SCIENTIFIC NOTEBOOK

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1. INITIAL ENTRIES

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By agreement with the CNWRA QA this NoteBook is to be printed at approximate quarterly intervals. This computerized Scientific NoteBook is intended to address the criteria of CNWRA QAP-001.

1.1. Objectives

The initial objectives of this task are two-fold: (1) to perform coupled thermal-hydrological (TH) modeling of the Large Block Test (LBT) conducted by Lawrence Livermore National Laboratory to test and verify analysis approaches for evaluation or prediction of the performance of the proposed geological repository at Yucca Mountain based on conceptual models using computer; and (2) to better understand the mechanisms of coupled TH processes. The ultimate goal may also include coupling of mechanical and chemical processes and their effects in near-field environment of the repository.

1.2. Technical Approaches

The modeling will use in-house numerical code, MULTIFLO. Model geometry, boundary conditions, and material properties in the DOE Large Block Test will be used as input. Modeling results will be compared with the available results from the LBT testing.

1.3. Data Sources

All the necessary data related to the LBT will be coming from various relevant technical and/or progress reports produced by Lawrence Livermore National Laboratory. Other necessary data will be obtained from the Yucca Mountain data systems, such as the *Reference Information Base* (RIB, DOE, 1995).

1.4. Computers, Computer Codes, and Data Files

Figure 2.4-1 Three-dimentional geometry of hte Large Block Test and quarter-symmetry section for thermal-hydrologic modeling**Table 1-1. Computing Equipment**

Machine Name	Type	OS	Location	Computer Code	Language
ULTRA	Sun Workstation	Solaris 2.5	Bldg. 189	Multiflo	Fortran 77

Table 1-1 lists computer equipment and computer codes. Table 1-2 provides names, type, and content of data files LBT analyses.

Table 1-2. Names, Type, and Content of Relative Files

File Name	Directory	Type	Content
Metra		executable	Executable of the TH part of Multiflo code
LBT-TH1.inp		text	Input data file for Multiflo analyses
		text	
		text	

2. IN-PROCESS ENTRIES

2.1. Summary of Large Block Test (LBT)

2.1.1 General Information and Objectives of the LBT

The LBT is one of a series of tests intended to assist in defining the physical processes that must be considered in models of a potential repository at Yucca Mountain. These include: laboratory tests of core-size samples, laboratory tests of ~1-m-scale block samples (small block tests), large block test, in situ tests [such as the single heater test (SHT) and the drift Scale Test (DST)], and confirmation tests.

The LBT is focused on what has been defined as the near-field environment (NFE) and the altered zone (AZ) environment (Wilder, 1997). Its purpose is to test the conceptualizations in a representative rock mass so that the tools are appropriate for characterization and analyses of YM (Wilder, et al., 1997)

The eastern slope of Fran Ridge, Nevada Test Site, was selected to be the LBT site because of its desirable rock type (outcrops of the Topopah Spring tuff), fracture characteristics, and accessibility. The rock at this site is near the interface between the lithophysal and nonlithophysal units of the Topopah Spring tuff, but it is mineralogically acceptable for the LBT.

The objectives of the LBT are (Wilder et al., 1997; Lin, 1993)

- To study coupled TMHC processes
  . controlled thermal boundary
  . controlled moisture boundary
  . scale sufficiently large to include multiple fractures and heterogeneities
  . allow for 3D characterization
  . provide for post-test characterization
- To test instruments and techniques
- To test waste package materials

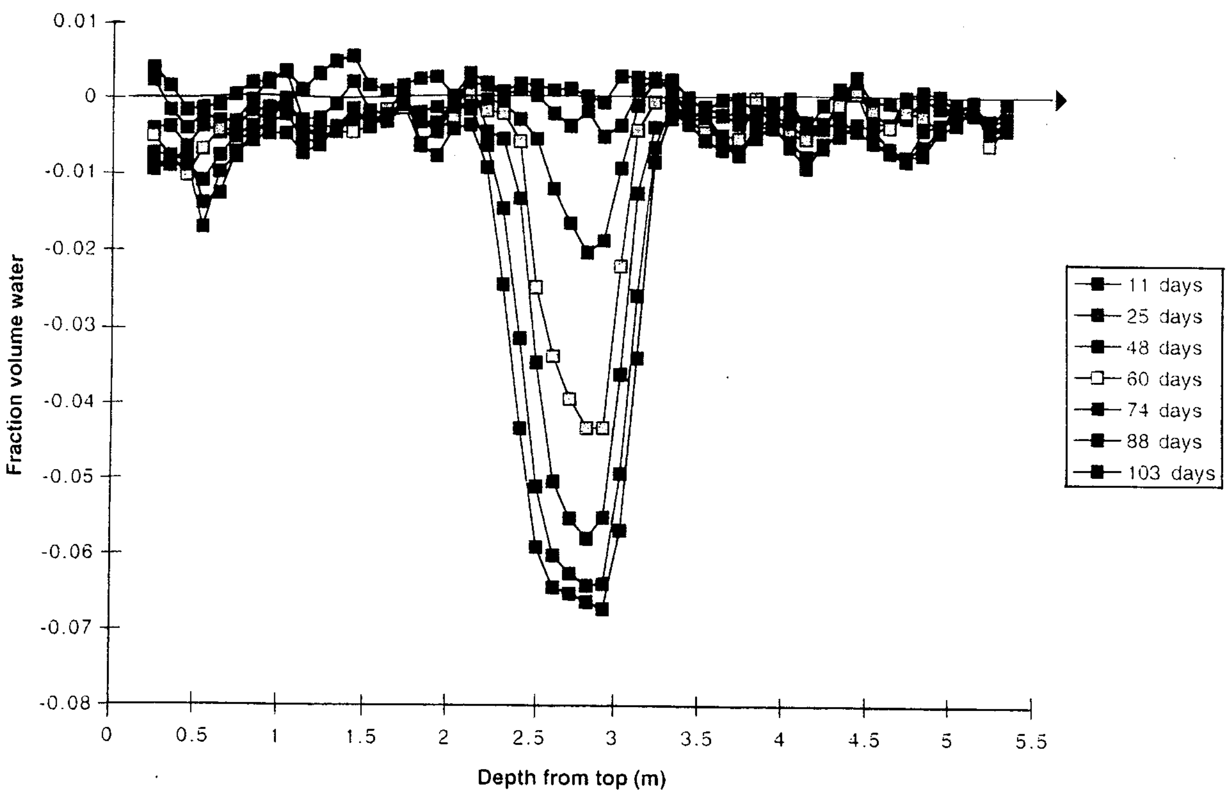
2.1.2 Pretest Characterization

- Fracture mapping and analysis:
  - maps of surface fractures on all five exposed surfaces
  - 3D physical model of fractures within the block

- Permeability measurements
  Determined properties of the matrix include: porosity, permeability, moisture retention curves, electrical resistivity versus moisture content, stress-strain curves, and acoustic wave velocity. The average porosity of the block was determined to be 11.55±2.28%.
  - air permeability (single hole, cross hole, tracer)

- Neutron logging and moisture conditions
  Figure 2.1-1 shows water saturation as a function of depth, determined from neutron logging in hole E4. The water saturation determined in other holes agrees well with the values shown here. Neutron logging was performed again to estimate the initial moisture content of the block before the experiment started.

