for the fracture data is listed in Table 1.

Table 2. Fractures Listed by XYZ Location, Taken from DTN: LL000116204243.035

Fracture No.	Dip Direction (°)	Dip Angle (°)	X coordinate (m)	Y coordinate (m)	Z coordinate (m)
1	199	75	-21.40	-8.26	4.11
2	86	83	-12.86	-10.11	-3.93
3	122	61	-13.52	-9.70	-1.38
4	28	13	-4.91	-8.32	5.57
5	51	6	-1.87	-6.60	6.35
6	9	31	-25.79	-8.20	1.57
7	21	62	-9.70	-6.54	5.51
8	20	84	-3.32	-8.33	5.71
9	22	68	-1.57	-8.28	16.26
10	20	82	-3.59	-6.59	6.17
11	20	84	-15.50	-8.28	4.63
12	124	81	-22.44	-8.17	0.58
13	100	88	-16.81	-8.13	-1.08

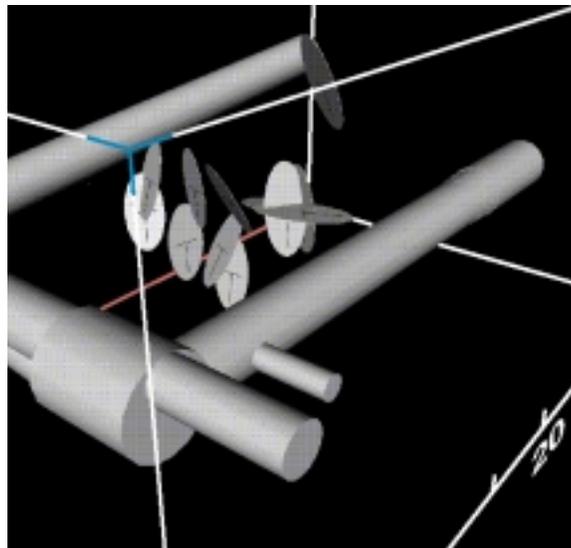


Figure 3. Spatial Locations and Orientations of the Major Fractures Used in the Basecase Analysis.

Model Geometry. The geometry of the simulation is as follows. Excavations representing the AOD, Cross Drift, Heated Drift, and Plate Loading Niche were excavated from a simulated block of rock with dimensions 110 m × 55 m × 50 m. Then fractures listed in Table 2 were introduced. These fractures are allowed to extend to the edges of the model domain. The model domain with fractures included is shown in Figure 4. Excavations are shown in Figure 5.

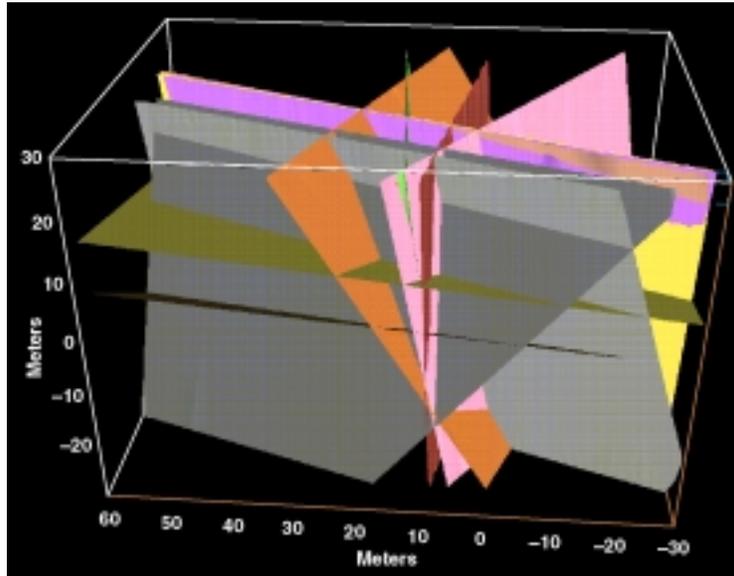


Figure 4. Model Domain with Fractures Included, Used for Basecase Simulation.

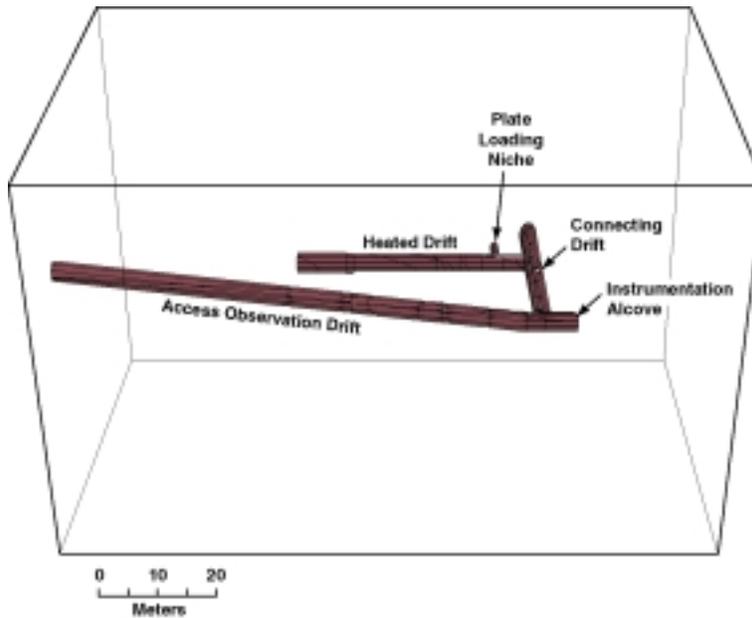


Figure 5. Excavations of Drifts and Niches Associated with the DST from the Model Domain.

Boundary Conditions. Boundary conditions were applied to the simulated rock mass as follows. The base of the model was considered to be a roller boundary so that no vertical displacement was allowed. However, horizontal displacements were allowed.

The vertical sides and top of the rock mass were considered stress boundaries, and an in situ stress condition was applied with a vertical stress of 9.7 MPa and a horizontal stress of 4.85 MPa (Schelling 1989). Stress gradients were 0.023 MPa per meter of depth for vertical stresses and 0.0115 MPa per meter of depth for horizontal stresses. The stress boundary is considered appropriate as rock surrounding the DST is at ambient conditions.

Rock Properties. Both the DST and LBT are sited in the middle nonlithophysal unit of the Topopah Spring Tuff. Input parameters for the TM emplacement drift base case are provided in Table 3 and are the same as those used for the emplacement drift analysis presented in CRWMS M&O 2001. Calculated or assumed parameters are listed in Table 4. Bulk and shear modulus can be calculated from the elastic modulus (E) and Poisson's ratio (ν) as

$$K = E/(3(1 - (2\nu))) \quad \text{and} \quad G = E/(2(1 + \nu))$$

(Jaeger and Cook 1979), and values are given in Table 4. The input values for joint normal stiffness and joint shear stiffness assume a joint spacing of 1 m and were calculated with a relationship given in the 3DEC User's Guide (Itasca 1998, Section 3, p. 94). The joint normal stiffness calculation used an intact rock elastic modulus of 33.03 GPa (DTN: MO9911SEPGRP34.000, Table 8) and a rock mass elastic modulus of 24.71 GPa (DTN: MO9911SEPGRP34.000, Table 10). Shear moduli for the joint shear stiffness calculation were obtained from the above elastic moduli and a Poisson's ratio of 0.21 (DTN: MO9911SEPGRP34.000, Table 11). The other input parameter values were taken directly from the Technical Data Management System. The input parameters are considered appropriate because they are derived from field and laboratory measurements of the host rock physical properties, or are based on EDA II design parameters.

Table 3. Input Parameters and Data Tracking Numbers

Item No.	Description	Value	Units	Data Tracking Number
Matrix Properties				
1	Dry Bulk Density	2270	kg/m ³	MO0003SEPDRDDA.000
2	Intact Rock Elasticity Modulus	33.03	GPa	MO9911SEPGRP34.000
3	Rock Mass Elasticity Modulus	24.71	GPa	MO9911SEPGRP34.000
4	Poisson's Ratio	0.21	none	MO9911SEPGRP34.000
Joint Properties				
5	Joint Friction	41	deg	MO0010RDDAAMRR.002
6	Joint Cohesion	0.09	MPa	MO9911SEPGRP34.000
Thermal Properties				
7	Thermal Conductivity	2.33	W/m-K	MO9911SEPGRP34.000
8	Thermal Expansion Coefficient	9.73E-6	deg C ⁻¹	SNL22100196001.001
Input Temperatures				
9	Input Temperatures	various	deg C	LL000114004242.090

Table 4. Calculated or Assumed Model Parameters

Description	Value	Units
Matrix Properties		
Rock Mass Bulk Modulus	14.2	GPa
Rock Mass Shear Modulus	10.2	GPa
Joint Properties		
Joint Tensile Strength	0	MPa
Joint Normal Stiffness	98.1	MPa/mm
Joint Shear Stiffness	40.5	MPa/mm
Joint Dilatation Angle	29	deg
Initial Joint Aperture	0.098	mm
Boundary and In Situ Stresses		
In Situ Stress (280 m depth)	5.54	MPa
Vertical Stress Gradient	0.021	MPa/m

Results for Drift-Scale Test

This section presents results of the model predictions of displacement for MPBX systems used in the DST, and compares the predicted displacements with those observed during the first 545 days of heating in the DST. For this analysis, comparisons are made for MPBX data collected for 10 of the 17 MPBX holes in the DST. The holes and anchors used are listed in Table 5.

Moreover, in the Qualitative Results discussion below, model predictions at a series of times are compared with observations. This is done for the deepest anchor in the MPBX holes listed in Table 5. The deepest anchor was chosen as it best represents the rock mass behavior. Note that for boreholes 42 and 43 anchor 1 is the deepest, while for the remainder of the holes anchor 6 is the deepest, i.e., farthest from the borehole collar.

Table 5. List of MPBX Anchors Simulated for DST

Hole	Anchor No.					
	1	2	3	4	5	6
42	1	2	3	4	5	6
43	1	2	3	4	5	6
81	1	2	3	4	5	6
82	1	2	3	4	5	6
147	1	2	3	4		
148	1	2	3	4		
149			3	4		
150		2		4		
156				4		
180				4		

Qualitative Results. Simulation of Mine-by—Prior to the excavation of the HD three boreholes were drilled from the AOD perpendicular to the planned location of the HD. These boreholes (42, 43, and 44) were instrumented with MPBX systems and deformations were recorded during the excavation of the HD. The borehole response due to the excavation was simulated using the DSDE model, and can be used to calibrate the bulk and shear moduli of the rock mass in the simulation.

The excavation of the HD was simulated by excavating the entire length of the HD at one time. Thus the time history of the HD excavation was not simulated, but the effect of the excavation on the rock in boreholes 42 and 43 was determined. Borehole 44 was not used in this analysis as the data for this borehole were judged to be of poor quality.

The deformation of the deepest anchors in holes 42 and 43 was simulated and the resulting total deformation is listed for the simulation in Table 6 along with total deformation as measured by the MPBX systems. The total deformation is shown graphically for holes 42 and 43 in Figure 6. This figure shows that the prediction overestimates the observed deformation by 45% in borehole 42, and by 32% in borehole 43. Thus both estimates are within an order of magnitude of the observations.

