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 objectives of this task are two folds: 1. establish procedures for TEF KTI implementation of EBSPAC and TPA codes for sensitivity analyses; and 2. carry out analyses to develop estimates of sensitivity of dose to gravity-driven refluxing and to thermally-induced perturbations in water flux through the repository.

1.2. Technical Approaches

Estimation of sensitivity of dose to gravity-driven refluxing and thermally-induced perturbations in water flux through the repository is to be accomplished using TPA code through EBSPAC module. While TPA code controls the probabilistic aspects of the input parameters and spatial discretization of the repository, EBSPAC evaluates the actual, deterministic effects of input parameters on various EBSPAC output parameters for each TPA sub-area. At the present stage, only EBSPAC will be used to analyze one particular sub-area witch corresponds to one basic unit consisting a column from ground surface to water table with cross section equals to a drift spacing and a waste package (WP) spacing. Following is a list of specific steps to be taken:

Determine cases to be considered

Baseline cases will be those listed in Table 1-1 which consider the effects of (1) three thermal loading (or two, the high and the low); (2) with and without ventilation; (3) with and without backfill. Additional cases may include:

<u>Backfill properties:</u>

backfill thermal conductivity (0.2, 0.6 2.0, 10.0 W/m-K)
backfill initial saturation (0.01, 0.5, 0.99)

<u>Effect of media properties (??):</u>

evaluate the hydraulic conditions at Yucca Mountain (YM) for different, yet reasonable,

Table 1-1. Cases for Parameter Sensitivity Analyses Using EBSPAC (Modified Based on Manteufel, 1996)

Set	AML (MTU/Acre)	Ventilation (up to 100 yr)	Backfill at 100 yr
1	80	N	N
2	80	N	Y
3	80	Y	N
4	80	Y	Y
5	40	N	N
6	40	N	Y
7	40	Y	N
8	40	Y	Y
9	20	N	N
10	20	N	Y
11	20	Y	N
12	20	Y	Y
y: yes N: no			

homogeneous hydraulic property values assigned to the Paintbrush Tuff (PTn) and Calico Hills (CHnv) units located above and below the proposed repository horizon, respectively, in the presence of heat-generating HLW (Green 1996).

geologic structure and features on the evolution of perched water body (??):

perched water (? Goodluck and Ross)

geologic structure and media hydrologic properties on temperature and saturation

Effect of a zone of higher permeability (width) intersecting the drift on thermohydrology of the drift (temperature, saturation, and relative humidity within the drift and at the drift wall).

Evaluation of baseline cases

The results of baseline cases listed in Table 1-1 from thermal model (Manteufel 1996, figure 5-1 in EBSPAC manual) will be used in EBSPAC to look at the effects of thermal load, ventilation, and backfill on various EBSPAC output parameters.

Effect of other cases

(Need more consideration as how to incorporate them)
[The effect of various factors on importance of various factors will be examined, including baseline factors list in Table 1. The sensitivities will be examined through comparisons of the statistical properties of the CCDFs. (Use of TPA??)]

1.3. Data Sources

To implement EBSPAC, TEF KTI will provide parameter estimates and the technical basis for those estimates. The primary parameters include:

Temperature and Relative Humidity Data (5.1.1 in EBSPAC report)

- WP temperature as a function of time
- WP relative humidity (RH) as a function of time
- drift wall temperature as a function of time (no longer used?)

These parameters are implemented in EBSPAC through tabular data files *tefkti.inp* and *floebs.dat*. Most of these parameters are obtained through the so called **Thermal Model**, which is a set of external calculations to EBSPAC developed within the TEF KTI. An example of such calculation is described in detail by Manteufel (1996).

Some basic cases to be studied for sensitivities using EBSPAC are listed in Table 1-1. Others may include variations of these basic cases considering other factors studied by TEF KTI in FY96 and FY97 sensibility study, namely:

<u>Effect of backfill on temperature and saturation:</u>

a. backfill thermal conductivity (0.2, 0.6 2.0, 10.0 W/m-K)
b. backfill initial saturation (0.01, 0.5, 0.99)

<u>Effect of media properties on prediction of moisture redistribution:</u> (?)

evaluate the hydraulic conditions at YM for different, yet reasonable, homogeneous hydraulic property values assigned to the Paintbrush Tuff (PTn) and Calico Hills (CHnv) units located above and below the proposed repository horizon, respectively, in the presence of heat-generating HLW (Green 1996).

<u>geologic structure and features on the evolution of perched water body</u> (?)

perched water (? Goodluck and Ross)

<u>geologic structure and media hydrologic properties on temperature and saturation</u> (?)