Figure 2.1-1 Water saturation as a function of depth determined from neutron logging in hole E4 (after Wilder et al. 1997)



2.1.3 Pretest predictive analyses

See Lee (1995a&b)

Assumptions:

Heating power levels in the boreholes are identical
Heat is delivered uniformly along the heated length of each borehole
Top-surface temperature was fixed at 60 C
Heating power varied to attain a maximum temperature of 138 to 140 C at the walls of the heater boreholes

Homogeneous and Heterogeneous Cases - 2D

. half-symmetry section of the block
. equivalent continuum model
. the heterogeneous permeability field had a "layer-cake" distribution because the permeability measured any depth was assumed to be constant for that depth
. main observations:
  - a distinct dryout zone was observed in and around the heater plane
  - well-developed condensation zones above and below the heaters in the homogeneous case
  - the heterogeneous case did not show a well-developed condensation zone above the heaters, instead, a distinct dryout zone and a well-developed condensation zone was observed only below the heater plane.
  - for heterogeneous case, there was a net loss of liquid above the heater plane, results show that saturation changes might be sensitive to permeability distribution
  - gas pressure was higher for the heterogeneous case.

TH discrete fracture model

. Fracture aperture: 200 μm
. Fracture spacing: uniform of 30 cm
. The fractures were vertical, parallel to the heater borehole axes, they were assumed to intersect the borehole axes and to occur midway between two boreholes
. main observations:
  - dryout and recondensation zones occur above and below the heater plane
  - dryout zone was thickest at the fractures and thinnest in the matrix, midway between the fractures
  - block fractures were not significantly affected by fracture location

3D TH model

. equivalent continuum and homogeneous
. heater load: 450 W per heater for six months (182.5 days), power was then turned off and cool-down was simulated for an additional six months.
. initial liquid saturation was 92% for case A.
. six additional cases as shown in Table 2.2-1, incorporating power failures

Simulation of tracer studies

see Wang and Ahlers (1996)

Thermal-mechanical predictive modeling

Flac and ABAQUS

. Assumptions in TM modeling:
- the large block is 3.0mx3.0m at the base and 4.5 m tall
- five heaters span the width of the block at a height of 1.5 m above the ground surface
- temperature at the plane of the heaters will eventually raise to about 140 C and a thermal gradient will be developed between the heater plane and the top of the block
- temperature at the top of the block will be maintained at a constant 60 C
- heater flux on the sides of the block will be maintained at zero (it should be noted that this is no longer a correct boundary condition assumption, in that computer controlled heaters are not part of the LBT; therefore there will be a flux that will be measured, but not controlled to be zero).
- the block will be essentially unconfined, with a m maximum horizontal stress of 0.2 MPa (30 psi) imposed on the sides of the block.

2.1.4 Instrumentation and Monitoring
See Wilder et al. (1997)

2.1.5 Useful Results

Air injection measurements
Don't really know how to use it.

Temperature: (very important)
- measured using resistance temperature devices (RTDs) both in boreholes and on the surfaces of the block
- fourteen boreholes: two vertical (TT1, TT2), seven horizontal (NT1-NT4, WT1-WT3), and five heater hoes (EH1-EH5)
- the RTDs in the holes were separated by a spacing of 20 cm, numbering starting from the bottom, or the end-side.
- heater turned on at 10 am on Feb 28, 1997 to a power level of about 450 w each
- figures 2.1-2 and 2.1-3 show the history of heating at TT1-14 and TT2-14, at 5 cm above and below the heater horizon, respectively. Notice power outages and rain falls.
- **Temperature files are available in spread sheets in the LLNL data base!!**
  Need the following temperature files:
  . temperature history at the heater plane
  . temperature history on the vertical side walls of the block

Electrical Resistance Tomography
- To measure changes in moisture content caused by temperature changes.
- **Need moisture data along the side walls of the block to control hydraulic flex**

Moisture content determined by neutron logging
. Background moisture: 60 to 80%, for a laboratory determined porosity of about 11%.
  - Figure 2.1-4 shows a typical pre-heat baseline fraction volume water content (in TN4), moisture content increases with depth and ranged between 0.08 and 0.1
. Heating phase moisture content:
  - See figures 5-32 through 5-36 of Wilder et al. (1997) for details.

Figure 2.2-2 Temperature history at TT1-14 (5 cm above the heater horizon) (after Wilder et al. 1997)

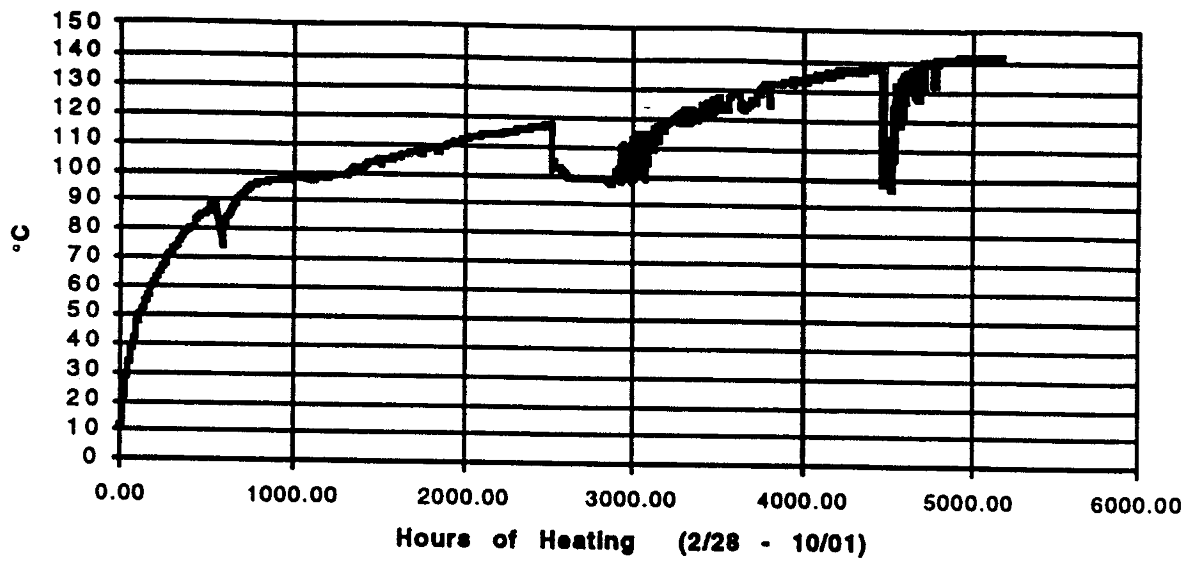


Figure 2.2-3 Temperature history of TT2-14 (5 cm below the heater horizon) (after Wilder et al. 1997)