Table 6. Deformation Due to Mine-by of HD

Borehole	Anchor 6 max (mm)	Predicted deformation (mm)
42	2.4	3.5
43	3.1	4.1

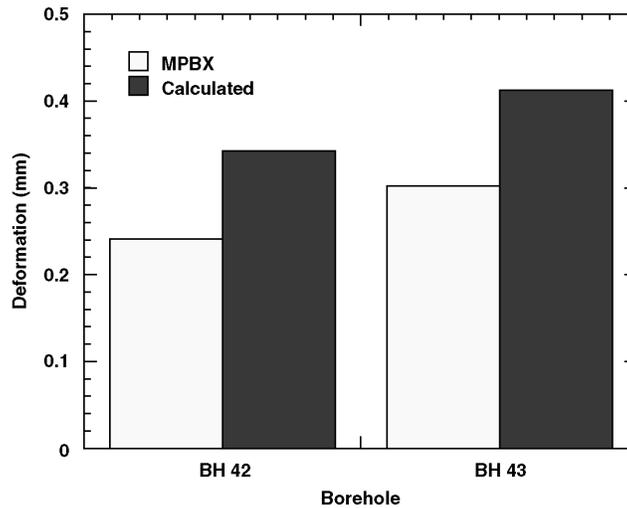


Figure 6. Total Deformation for Boreholes 42 and 43 During Mine-by, Prior to Heating.

Heating Phase of DST—

Boreholes 42 and 43: These boreholes extend from AOD toward the HD and were used for mine-by as discussed above. Observed and predicted deformations for these boreholes after heating started are shown in Figures 7 and 8. Figure 7 shows that for the first 250 days, the basecase model simulated deformation very well for Borehole 42. After 300 days, the observed deformation rate is higher than predicted, and the fit is not as good.

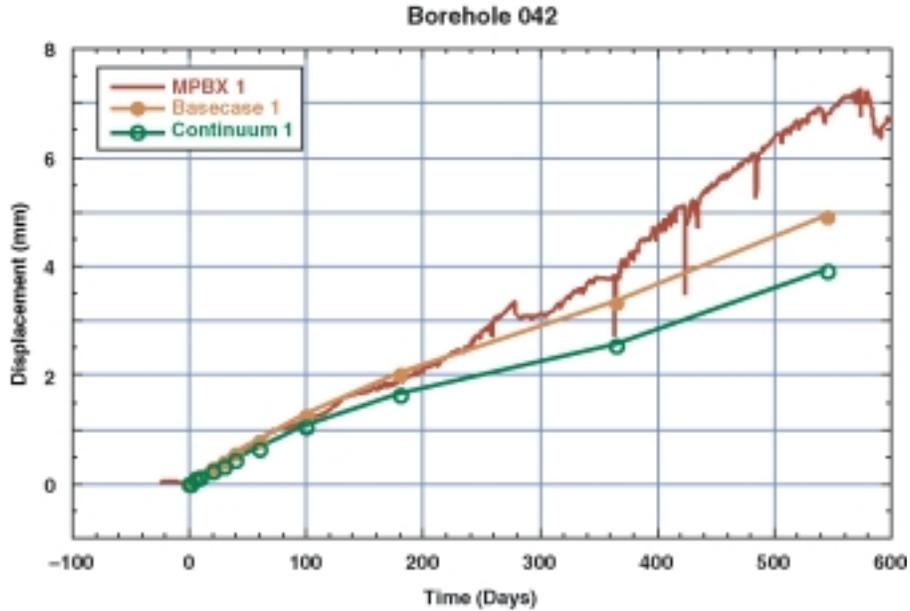


Figure 7. Observed and Predicted Deformation for BH 42.

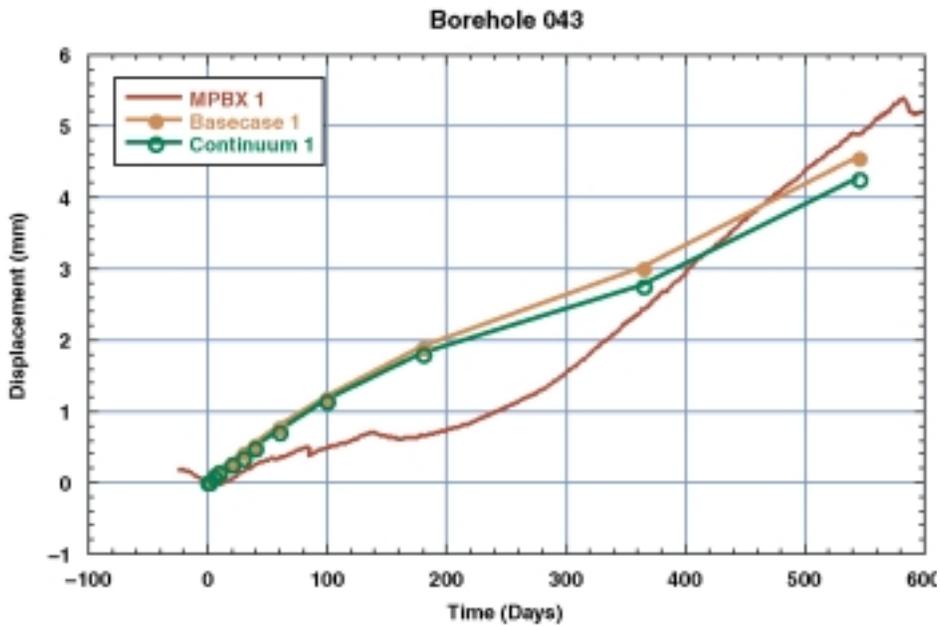


Figure 8. Observed and Predicted Deformation for BH 43.

At 240 days the basecase model matches the prediction to better than 10%, but at 545 days the basecase model predicts 70% of the observed value. The continuum model underpredicts the deformation throughout the 545-day period and, at 545 days, the value predicted by the continuum model is 57% of the observed value.

Observed and predicted behavior for BH 43 is shown in Figure 8. This hole is roughly parallel to BH 42 (see Figure 1) and, as expected, the predicted deformations are similar to those predicted for BH 42, with the basecase model predicting more deformation than the continuum model.

However, the observed deformation for BH 43 anchor 1 shows a much different trend than deformation observed for borehole 42, with a low rate of deformation for the first 200 days of heating. After 200 days, the deformation rate increases dramatically to slightly less than the 0.016 mm/day observed for BH 42 after approximately 300 days.

Boreholes 81 and 82: Figures 9 and 10 show results for boreholes 81 and 82. These boreholes are parallel to the HD, 3.4 m above the center of the wing heaters, and are collared in the connecting drift. These figures show that both the basecase and the continuum models substantially underpredict the observed deformation for Anchor 6 in each of these holes.

The data show very little movement for the first 20 days, followed by increasing deformation (expansion), with holes 81 and 82 showing 5 and 6 mm of expansion, respectively, by 545 days of heating. In contrast, the predictions show negative deformation (compression) for the first 80 days, followed by expansion, but the predicted rate of expansion is much slower than that observed.

The observations and model predictions follow the same general trend between 80 and 400 days, during which both observed and predicted displacements rise at a diminishing rate. After 400 days, the observed displacements rise at an increasing rate, a feature which is not matched by the model. The total predicted deformation of approximately 1 mm is a factor of 6 lower than the 6 mm observed.

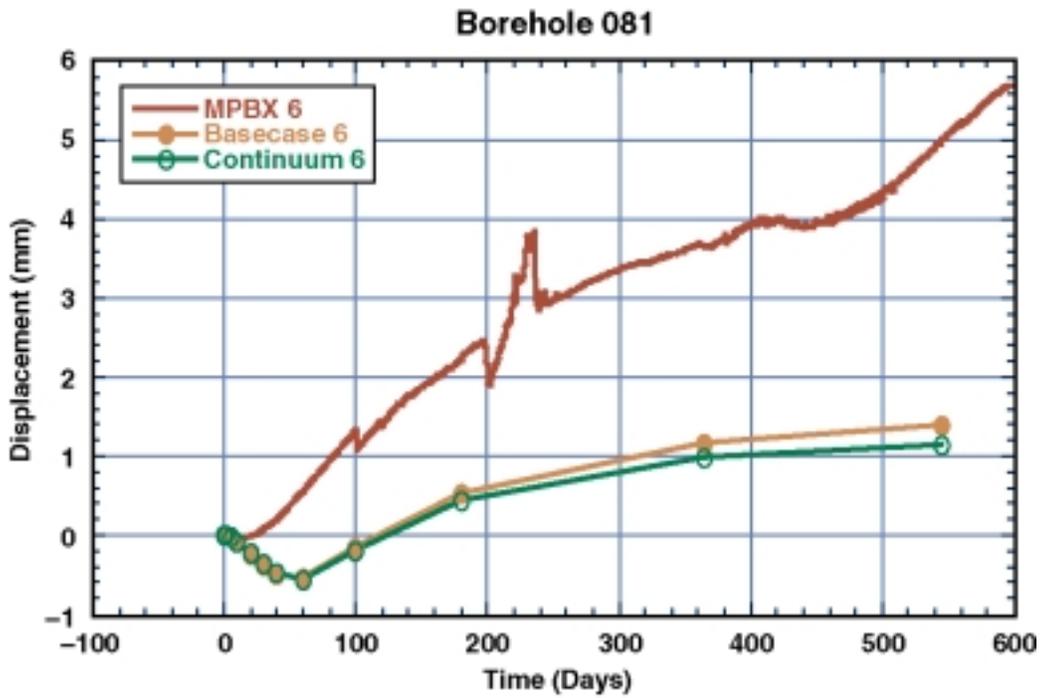


Figure 9. Observed and Predicted Deformation for BH 81.

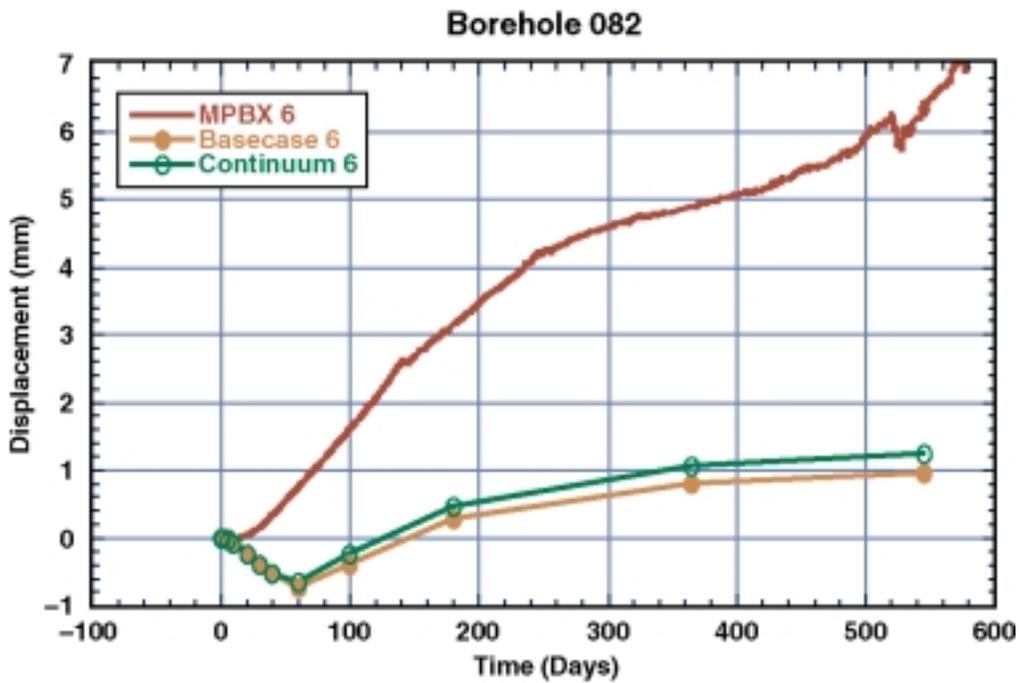


Figure 10. Observed and Predicted Deformation for BH 82.