Effect of a zone of higher permeability (width) intersecting the drift on thermohydrology of the drift (temperature, saturation, and relative humidity within the drift and at the drift wall).

Water Flow Data (5.2.2 in EBSPAC report)

- rate of flow into EBS.

The infiltration of meteoric water and its arrival at the WP is a function of the hydro-stratigraphic conditions above and below the repository horizon. The carrying capacity of the fractures and matrix above the repository, as well as horizontal diversion depending on the dip of fractures and matrix above the repository, as well as horizontal diversion depending on the dip of the bedding planes, and thermal conditions will dictate the rate of infiltration into the EBS. In some instances the infiltrating water may reach the EBS by matrix-only flow. EBSPAC uses the funnel flow concept adopted in SOTEC to represent flow into the EBS. The funnel flow concept assumes that flow through fractures over a wide area will converge to focused spots on the drift and will result in dripping of water on the WP. The average fracture infiltration rate can be specified as a function of time for more realistic input of infiltration data. Detailed calculation of infiltration performed elsewhere (Stothoff, 1996, Stothoff et al, 1996) will provide average fracture infiltration rate.

Other input for EBSPAC (??)

- critical RH above which the water vapor condenses
- thickness of water film on the WP surface (a uniform thickness all around the WP is assumed)
- backfill porosity corresponding to zone 1
- funnel factor or fractional area for capture of darcy flow onto WP
- water level inside the WP expressed as a fraction of WP internal diameter

1.4. Computers, Computer Codes, and Data Files

Table 1-2. Computing Equipment

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

Table 1-2 lists computer equipment and computer codes. Table 1-3 provides names, type, and content of data files for EBSPAC analyses.

Table 1-3. Names, Type, and Content of Relative EBSPAC Files

File Name	Type	Content
ebspac_fail.x	executable of EBSPAC code	executable of EBSPAC code
TEFKTI.inp	text	input temperature and RH data file for EBSPAC from TEF KTI
Example_fail.inp	text	EBSPAC input data file
temphumd.dat chloride.dat	text	EBSPAC output data files

2. IN-PROCESS ENTRIES

2.1. Establishment of EBSPAC and TPA Implementation Procedures

Result from four cases of MULTIFLO analyses on the effect of thermal conductivity of backfill materials were used to establish EBSPAC and TPA implementation procedures for TEF KTI.

2.1.1 Thermal-Hydrological Model - Effect of Thermal Conductivity of Backfill Materials

The six-layer ECM hydro-stratigraphic model of YM taken from TSPA-95 was used in analyses of the effect of backfill thermal conductivity. The analyses considered two-phase, nonisothermal flow using computer code MULTIFLO. The numerical model extended from ground surface to water table (at 654 m depth) and included one half of an "unit cell" width (from the center of emplacement drift to the center of the pillar). The model was discretized into 19 elements along the horizontal direction and 43 elements along the vertical direction. The vertical boundaries were modeled as symmetric boundaries (i.e., no heat and no fluid flow). The upper boundary was assigned a uniform, steady infiltration of 0.3 mm/yr.

The modeling started with an initial simulation to achieve steady-state conditions under 0.3 mm/yr infiltration at the top boundary. A 5x5 m^2 emplacement draft was, then, "excavated" by changing the corresponding material properties to "air" properties and a decay heater source with initial heat load of about 84 kW/acre was emplaced. The simulation continued to 100 years with "air" filling the emplacement drift before backfill was emplaced.

Figure 1 shows the time history of WP temperature with backfill thermal conductivities ranging from 0.2 W/m-K to 10 W/m-K. This figure shows that lower backfill thermal conductivity resulted in higher WP temperature. This effect is most pronounced immediately after the emplacement of backfill and gradually becomes insignificant with time. It is interesting to notice that although backfill thermal conductivity affects temperature at the WP, it has little effect on temperature at the drift wall.

2.1.2 EBSPAC Analyses

Output data files from MULTIFLO that contain time history of temperature and relative humidity (RH) at the WP and temperature at drift wall for all four cases described in the previous section were used as input for EBSPAC analyses. A fortran program was developed to read data from MULTIFLO output history files for each of the analysis cases and write out in the format required by EBSPAC. The fortran program is included in Appendix A. EBSPAC input file is included in Appendix B. Table 2-1 lists names and contents of all data files in those analyses.

EBSPAC analyses for all four cases show that no WP failure occur during the simulation time period (10000 yr). Also, backfill thermal conductivity does not appear to significantly affect other EBSPAC output parameters neither. For example, Figure 2-2 depicts the remaining WP overpack thickness as a function of time for all four cases. Although the curves appear to diverge as time increases, there is no significant difference.