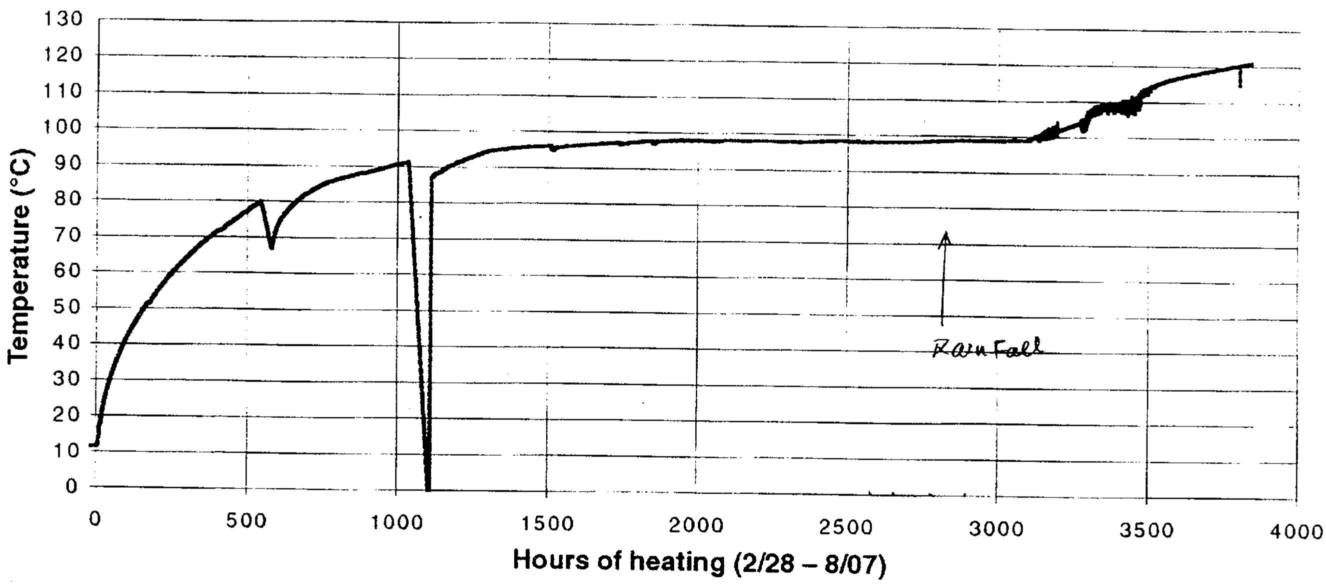


Figure 5-3.

TT2-14

Figure 2.1-4 A typical pre-heat baseline fraction volume water content (in TN4). Moisture content increases with depth and ranges between 0.08 to 0.1 (after Wilder et al. 1997).

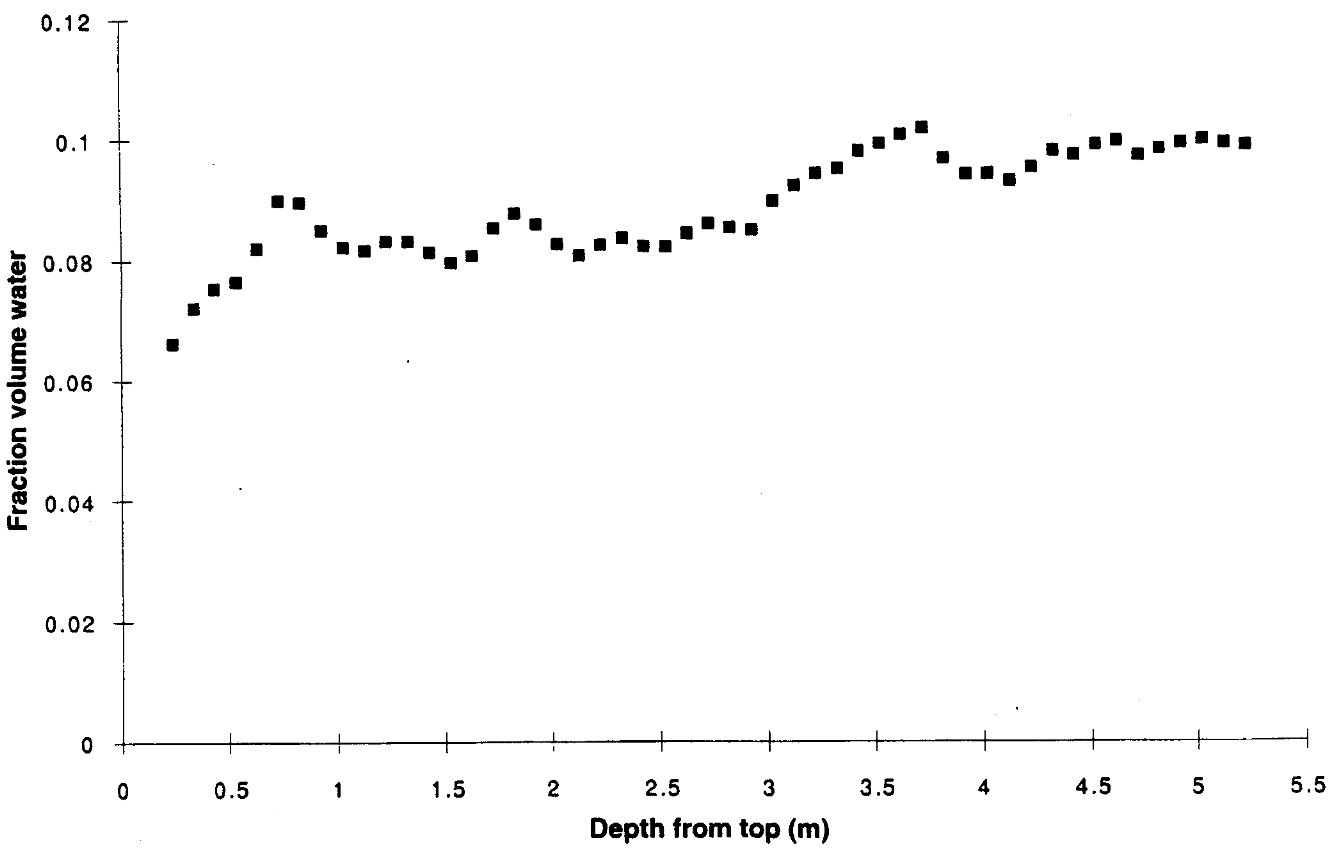


Figure 5-30.