Boreholes 147, 148, and 149: These boreholes are located in the crown of the HD, approximately 13 m from the bulkhead, and form along with BH 150 the first fan of three MPBX holes in the HD. The observed and predicted deformations for boreholes 147, 148, and 149 Anchor 4 are shown in Figures 11, 12, and 13.

Results for BH 147 (Figure 11) show that observed deformation begins immediately upon start of heating, while the predicted deformation doesn't begin until 40–50 days after heating. After 50 days the predicted slope is very similar to observation, and overall magnitude at 545 days is 5 mm for prediction vs. approximately 5.5 mm for observation. Thus the predicted value is 90% of the observed value. The basecase model predicts larger magnitude of deformation and starts somewhat sooner than the continuum model. Note that the sharp drops in deformation are interpreted to be associated with temperature changes in the borehole and not actual rock movements.

Predicted and observed deformations for BH 148 are shown in Figure 12. This hole is angled toward the AOD. This figure shows that the observed displacement increases much more quickly after the start of heating than does the predicted displacement, but the difference is not as great as observed in BH 147.

A change in slope occurs at approximately 20–30 days, after which the slope is linear until approximately 250 days, when the rate of displacement decreases somewhat. The simulated deformation shows a lag in initial response similar to that predicted for BH 147. After approximately 60 days the slope of the basecase model matches the observation very well, while the expansion rate for the continuum model is too high. At 400 days the basecase model matches the observed value almost exactly.

Predicted and observed deformations for BH 149 are shown in Figure 13. This figure shows that the basecase model predicts behavior very well. This hole is vertical in the crown (see Figure 1).

In initial behavior, the rock deforms during the first 10 days, while the predicted deformation does not start until after day 20. Agreement with data at 545 days is excellent, within 5%. The basecase model fits somewhat better than the continuum model

Examination of the three holes (147, 148, 149) as a group shows that deformation for BH 147 is greater than for BH 148 and 149. That is, at 400 days, boreholes 147, 148, and 149 show 4.4, 3.4, and 3.6 mm of displacement, respectively. This indicates that rock on the side away from the AOD is deforming more than the rock between the HD and the AOD. The basecase model predicts 3.6, 3.4, and 3.4 mm, respectively, while the continuum model predicts 3.4, 3.8, and 3.8 mm, respectively, for these boreholes at 400 days. Thus, the basecase model correctly predicts the trend of the measurement, as it indicates larger deformation for BH 147, and equal deformation for boreholes 148 and 149. The continuum model does not capture this behavior as well.

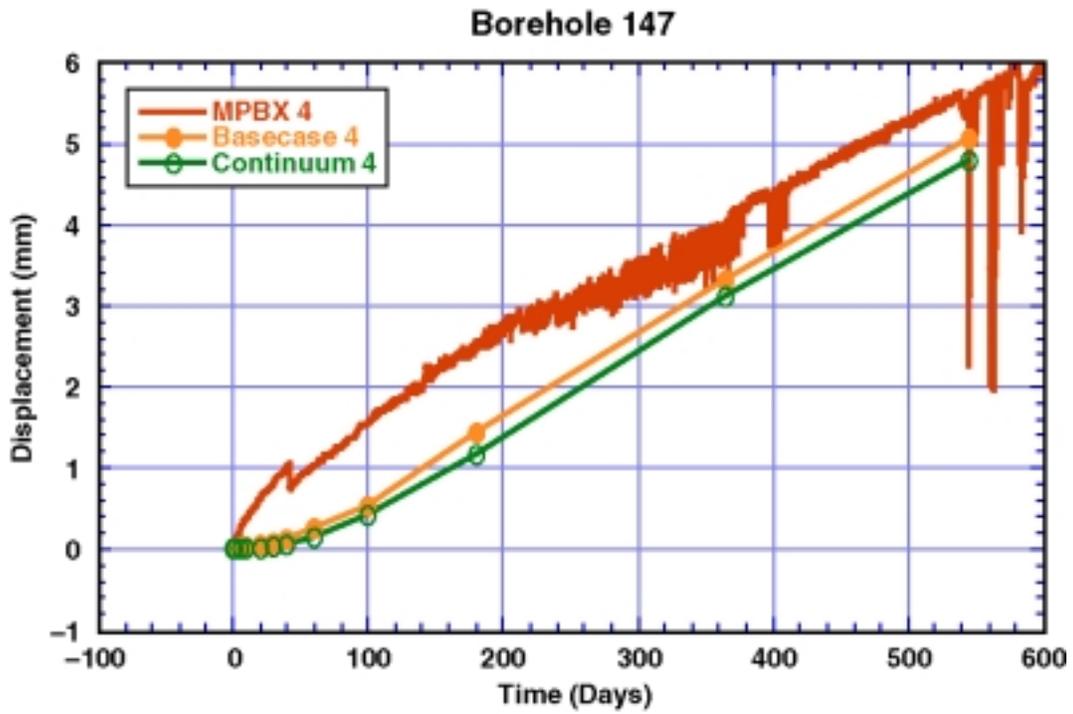


Figure 11. Observed and Predicted Deformation for BH 147.

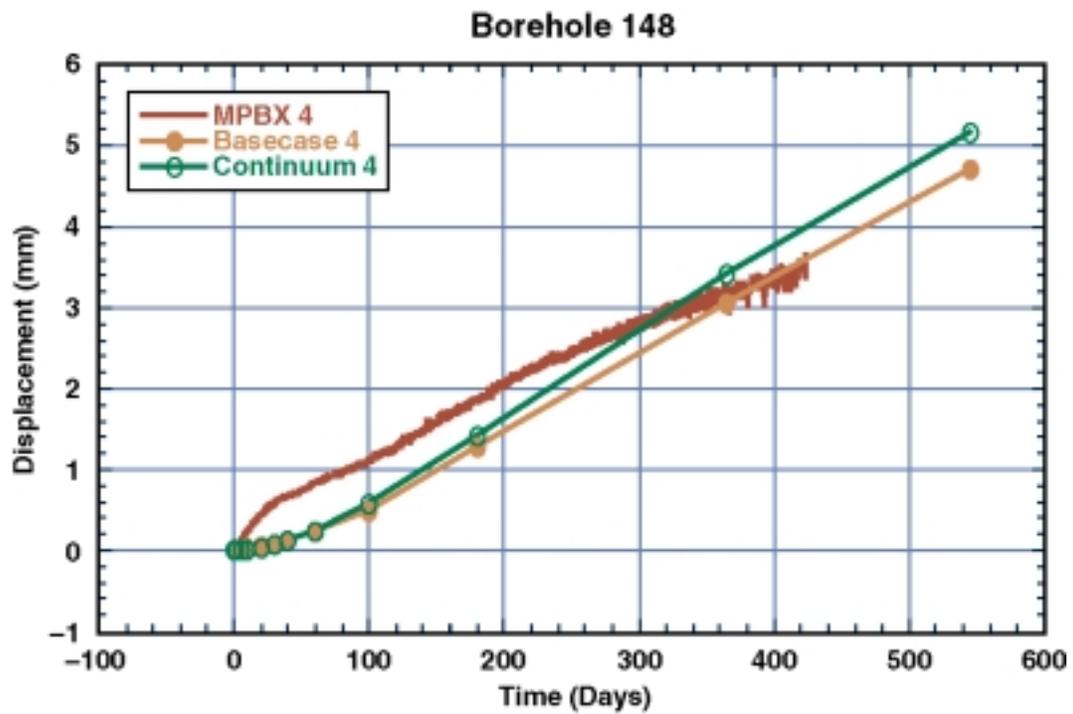


Figure 12. Observed and Predicted Deformation for BH 148.

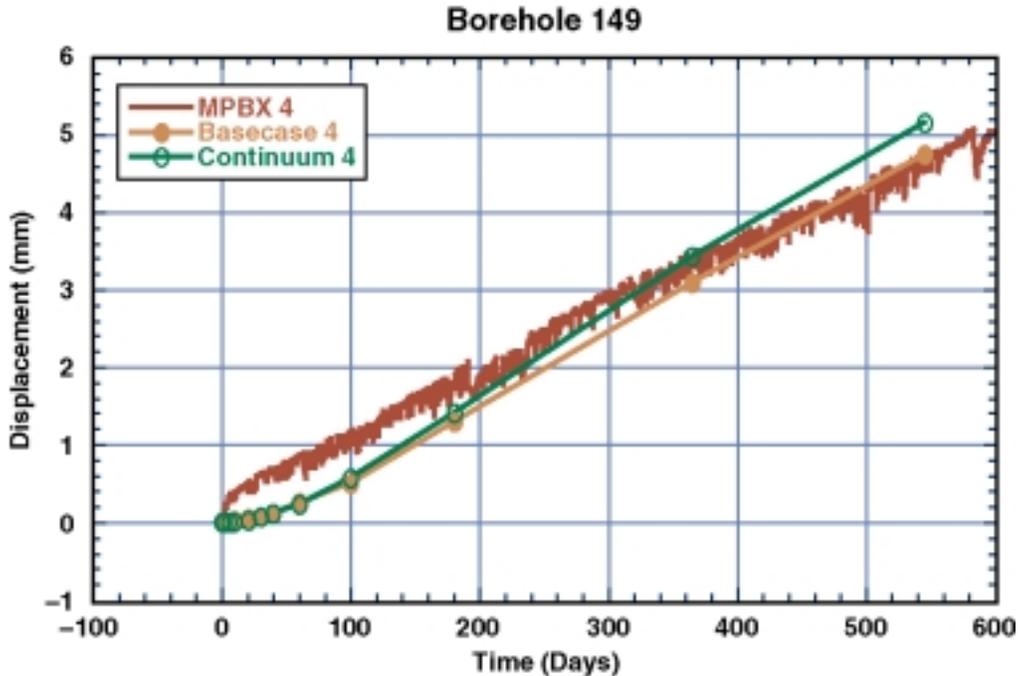


Figure 13. Observed and Predicted Deformation for BH 149.

Borehole 150: Results for BH 150 are shown in Figure 14. This is a vertical down hole in the floor of the drift, and is in the same cross-section as boreholes 147, 148, and 149. Again, the predicted deformation lags the observations during the first 20 days of heating, after which the slopes are similar.

The basecase model is closer in magnitude to the observed deformation at MPBX 4 by about 0.3 mm (day 545) than the continuum model, and the deformation rate appears to be slowing in the data. This change in rate is not predicted by the model. The magnitude of the prediction at day 545 is well within 10% of the observed value (4.8 mm predicted by the basecase model vs. 5.0 mm observed).

Borehole 156: This is a vertical up hole located in the middle fan of the MPBX holes shown in Figure 1. Observed and predicted deformations are shown in Figure 15. For this hole, predictions show a small negative deformation for the first 100 days, while observations during this time show a rapid expansion. After 100 days the slope of the predicted deformation is very similar to that of the observed. At 545 days the estimate of 3.5 mm is within 20% of the 4.7 mm observed value.