2.1.7 Calendar of Large Block Test

Table 2.1-1 Calendar of major events during Large Block Test

Events	Dates			Remarks
	Absolute dates	Relative hours	Relative days	
Heaters energized	2/28/97 (10 am)	0	0	Heater power is 450 W/heater
Power outage		580		
Power outage		1120		
Power outage		1520		
Power outage		1740		
Power outage		1860		
June event (first rain fall)	6/13/97	2520	105	Estimated to be 0.6-0.7" at YM, no actual measurement
Refluxing of condensed water in the borehole?		2900		Fluctuation of T starting at 2900 in Figure 2.2-2
Mal-functioning of data acquisition system		3200-3280		Appear to be a smooth line in Figure 2.2-2
Refluxing of condensed water in the borehole?		4520		Fluctuation of T starting at 4520 in Figure 2.2-2
Sept event (second rain fall)	9/02/97	4475	186	Reported 5.0" at YM, no actual measurement
Power rampdown to maintain T at 140 C	10/6/97 (12 pm)	5282	220	**Need to know the actual power**
Cooling started by shot down heaters	?	?	?	Need to model cooling rate and when cooling phase started?

Table 2.3-2 Easy calendar of the Large Block Test

Date	2/28	3/31	4/30	5/31	6/30	7/31	8/31	9/30	10/6*	10/31	11/30	12/31	1/31	2/28
Hrs	0	31	60	92	122	153	184	214	220	245	275	306	337	365
* heater turned on														

2.2. Parameters Needed for TH Coupled Analyses Using *Multiflo*

2.2.1 Summary of Parameters

a. Matrix hydrologic parameters
- porosity
- permeability
- residual saturation
- van Genuchten α
- van Genuchten β

b. Fracture hydrologic parameters
- porosity
- permeability
- residual saturation
- van Genuchten α
- van Genuchten β

c. Matrix thermal Properties
- Thermal conductivity
- density
- specific heat (dry)

d. Other properties or parameters
- infiltration
- head load
- with/without backfill
- maximum cut off value for capillary pressure
- residual gas saturation

2.2.2. Parameters for the LBT Modeling

2.2.2.1 Case 1 (LBT1.dat)

- Parameters are taken from DOE pretest predictive analyses, see Wilder et al., 1997, unless noted otherwise. As described by Wilder et al. (1997), these parameters used rock properties from the *Reference Information Base* (RIB, DOE, 1995), with the bulk permeability adjusted to approximate the median value obtained by single-borehole air-injection measurements on the block.
- The initial liquid saturation for Case A was 80% of pore volume, the approximate medium number from the single-borehole air-injection measurement shown in Figure 2.1-4.
- Parameters are summarized in Table 2.2-1. Case A uses parameters of Tsw2.

Table 2.2-1. Matrix thermal and hydrologic properties and fracture hydrologic properties

Parameters		TSw2[a]	Tsw35[b]	TSw[c]
Matrix thermal and Hydrologic Properties				
Thermal Conductivity	Dry	2.10	1.56	2.10
	Wet[5]	2.10	2.33	2.78
Specific Heat [J/(kg-K)]		928	948	840
Density (kg/m^3)		-	-	2580
Porosity		0.11	0.11	0.139
Ksat (m/s) [Permeability (m^2)]		(4.00e-18)	(1.01e-15)	2.089e-11 (2.131e-18)
Residual Saturation		-	-	0.045
	α (m^{-1}) (Pa^{-1})	6.40e-7	7.72e-7	1.355e-2 (1.355e-6)
	β (Pa^{-1})	b=1.47	b=1.47	1.799
	$\lambda = 1 - 1/\beta$			0.444
Fracture Hydrologic properties				
Porosity		1.19e-4	2.34e-4	1.800e-3[c1]
Ksat (m/s) [Permeability (m^2)]		8.33e-10	6.55e-9	3.900e-12[c2]
Residual Saturation		-	-	0.04
van Genuchten Parameter	α (m^{-1}) (Pa^{-1})	1.34e-3	6.86e-4	13.1 (1.31e-3)
	β	b=3.00	b=3.00	4.23[c3]
	$\lambda = 1 - 1/\beta$			0.764

[a]TSw2 properties were obtained from Klaveter and Peters (1986), with some modification by Wilder et al. (1997).

[b]tsw34 properties were obtained from Lawrence Berkeley National Laboratory (LBL) parameter set 4 (Bodvarsson and Bandurraga, 1996) and used by Wilder et al. (1997).

[c]TSw properties are presented only for the purpose of comparison. These properties were from TSPA-93 mean values as documented in Section 4 of Scientific Notebook No. 204, unless noted otherwise as followings:

[c1]TSPA-93 values lead to excessive computer time. Therefore, these values were taken from ???

[c2]TSPA-93 values lead to excessive computer time. Therefore, these values were taken from TSPA-95 Table 4-2-2
[c3] Parameter statistics not available in TSPA-93. Values are from TSPA-95 Table 4.2-2

Other useful parameters:

Bulk permeability (m^2): 9.87e-12 to 3.30e-15 for TSw2, 1.59e-12 for tsw34

2.2.2.2 Other Cases

- Six additional runs are conducted using two rock property sets with different initial liquid saturations to study the effect of rock properties and initial conditions on the calculated rock response.
- Parameters for these six additional cases are given in Table 2.1-2.

Table 2.2-2 Initial liquid saturation for the six cases

Case No.	Rock Unit	Liquid Saturation
Case 1	TSw2	0.92
Case 2	TSw2	0.70
Case 3	TSw2	0.65
Case 4	tsw34	0.92
Case 5	tsw34	0.70
Case 6	tsw34	0.65

2.2.4 Other Parameters

- maximum cut off value for capillary pressure (50, according to previous multiflo calculation)
- residual gas saturation (0, according to previous multiflo calculation)

2.3. Tentative Plans and Assumptions for LBT Modeling

2.3.1 Homogeneous Case, ECM Modeling

Homogeneous block having the dominant bulk permeability as measured by single-borehole air injection

2.3.2 Homogeneous Case with Fractures

2.3.3 Heterogeneous Case, ECM Modeling

Heterogeneous block with the permeability profile obtained from air injection. The heterogeneous permeability field had a "layer-cake" distribution because the permeability measured at any depth was assumed to be constant from that depth

2.4. Model Geometry and Boundary Conditions

2.4.1 Homogeneous Cases

A quarter-symmetry section was modeled, similar to the section used for the conduction-only model (Lee, 1995b). The grid is rectangular with ? nodes. Grid dimensions vary from ? cm at the heater boreholes to a maximum of 20 cm (?) within the block.

The geometry of the LBT and the quarter-symmetry section are depicted in Figure 2.4-1. Mesh for Multiflo calculation is shown in Figure 2.4-2.

2.5. Modeling Process and Results

2.5.1 Basic Data

The rock was heated at 450 W per heater for six months (182.5 days) (or other arrangement, need to double check on this in Wilder's report) until temperature at the wall until the maximum temperature reaches 140 C at the walls of the heater boreholes.

It is assumed that heating power levels i the boreholes are identical and that heat is delivered uniformly along the heated length of each borehole

The top-surface temperature of the block was fixed at 60 C.

The Side-surface temperature ?? (how to control?)

Incorporating power failures that occurred during the test in these test cases of A (i.e., A1 through A2), but not in Case A.

Important Times (dates):

Heater Turned On: February 28, 1997, at 10 am.
Temperature reach 140 C: November 6, 1997 ?
Temperature maintained at 140 C: 12/6/1997 - 1/5/98
Start controlled cool down: 1/5/98

Heater Power Level: 450 w each

Background Temperature: 13 C (was collected for 18 hours, need to find these data)

Background moisture saturation levels: 60-80% for porosity of about 11%, not significantly affected by cutting the block.
Fraction volume water content is 0.08 to 0.1 and increases with depth (see figure 2.1-4). Since the porosity of the core samples of the large block was determined to be 10.4 +- 1.3%. The fraction volume water contents of 0.08 to 0.1 correspond to a range of saturation levels between 77 and 96% (Wilder, et al. 1997).

Rain Falls: a. 118 days after heating, b. 185 days after heating

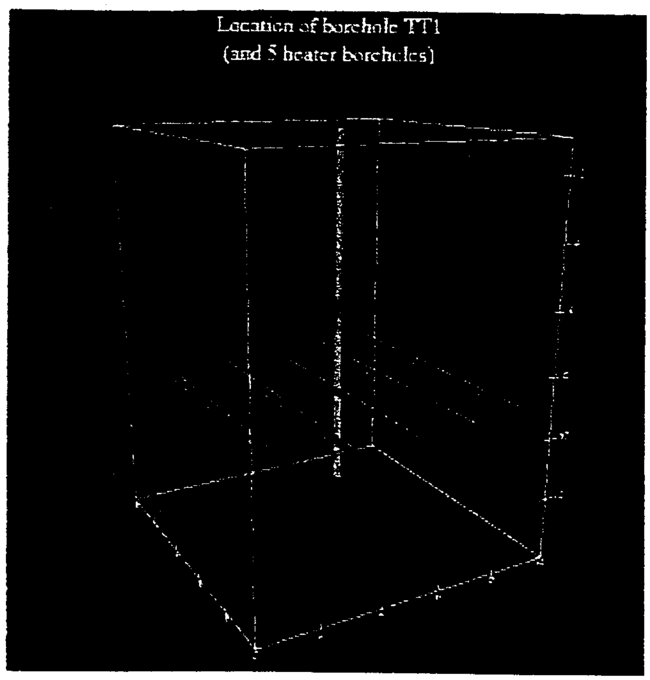


Figure 2.4-1 Three-dimentional geometry of hte Large Block Test and quarter-symmetry section for thermal-hydrologic modeling.

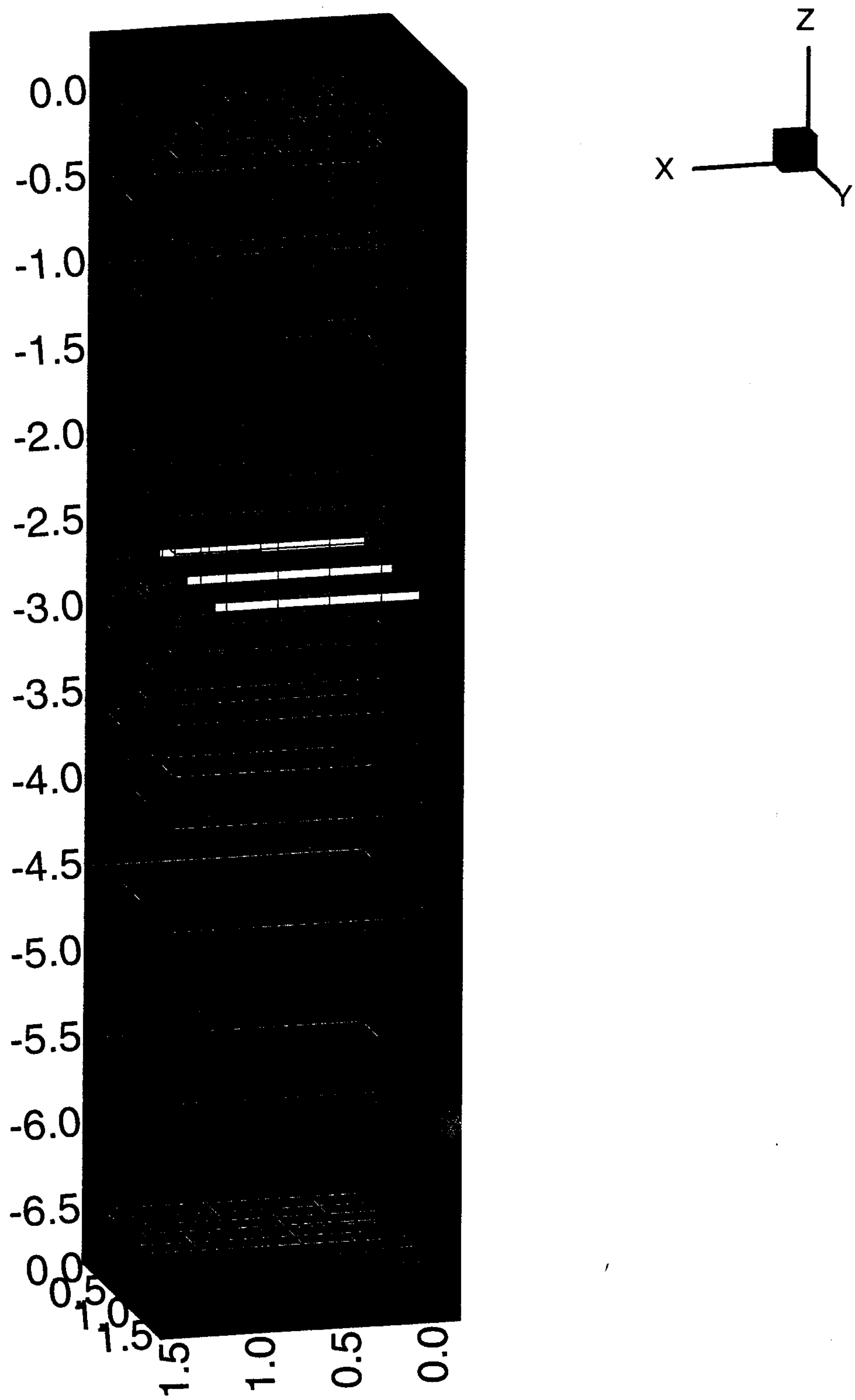


Figure 2.4-2 Mesh for Metra simulation of the quarter-symmetry section of the Large Block Test