Borehole 180: This is another vertical up-hole in the crown. Results of observations and predictions (Figure 16) are similar to those for boreholes 149 and 156. That is, the model shows low or negative expansion for the first 100 days and lags the observed deformation. The slope of the model and the observations after 100 days are very similar through 330 days. Observed deformation data are unavailable between 330 and 540 days. Data are available after 540 days, and the predicted value of 3.5 mm is within 10% of the observed value of 3.7 mm at 545 days. Continuum and basecase model predictions are very similar, as there are few fractures currently mapped in this region.

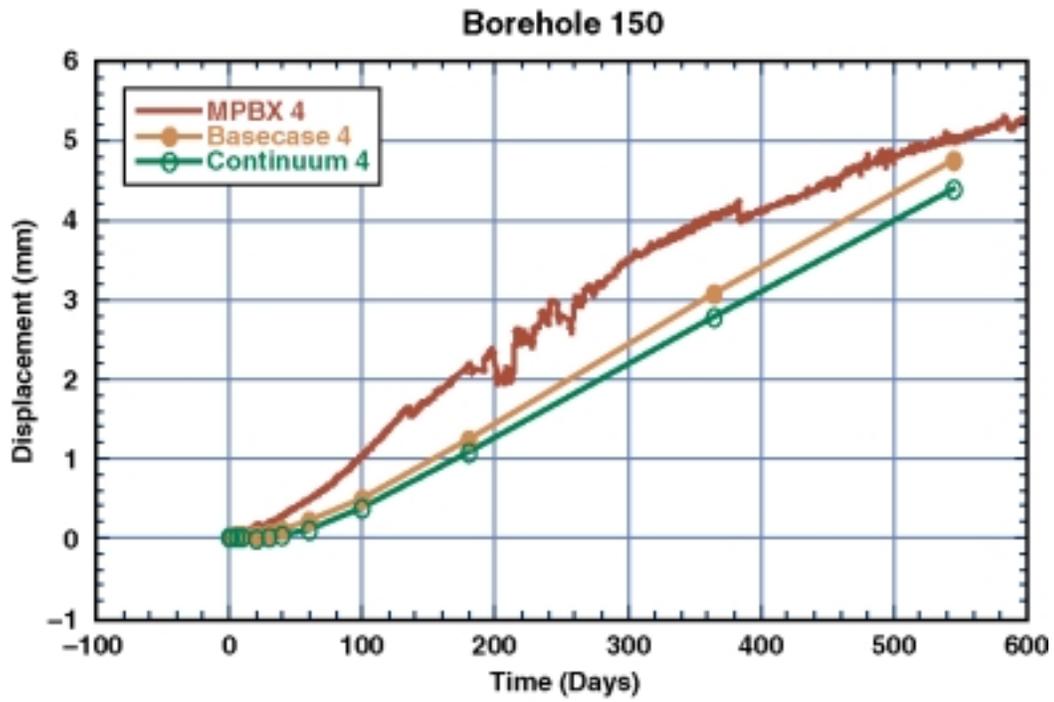


Figure 14. Observed and Predicted Deformation for BH 150.

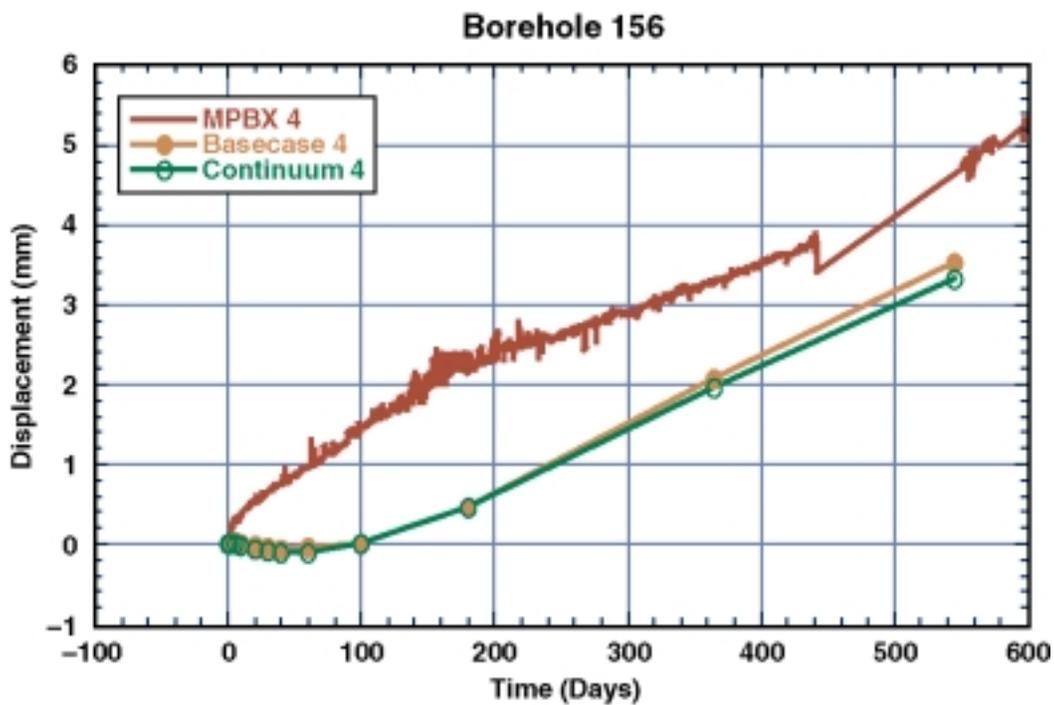


Figure 15. Observed and Predicted Deformation for BH 156.

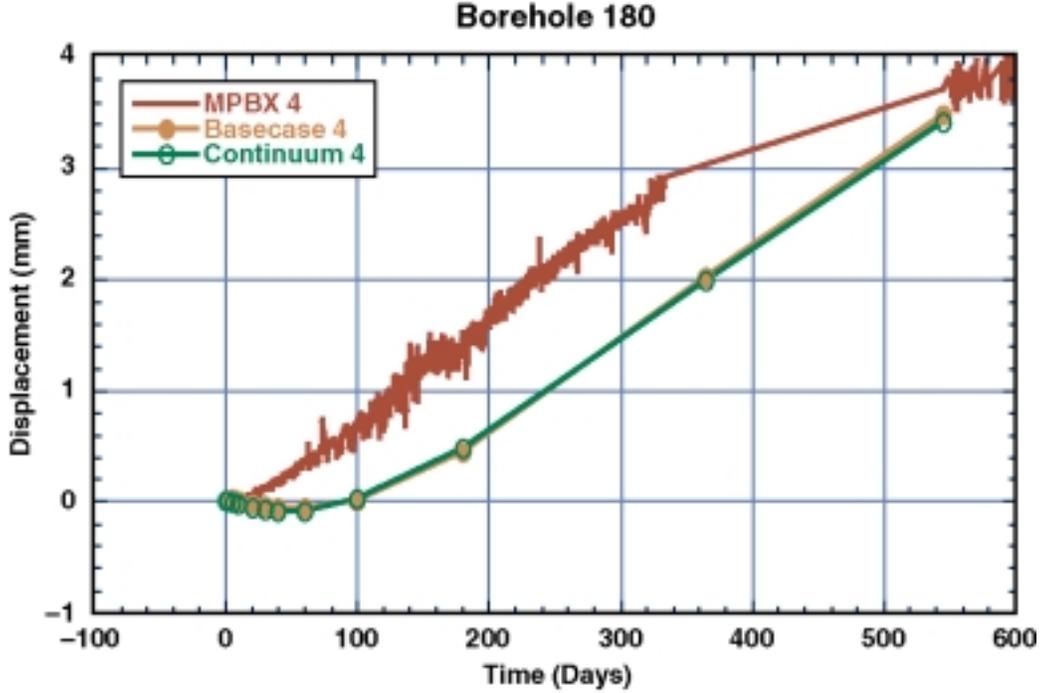


Figure 16. Observed and Predicted Deformation for BH 180.

Statistical Validation of THM Model. In addition to the qualitative comparison of predicted and observed deformation for the DST, three statistical measures were used to compare measured and simulated displacements. These measures are the root-mean-square difference (RMSD), the mean difference (MD), and the normalized-absolute-mean difference (NAMD). The application of these statistical measures provides a quantitative approach that complements the qualitative comparison of the predicted and measured deformations. These statistical measures are based on standard statistics (Bowker and Lieberman 1972) which have been modified to better adapt to interpretation of measured and simulated behavior in the thermal test.

The root-mean-square difference (RMSD) for a specific time after the start of heating is defined as:

$$RMSD = \left[\frac{\sum_{i=1}^N (d_{sim,i} - d_{meas,i})^2}{N} \right]^{1/2}$$

where $d_{sim,i}$ and $d_{meas,i}$ are the simulated and measured displacements for the i th MPBX anchors. N is the number of anchors compared at a particular time. The anchors used in this analysis are listed in Table 5. The smaller the RMSD the better the agreement between simulated and measured displacements.

The mean difference (MD) for a specific time is defined as:

$$MD = \frac{\sum_{i=1}^N [d_{sim, i} - d_{meas, i}]}{N}$$

A positive MD indicates an overestimate or overprediction of displacements, whereas the converse applies for a negative MD.

The normalized absolute mean difference (NAMD) for a specific time is computed using:

$$NAMD = \sum_{i=1}^N \left| \frac{d_{sim, i} - d_{meas, i}}{d_{meas, i}} \right| * \frac{1}{N}$$

The NAMD provides a percentage of the absolute difference between measured and simulated displacement relative to the measured displacement.

Figure 17 shows the time history for each of the three statistical measures (RMSD, MD, and NAMD) used to assess the agreement between measured and calculated displacements for both the base case (discrete model) and the sensitivity case (continuum model).

The overall agreement is reasonable for this initial analysis of the mechanical behavior in the DST. Also, it appears that the two cases considered (discrete and continuum models) do not differ substantially in their ability to simulate the measured displacements. These findings will need to be updated in future statistical analyses that will involve a more robust comparative analysis by including substantially more MPBX anchors. The RMSD shown in Figure 17 shows a general linear increase after the initial 20 days of heating for both cases considered. The 500-day magnitudes are slightly less than 3 mm. Figure 17 shows that the MDs for both cases are also quite similar for the times considered. These MDs, which are averages of all MDs determined at a specific time, range from 0.0 mm to -0.5 mm over the initial 500 days of heating. Upon further examination of the MDs for individual anchor locations, the MD ranges from -4.5 mm to 2.5 mm. Consequently, the MDs in this analysis tend to offset each other, resulting in the trends shown in Figure 17. The NAMDs shown in the figure are as high as 250 percent during the initial 100 days of heating. Thereafter, they are better but still average approximately 150 percent over the next 400 days. Upon examination of individual MPBX boreholes/anchors, it becomes apparent that a few of the MPBX boreholes contribute to the substantially large NAMDs. In some instances, these large NAMDs reflect comparatively small measured displacements. This behavior is noticeably present in the long longitudinal MPBX boreholes (81 and 82) that are slightly above and outside the Heated Drift. This general and unfavorable trend suggests that modeling of the displacements parallel to the axis of the Heated Drift will need to be reevaluated including characterization of fractures or discontinuities.