Other Dates:

Cutting started: 12/93

2.5.2 Case 1 (LBT1.DAT)

Input Notes:

1. Hydro properties used TSPA-95 properties, because LLNL predictive properties yielded low temperature

Major Results:

1. Figure 2.5-1 and 2.5-2 show history of temperature and liquid saturation at a few points. As figure 2.2-1 shows that temperature at the heater plane is close to 140 C, however, it never reach 140 C. Monitoring points selected are not very effective for monitoring saturation.
2. Figure 2.5-3 and 2.5-4 show temperature and liquid saturation profile along a vertical line through the center of the block. Temperature profile looks very good and is comparable with those obtained by LLNL. However, the water saturation profile looks a lot different from those of LLNL. The main reason is because water content at the top. Should top boundary have 0.99 gas saturation (in another word, 0.01 water saturation)? Does 0.99 gas saturation means steam could move away from the top surface?

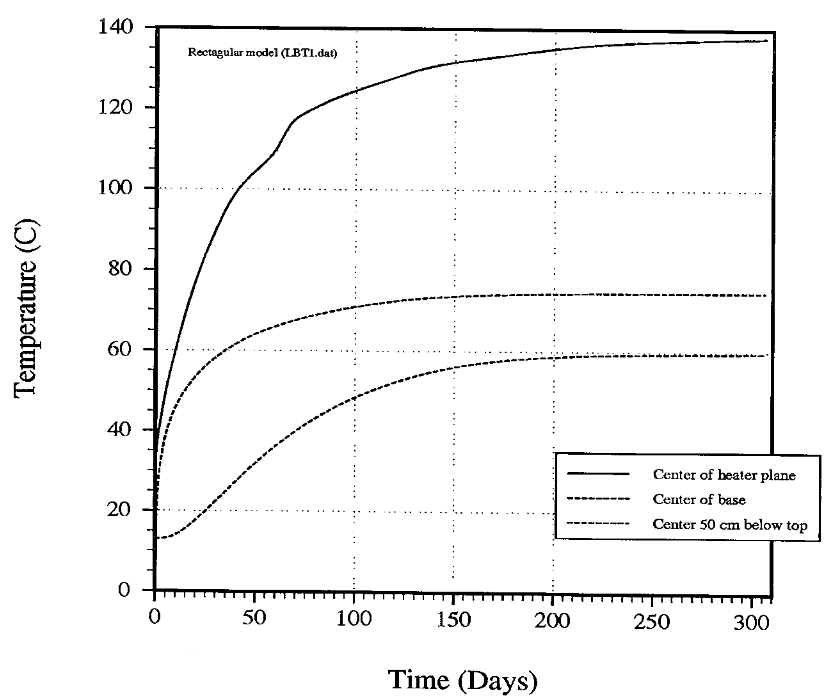


Figure 2.5-1 Temperature histories at a few points in the 3D LB model from LBT1

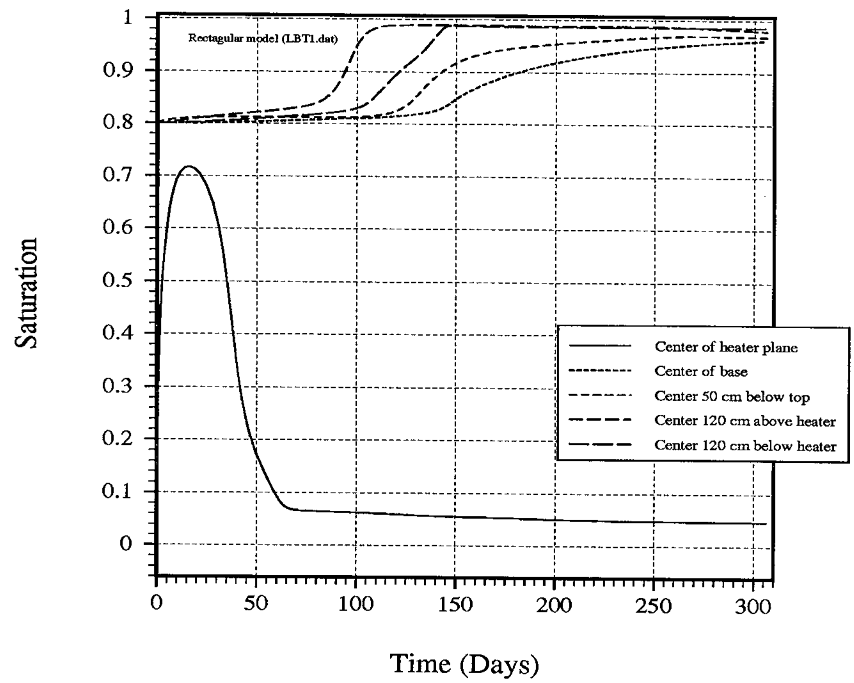


Figure 2-5.2 History of water saturation at a few points in LB model from LB1.dat