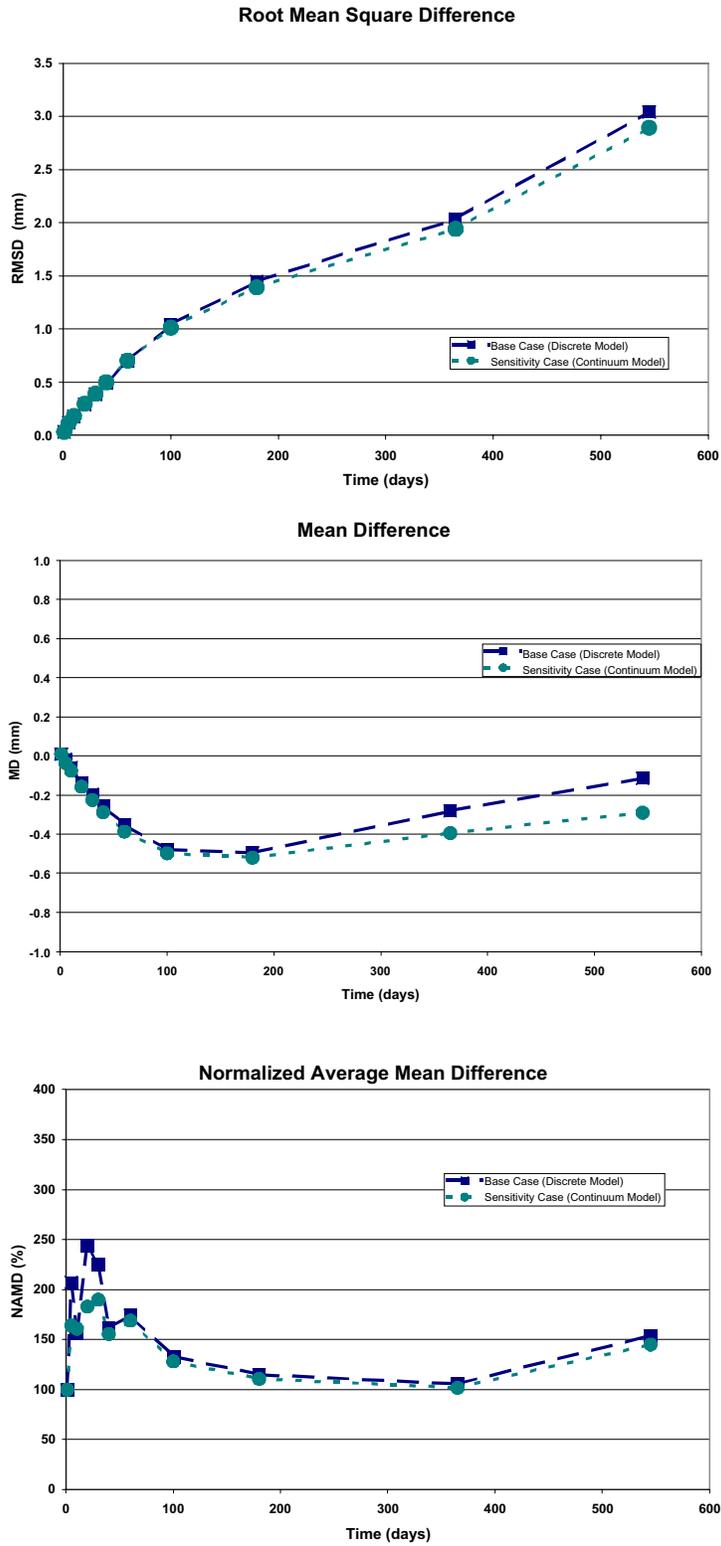


Figure 17. Statistical Measures for Comparative Analyses of Drift-Scale Test Displacements.

Large Block Test

Test Description and Model Development

The Large Block Test (LBT) was conducted at Fran Ridge, near Yucca Mountain, Nevada, and comprised one phase of the field-scale thermal testing program of the Yucca Mountain Site Characterization Project. The particular objective of the LBT was to monitor and characterize coupled THMC processes in an isolated block of fractured rock subject to a one-dimensional thermal gradient (Wilder et al. 1997). Because the block is an unconfined and well-mapped fractured rock mass, it is a good candidate for analysis using discontinuum models.

The LBT was conducted on a rectangular prism of rock 3 m × 3 m in cross-section and 4.5 m high that was exposed from an outcrop by excavating the surrounding rock. Detailed geologic mapping showed that two subvertical sets of fractures and one set of subhorizontal fractures intersect the block. The subvertical fracture sets are approximately orthogonal, with spacings of 0.25 to 1 m and are oriented generally in the NE–SW and NW–SE directions. Moreover, a major sub-horizontal fracture is located approximately 0.5 m below the top surface.

To create a one-dimensional thermal field within the block, heaters were placed in the rock to simulate a plane heat source at a height of 1.75 m from the base of the block, and a steel plate fitted with heating/cooling coils was mounted on the top of the block. This plate was connected to a heat exchanger to allow thermal control of the top surface. The block was heated for more than 12 months, from Feb. 27, 1997, until March 10, 1998.

The overall three-dimensional mechanical response of the rock to the heating was monitored using six multiple-point borehole extensometers (MPBXs). Three were oriented horizontally in the N–S direction; two were oriented horizontally in the E–W direction, and one was oriented vertically. The geometry of the heaters, MPBX holes, and one temperature hole is shown in Figure 18.

A THM model for the LBT has been formulated using the general approach presented above. This model incorporated the general geometry of the LBT. Data for the simulations is given in Tables 1, 3, and 4. The input and output files for the Large Block Test model validation simulations have been submitted to the TDMS (DTN: LL010703623123.01).

Temperatures. Deformation of the LBT was calculated at times of 0, 10, 25, 55, 85, 115, 145, 182, 200, 275, 340, 350, 375, 385, 395, 410, 430, and 450 days after the start of heating. The temperatures in this analysis were derived from the TH analysis reported in CRWMS 2000, Section 6. Files containing Cartesian coordinates and temperatures for the model region simulated by NUFT were obtained at each time. The NUFT model assumes symmetry in the block; consequently these files contained values for one quadrant of the region simulated in 3DEC. The 3DEC calculations include the entire volume of the block, as the fractures are not symmetric. A 3-dimensional temperature field for 3DEC was produced from the NUFT temperatures by reflecting the temperatures about the appropriate vertical planes. This was done as follows. Temperatures from the NUFT model and their coordinates were input into EarthVision along with an array of grid points generated by 3DEC for the LBT model domain at each calculation time. EarthVision performed a three-dimensional interpolation of the 3D NUFT

model temperatures to provide an interpolated temperature for each calculation time at each of the 3DEC model grid points. The grid point temperatures were then input into 3DEC as a separate input file for each calculation time.

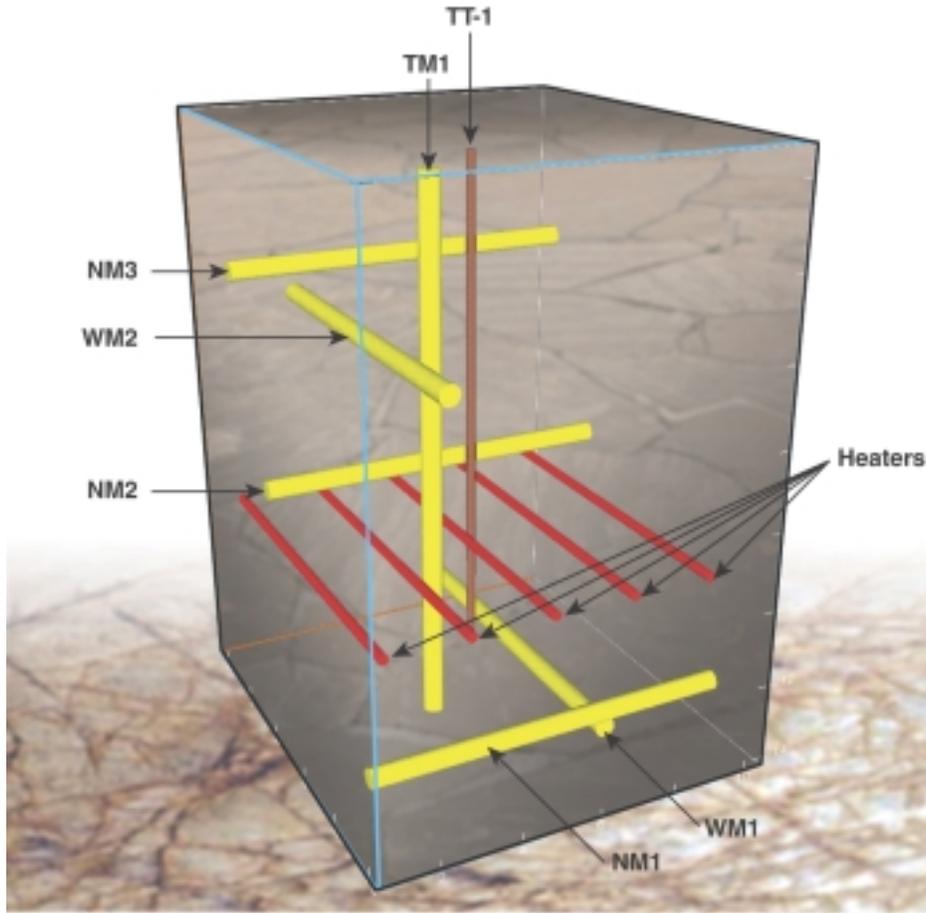


Figure 18. MPBX Borehole Locations in the Large Block Test.

Fractures. Fractures used in the simulations were taken from the LBT fracture data set described in Wilder et al. (1997, Section 2.2). Particular fractures used in the simulations are discussed below. The fractures were assumed to have no tensile strength.

Model Geometry. The spatial domain for the LBT model is shown in Figure 19, top left. This model domain extends 23 m beneath the ground surface and 23 m out from each vertical face of the LBT, so that the fixed displacement boundary conditions can be applied far from the heated portion of the block. At these distances thermal expansion cannot reasonably be expected, so that fixed displacement boundary conditions may be applied with confidence.