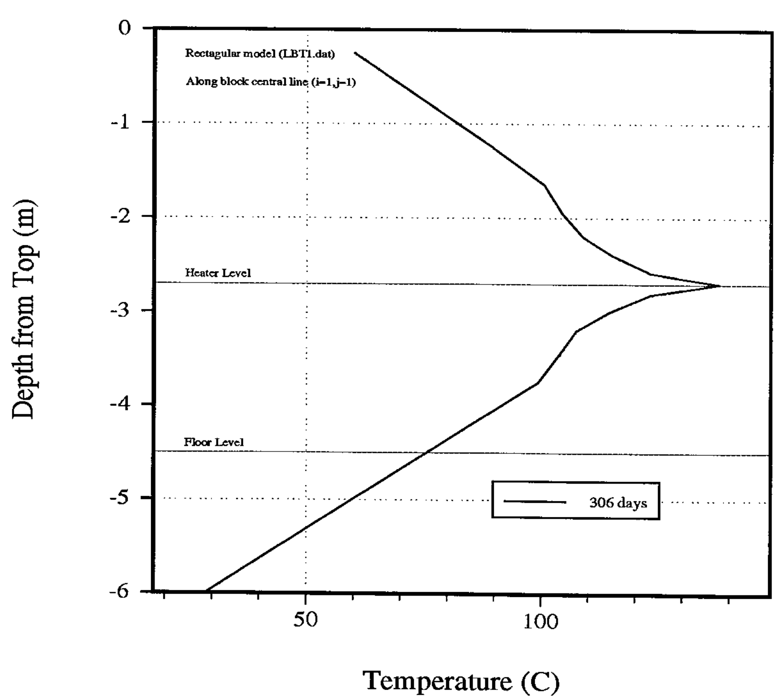


Figure 2-5.3 Temperature © along a vertical line through the center of the Large Block Model

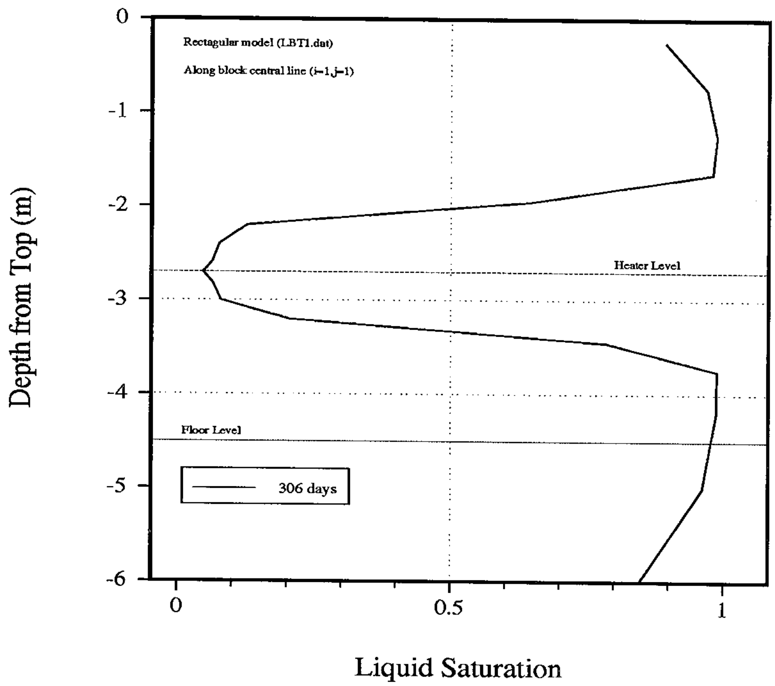


Figure 2.5-4 Water saturation along a vertical line through the center of the Large Block from LBT1.dat.

2.5.3 Case 2 (LBT2.DAT)

- Added monitoring point at 40 cm below and above the heater plan
- change boundary condition at the top boundary to have gas content of 0.99
- change hydro properties to those of LLNL

The initial calculation of *LBT2.dat* did not maintain the water saturation at the top surface close to zero. It was concluded that *Bcon* is not effective. The initial gas saturation should be changed to 0.99 for the top layer (using *Init*). Also, the volume of the top layer should be changed to very large so that it becomes a water sink. Results after these adjustment are shown in Figure 2.5-5 through 2.5-8.

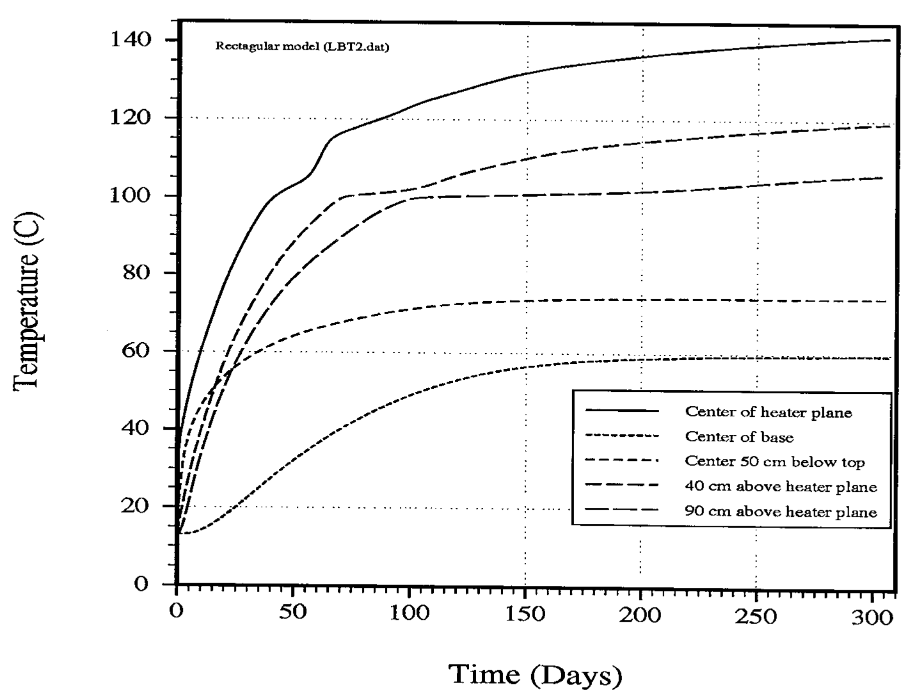


Figure 2.5-5 Temperature histories at a few points in the 3D LB model from LBT2.DAT