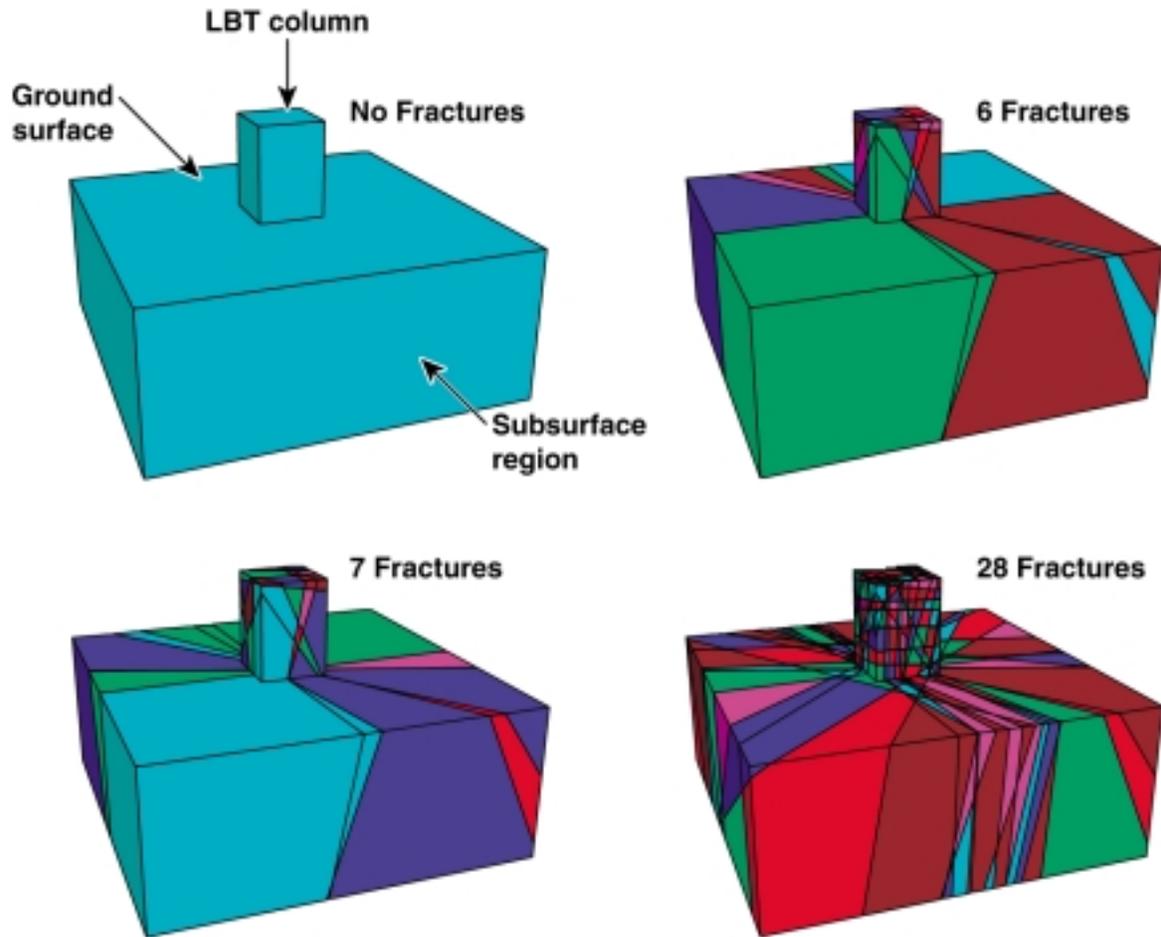


Figure 19. Spatial Domain for the Model.

Boundary Conditions. Roller boundary conditions were imposed on the four vertical sides and on the base of the subsurface region. These boundary conditions impose a zero displacement restriction on normal displacements along these surfaces, but allow parallel (in plane) displacements. Thus, horizontal displacements are permitted along the base of the block and vertical displacements are permitted along the sides of the subsurface region. Fixed displacement boundary conditions provide an upper bound on thermal stresses because outward displacements of the model sides, which would relieve built-up stresses, are not allowed.

The base of the block was fixed in the vertical direction to prevent the rock at 23 m below the LBT from moving vertically. The top of the block is allowed to move vertically. This is appropriate because the LBT column is unconfined, whereas the base of the model is supported by the underlying rock. A fixed stress boundary condition, equal to atmospheric pressure, is applied to the top and sides of the LBT columnar region and to the ground surface region in the model.

Rock Properties. Input parameters for the LBT simulation are provided in Table 3. Calculated or assumed parameters are listed in Table 4.

Simulations. A series of simulations (referred to as “Models” in the following discussion) were conducted to evaluate the effect of number of fractures and of Coefficient of Thermal Expansion (CTE) on the mechanical behavior. The simulations are listed in Table 7 and the fracture geometries of the model domain for the various simulations are shown in Figure 19.

Table 7. Summary of THM Simulations of the LBT

Simulation #	Number of Fractures	CTE ($\times 10^{-6}/^{\circ}\text{C}$)	Comment
1	0	5.27	Continuum model
2	6	9.73	High CTE with 6 major fractures
3	6	5.27	Low CTE with 6 major fractures
4	7	5.27	Same as 3 with one additional fracture
5	28	5.27	All fractures included in fracture analysis

Results for Large Block Test

The 3DEC model was configured to produce displacement values at the locations of the MPBX anchors discussed above. Deformation in the vertical direction was monitored in hole TM1, and predicted displacement is compared with observed displacement for anchor TM1-4 in Figure 20a for the first 100 days of heating. This figure plots results for each simulation along with the observed displacement and shows that while Model 2 with high CTE matches the early thermal deformation up to 20 days, it overpredicts the deformation at 100 days by more than a factor of 2. Predictions produced by the other four models, with lower CTE, are quite acceptable as they underpredict the magnitude of the displacement by only a few tenths of a millimeter. The continuum and fractured models produce similar estimates, and the response of all of these models lags the observed deformation during the first 40 days. Thus, the number of fractures had very little effect on predicted deformation for the vertical direction.

Predicted deformation during cooldown is compared with field measurement at anchor TM1-4 in Figure 20b. This plot shows that the continuum model (Model 1) fits both the shape and magnitude of the observations, while Model 3 with six fractures also approximates the observations quite well.

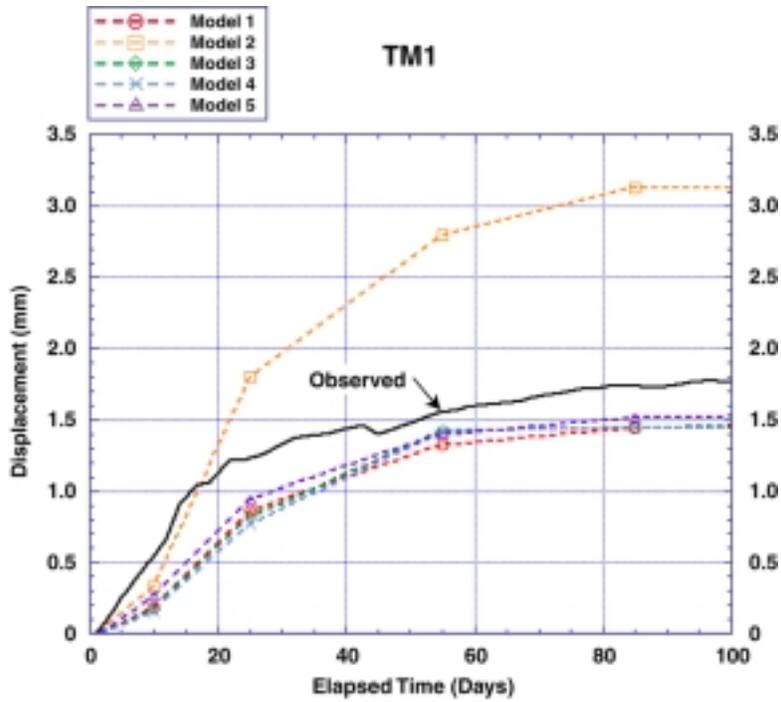


Figure 20a. Simulated Deformation in the Vertical Direction Compared with Observed Displacement for Anchor TM1-4.

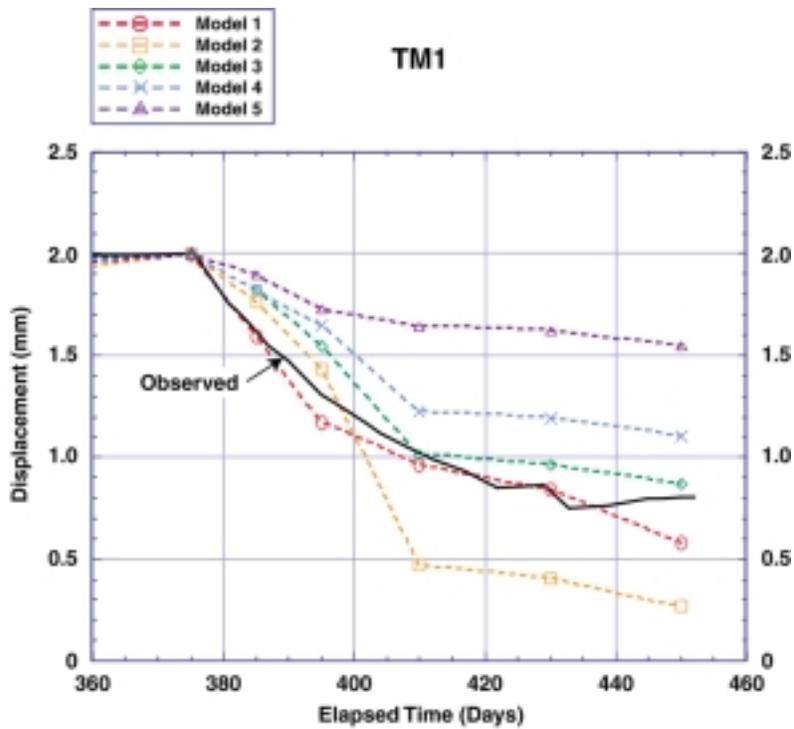


Figure 20b. Predicted Deformation during Cooldown Compared with Field Measurement at Anchor TM1-4.

MPBX holes NM1 and WM1 were located close to the bottom of the block and in orthogonal directions. Measured and predicted displacement values for anchor NM1-4 are plotted in Figure 21a. This figure shows that at this location, Model 3 provides the best match to the observations. Model 2 overpredicts displacement by nearly a factor of 2, while the continuum model (Model 1) underpredicts the deformation. Models 1, 3, 4, and 5 bracket the observed values, with Model 1 underpredicting for the first 100 days and Models 4 and 5 overpredicting at 100 days. This plot indicates that while Model 3 (6 fractures) slightly underpredicts deformation, adding one fracture (Model 4) caused more displacement at this location, but adding many fractures (Model 5) caused underprediction during the first 25 days and overprediction after 25 days.

Results for NM1-4 during cooldown are shown in Figure 21b. This figure shows that at this location Model 3 matches the magnitude of the displacement, but does not accurately predict the cooling path. Model 2 overpredicts the displacement and best approximates the slope of the curve during the first 20 days of cooling. Models 1, 4, and 5 underpredict the amount of recovery during cooldown. The least contraction is predicted by Model 5, the highly fractured rockmass.

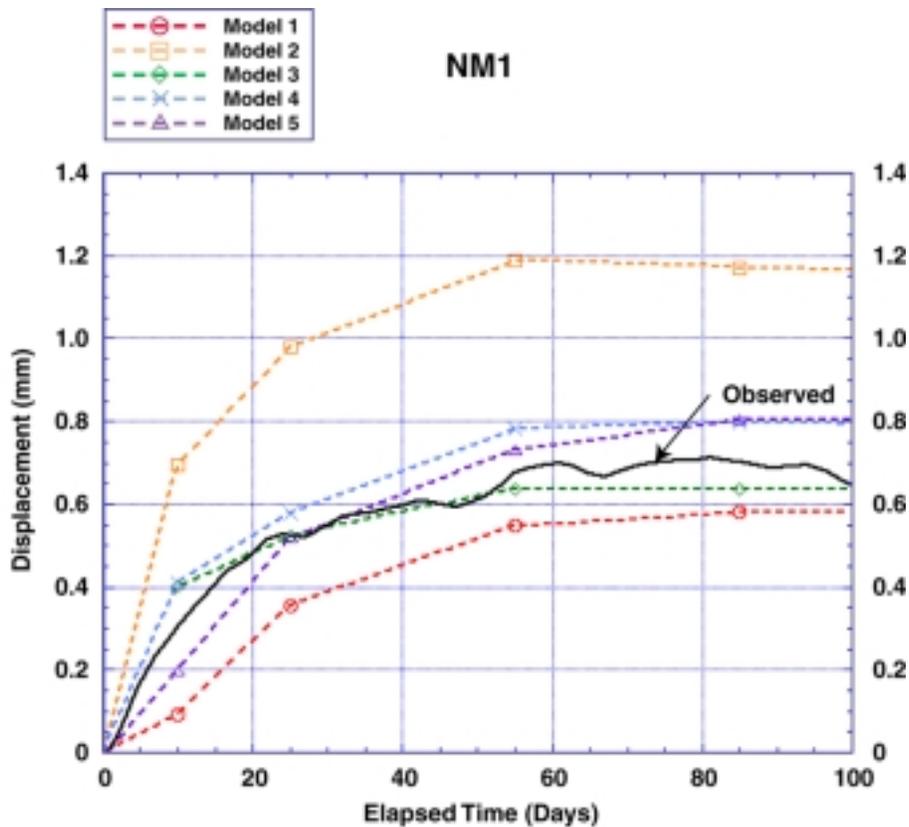


Figure 21a. Measured and Predicted Displacement Values for Anchor NM1-4.