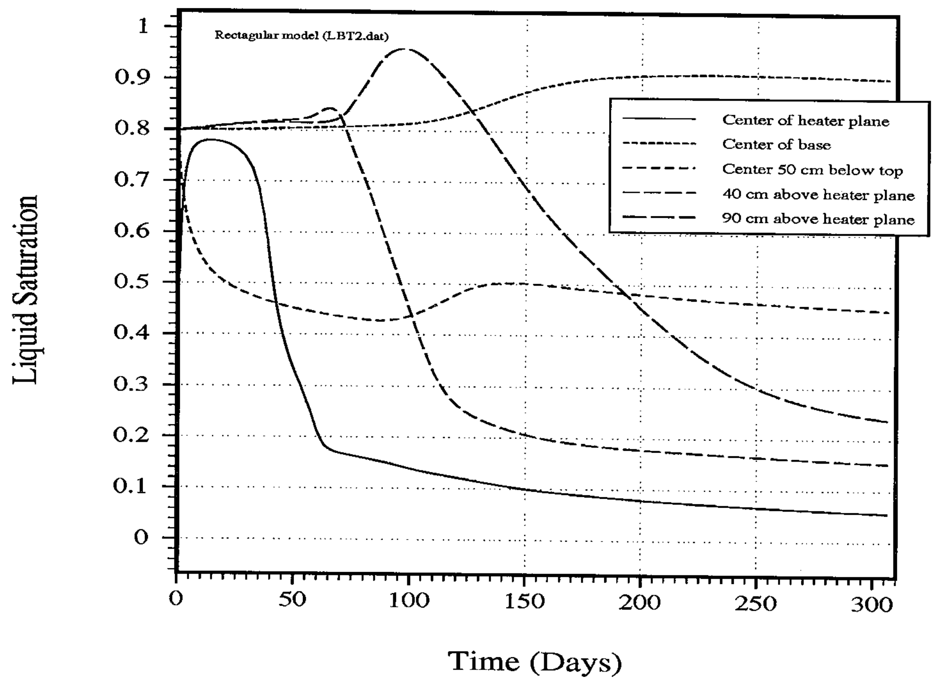


Figure 2.5-6 Histories of water saturation at a few points in the LB model from LBT2.dat

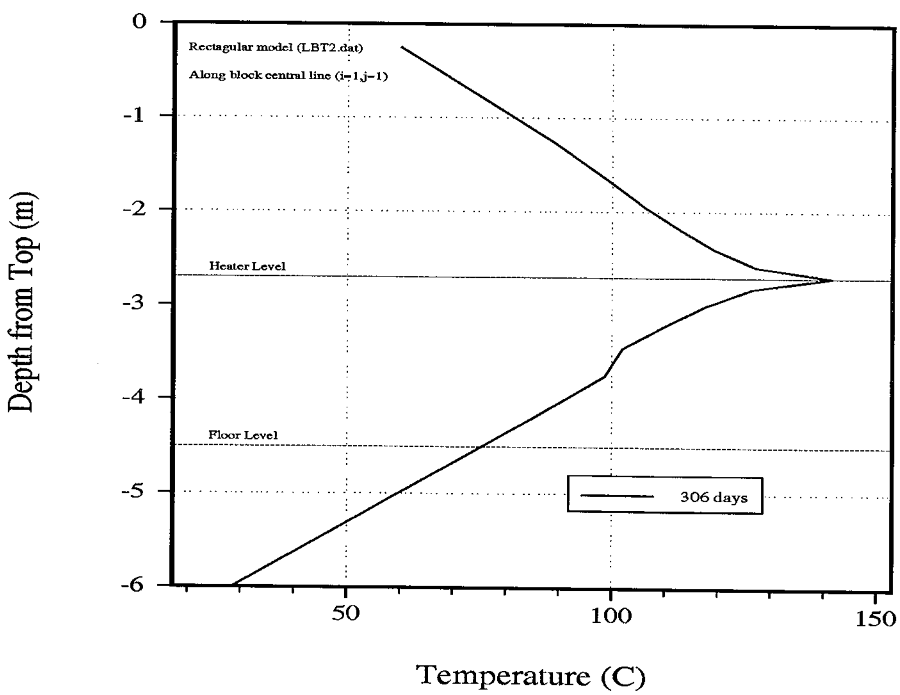


Figure 2.5-7 Temperature along a vertical line through the center of the Large Block model from (LBT2.dat)

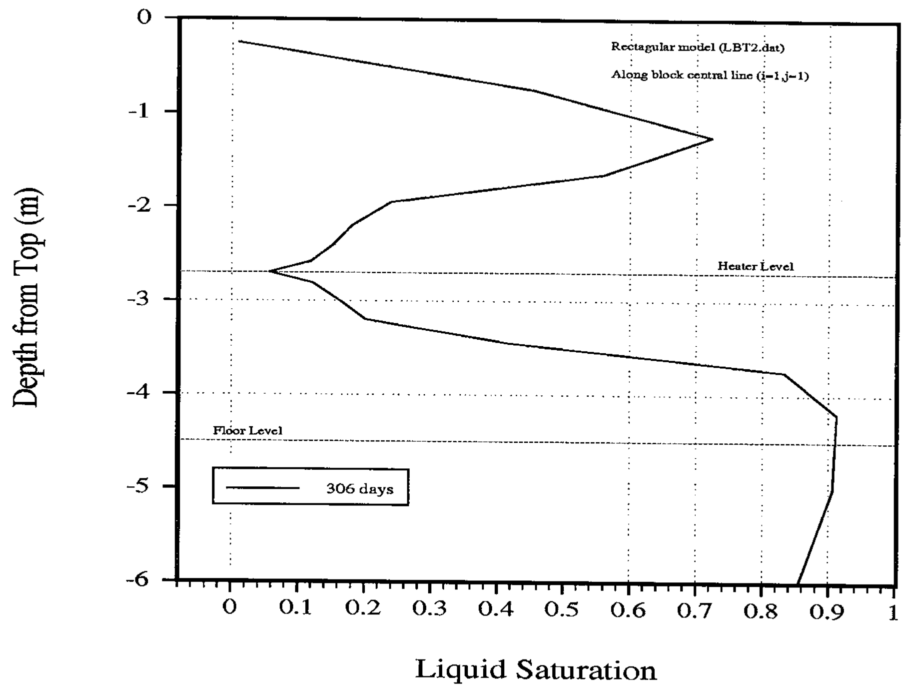


Figure 2.5-8 Water saturation along a vertical line through the center of the Large Block Model from LBT2.dat.

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Appendix A

Not used. RC 12/08/98

Appendix B

Not used. RC 12/08/98

______________________Reply Separator______________________
Subject: Re:Electronic Scientific Notebooks
Author: Rui Chen
Date: 12/8/98 8:09 AM

Bruce,

No input were made to scientific notebook No. 254 during the last printing period (July through September), since the work "TH Modeling of Large Block Test" under the TEF KTI was discontinued. Also, no additional input will be made in the future. Please close this notebook.

Thanks,

Rui

12/08/98

QAP-001 ______________________Reply Separator______________________
Subject: Electronic Scientific Notebooks
Author: Bruce Mabrito
Date: 12/4/98 10:09 AM

From the Electronic Scientific Notebook "call" at the end of September, all CNWRA staff members have turned in their respective copies (or responded that there are no entries) except for Rui Chen (Electronic Scientific Notebooks No. 254 and 274) and Chuck Connor (Electronic Scientific Notebook No. 267).

There will be another quarterly call for Electronic Scientific Notebooks at the end of December.

Please provide either Maria Padilla or me with the unbound printed pages of your Electronic Scientific Notebook or an electronic message stating there have been no entries as soon as possible. Thank you.
Bruce x 5149

I have reviewed this scientific notebook and found it to be consistent with QAP-001 requirements 12/11/98