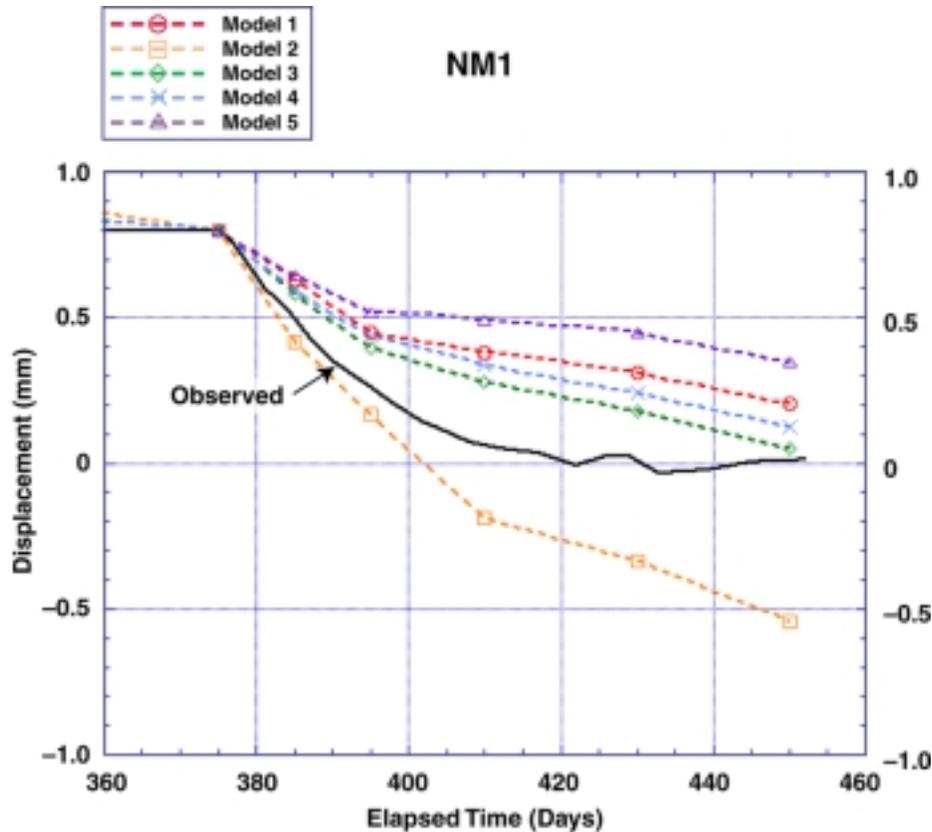


Figure 21b. Results for NM1-4 During Cooldown.

Data and predictions for the first 100 days of heating for WM1 are shown in Figure 22a. This plot shows similar results to Figure 21a in that Model 2 overpredicts by nearly a factor of two, and models 1, 3, 4, and 5 bracket the behavior. The highly fractured model (Model 5) best approximates the response during the first 20 days; Models 3 and 4 overpredict the displacement during the first 10 days, but are within about 0.05 mm of the observed displacement at 100 days. Model 1 underpredicts the displacement by between 0.1 and 0.15 mm throughout this time interval.

Modeling results for WM1 during the cooldown period are shown in Figure 22b. These results are similar to the results for NM1 in that the continuum model (Model 1) most closely approximates the observed cooldown. The high CTE model (Model 2) overpredicts the deformation, while the other models underpredict the displacement. Interestingly, these results show that adding fractures to the model causes less recovery during cooldown. This may be because fracture slip is essentially unrecoverable under unconfined stress conditions.

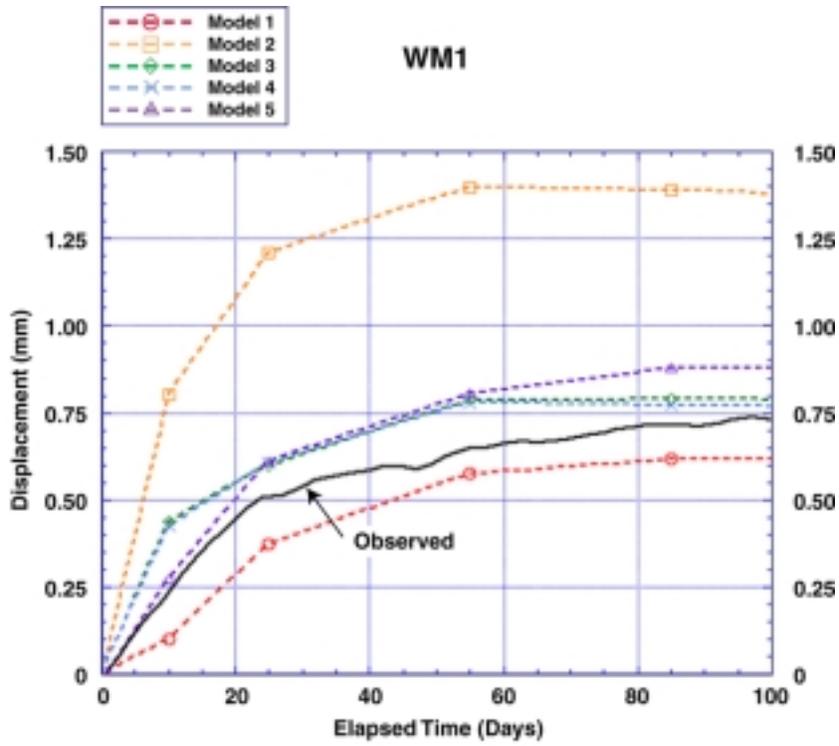


Figure 22a. Data and Predictions for the First 100 Days of Heating for WM1.

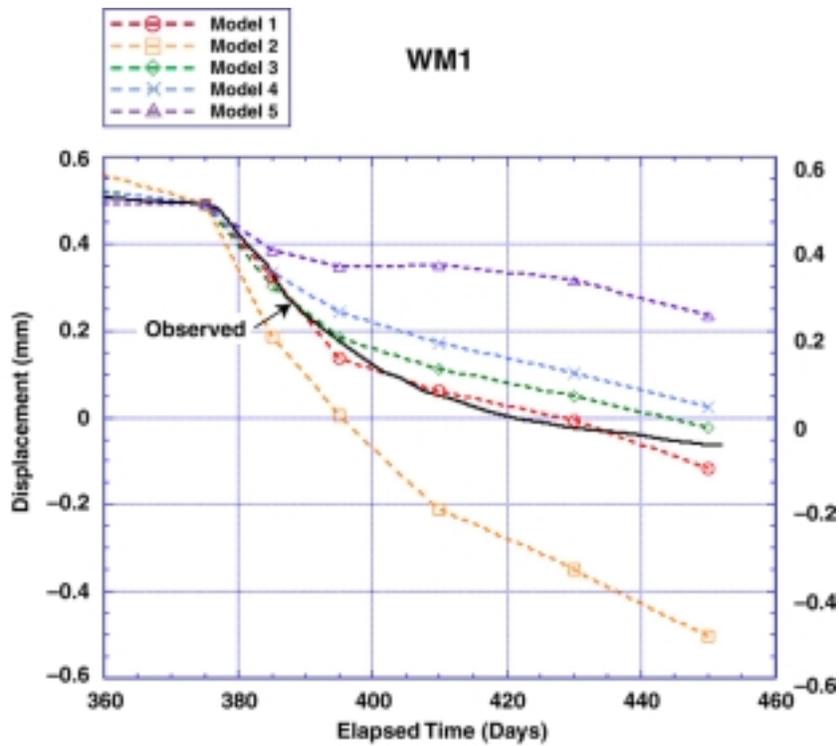


Figure 22b. Modeling Results for WM1 During the Cooldown Period.

Figure 23 presents simulated and observed displacements for borehole NM2, which was located near the heater plane. This figure shows that the continuum model (Model 1) underpredicts the displacement for anchor NM2-4, while the high CTE model (Model 2) predicts the deformation relatively well during the first 10 days, but overpredicts the magnitude of the total deformation at 40 days by nearly a factor of 2. Models 3, 4, and 5 produce similar results, and both Models 4 and 5 cross over the observed deformation at 40 days. Of these three models, Model 5 provides the best fit to the data for the first 40 days, indicating that rock in this region is highly fractured.

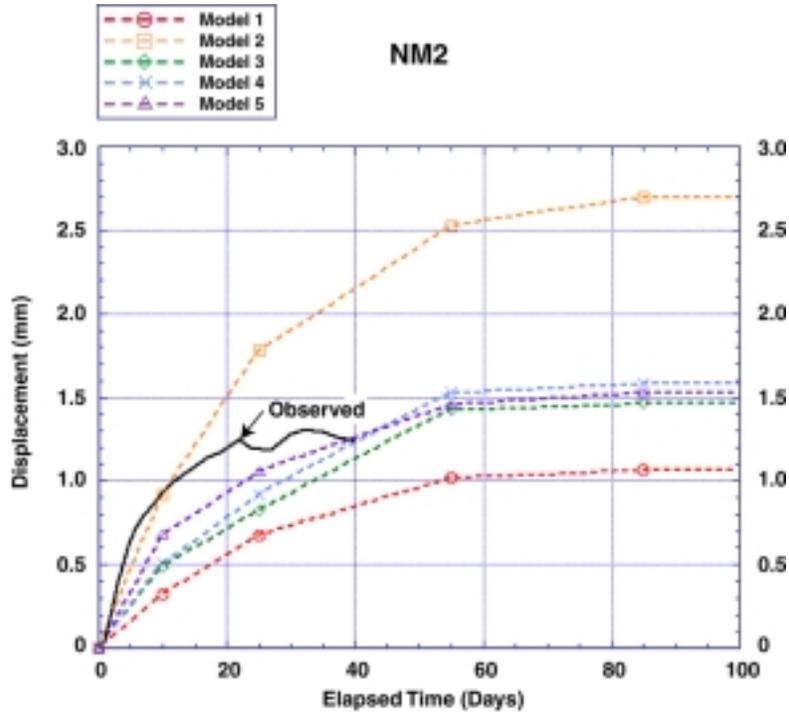


Figure 23. Simulated and Observed Displacements for Borehole NM2.

The MPBX instrumentation in borehole WM2 functioned throughout the test and data for anchor WM2-4 for the entire test is shown along with simulated displacements in Figure 24. This figure shows that for this anchor, Models 3 and 4 did a good job of predicting the deformation over much of the test duration. Model 3 predicts slightly less displacement than Model 4, and from 50 to 100 days Model 4 is closer to the observations, while from 120 to 220 days Model 3 fits slightly better. Models 3 and 4 also capture the cooldown relatively well. They underpredict the total amount of cooldown displacement, by 0.4 mm, and also show some contraction of the block about 270 days that is not reflected by the observation. Models 1 and 5 both underpredict maximum deformation by significant amounts (1.6 and 1 mm respectively). Model 2 overpredicts the maximum deformation, but does show the best fit to displacement during the first 20 days of heating. Model 5 does not show contraction with cooldown and Model 1 underpredicts the magnitude of the cooldown displacement. Model 2 correctly predicts the relative change in displacement during cooldown (1.8 mm) but the final value of 2.6 mm displacement is too high.

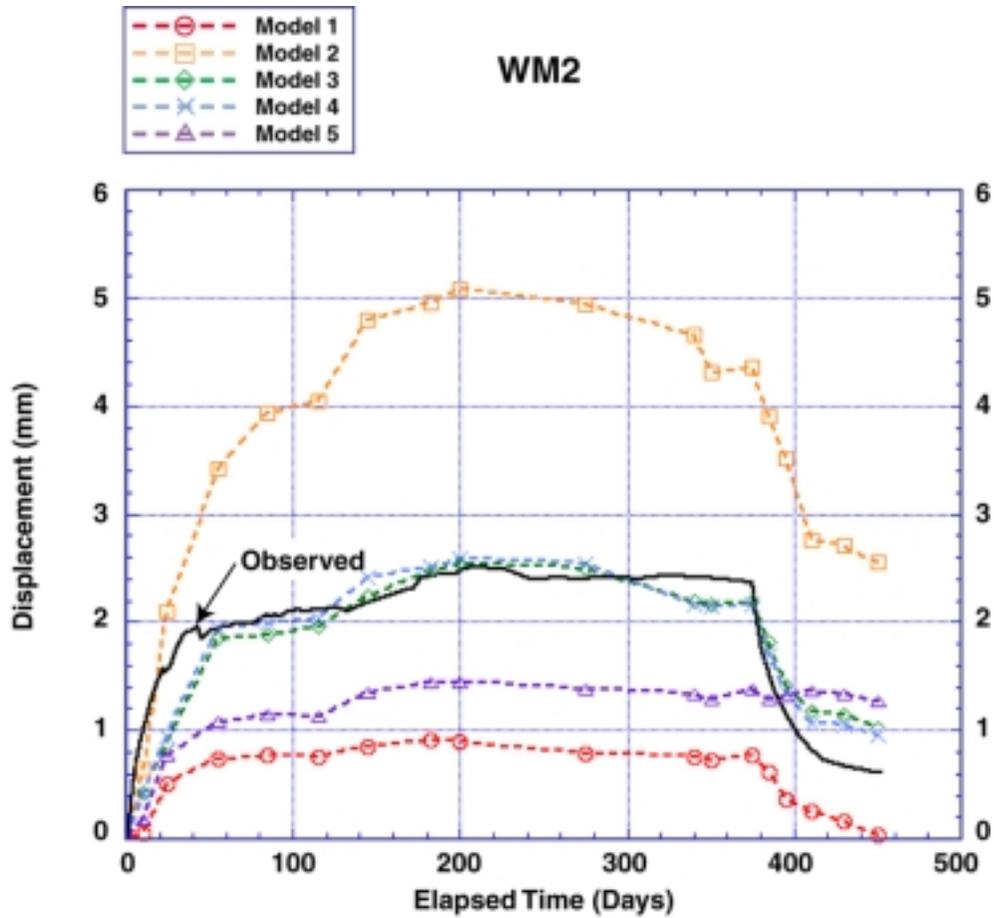


Figure 24. Data for Anchor WM2-4 for the Entire Test Shown Along with Simulated Displacements.

Continuous data are also available for anchor 4 of borehole NM3, the uppermost horizontal MPBX borehole in the block, and these data are shown with the model predictions in Figure 25. While the measured NM3-4 displacements are similar to those for WM2-4, with a maximum displacement between 2.5 and 3 mm, all of the models underpredict the measured NM3-4 displacements. This result differs considerably from that of the other MPBX boreholes. Adding one fracture to Model 3 to create Model 4 did increase the predicted NM3-4 displacements, but the increase was only a small fraction of that needed to compare well with the observations.

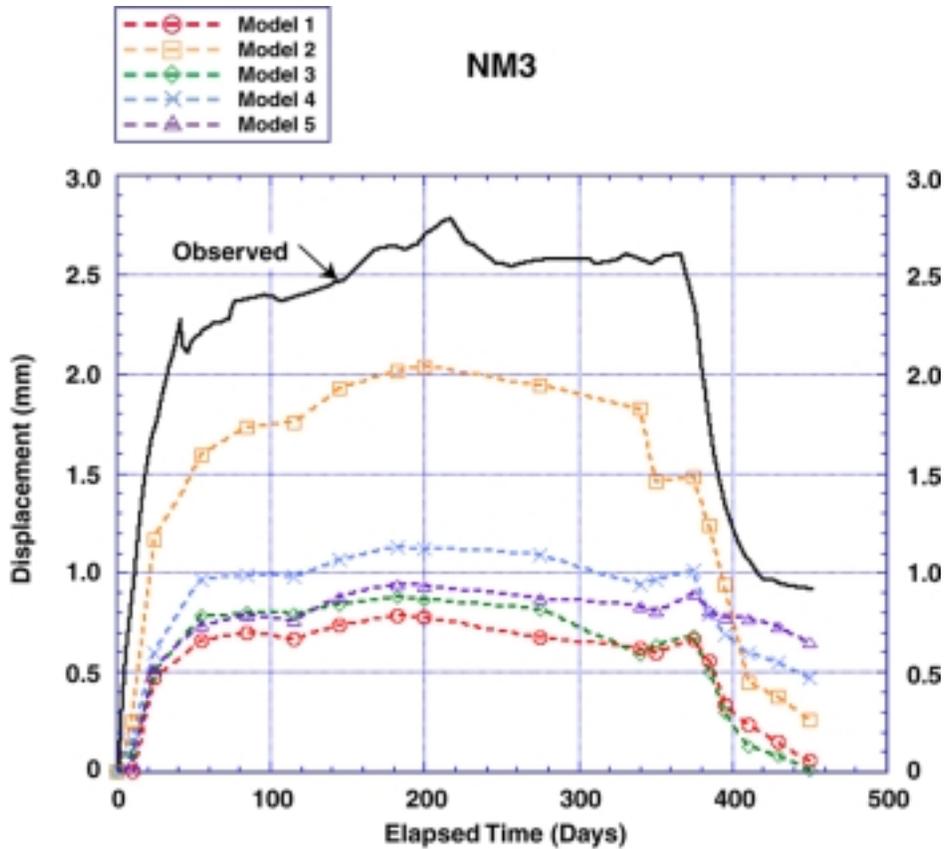


Figure 25. Continuous Data for Borehole NM3, Anchor NM3-4, Shown with the Model Predictions.

The results discussed above indicate that Models 3 and 4 provide the best overall fit to the observations. Model 1 fits the results at the bottom of the block relatively well.

The difference between the measured and predicted deformation during the first 50 days of heating is of interest as it relates to the transient response of the rock to the temperature field. Figures 21a and 22a show that for horizontal boreholes near the base of the block, deformation in Models 3 and 4 lead the observed displacements during the first 20 days. Figures 23, 24, and 25 show that the observed deformation leads the predictions during the first 40 to 60 days of heating. Predicted and observed results for anchor WM2-4 for the first 100 days of heating are replotted in Figure 26 along with temperature data for the plane of the heater and the plane of WM2, respectively. This figure shows that during the first 30 days the observed deformation (WM2-4) can be correlated with temperature at the heaters (TT1-14), while the predicted deformation is correlated with temperature at the borehole location (TT1-22). This indicates that movement of the rock above the heater may be due to a far-field effect, and may imply that movement along fractures serves to propagate deformation.

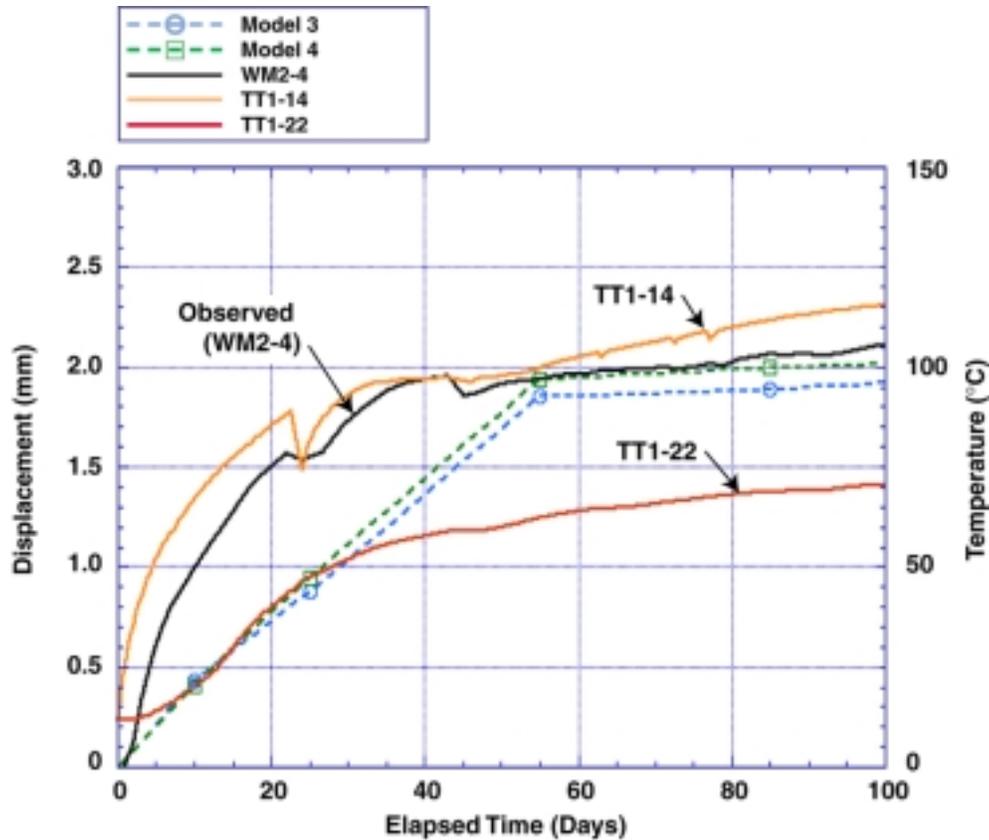


Figure 26. Predicted (Model 3, Model 4) and Observed (WM2-4) Displacements for Anchor WM2-4 during the First 100 days of Heating along with Temperatures for the Heater (TT1-14) and WM2 (TT1-22) Planes.

Conclusions

The coupled THM models have been formulated for the DST and the LBT and predictions of deformation have been made using the model in both a continuum mode and in formulations containing discrete fractures. Comparison of the predicted deformation with observations made using MPBX instrumentation shows that generally the predictions capture both the trend and the magnitude of the observations. Moreover, for both the DST and the LBT, the models containing discrete fractures more accurately predict the deformation behavior than do the unfractured models.

This work indicates that not all fractures are active in the tests, and for the LBT, the deformation was controlled by a subset of 6-10 major fractures.

A CTE value of $5.27 \times 10^{-6} / ^\circ\text{C}$ is appropriate for the LBT. This is consistent with the value determined for the Single Heater Test. However, a higher value of $9.73 \times 10^{-6} / ^\circ\text{C}$ provided a good fit to deformation in the DST.

The transient response of the predicted deformation at early times lags the observed deformation in both tests. This is caused in part by the lag in predicted temperatures when compared to observed temperatures. The thermal models must be improved in early times in order to correctly predict the TM behavior.

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