2.1.3 References

Green, R.T. 1996. The effect of media properties on prediction of moisture redistribution at a high-level nuclear waste repository. *Proceedings of the Seventh Annual International Conference on High-Level*

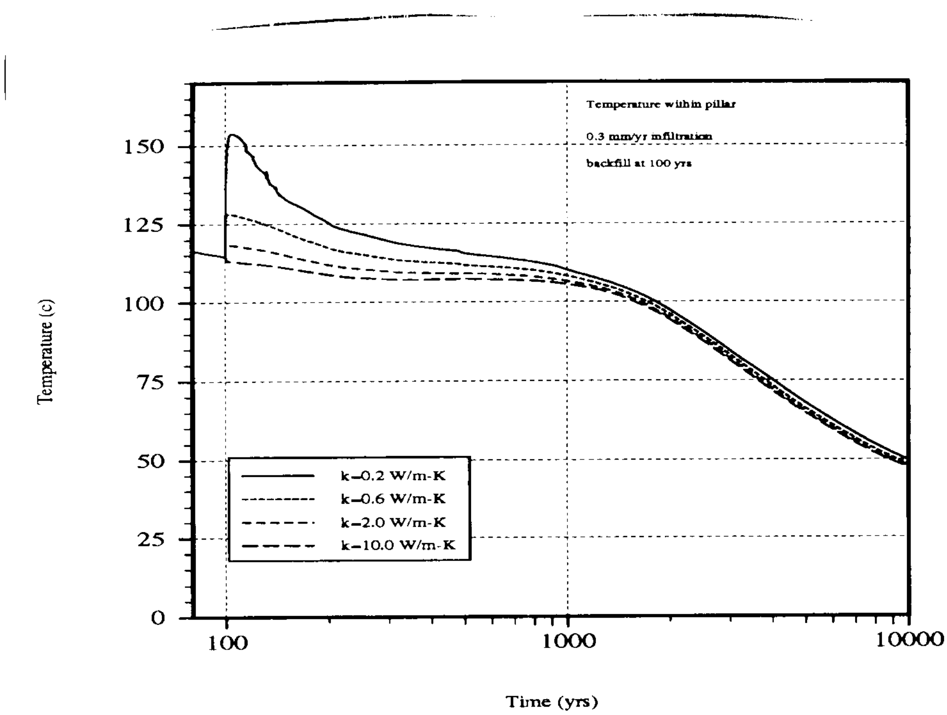

Figure 2-1 Time history of temperature at the WP with backfill thermal conductivity ranging from 0.2 W/m-K to 10 W/m-K.

Radioactive Waste Management. La Grange, Park, IL: American Nuclear Society.

Manteufel, R.D. 1996. Effects on ventilation and backfill on a mined waste disposal facility. *Nuclear Engineering and Design*. Submitted for publication (ask Randy for a copy)

Sothoff, S.A. 1996. Sensitivity of Long-Term Bare-Soil Infiltration Simulations to Hydraulic Properties in an Arid Environment. *Water Resource Research*. Submitted for publication (ask Stuart for a copy)

Stothoff, R.D., H. Castellaw, and A. Bagtzoglou. 1996. Simulating the Spatial Distribution of Infiltration at Yucca Mountain. *Water Resource Research*. Submitted for publication (ask Stuart for a copy)

Table 2-1: Names and Content of Data files for EBSPAC analyses of the Effect of Backfill Thermal Conductivity

File Name	Content
bk1_precls_tmp.xyp bk1_poscls_tmp.xyp bk2_poscls_tmp.xyp bk3_poscls_tmp.xyp bk4_poscls_tmp.xyp	Temperature at waste package and drift wall as functions of time from MULTIFLO analyses
bk1_precls_rh.xyp bk1_poscls_rh.xyp bk2_poscls_rh.xyp bk3_poscls_rh.xyp bk4_poscls_rh.xyp	Relative humidity at waste package as a function of time from MULTIFLO analyses
temphumd.f	Fortran file for reading MULTIFLO output data and writing the data for EBSPAC input
bk_cond.inp	Temperature and humidity history data in EBSPAC specified format for all four cases of backfill thermal conductivity
bk_cond_fail.inp	EBSPAC input file
rthick_his_comb.xpb tmp_his_comb.xpb	Xplot batch files for plotting analysis results
temphumd_bk1.dat temphumd_bk2.dat temphumd_bk3.dat temphumd_bk4.dat	EBSPAC output data file containing temperature and humidity data for corrosion analyses, and WP failure time
chloride_bk1.dat chloride_bk2.dat chloride_bk3.dat chloride_bk4.dat	EBSPAC output data file containing remaining WP thickness

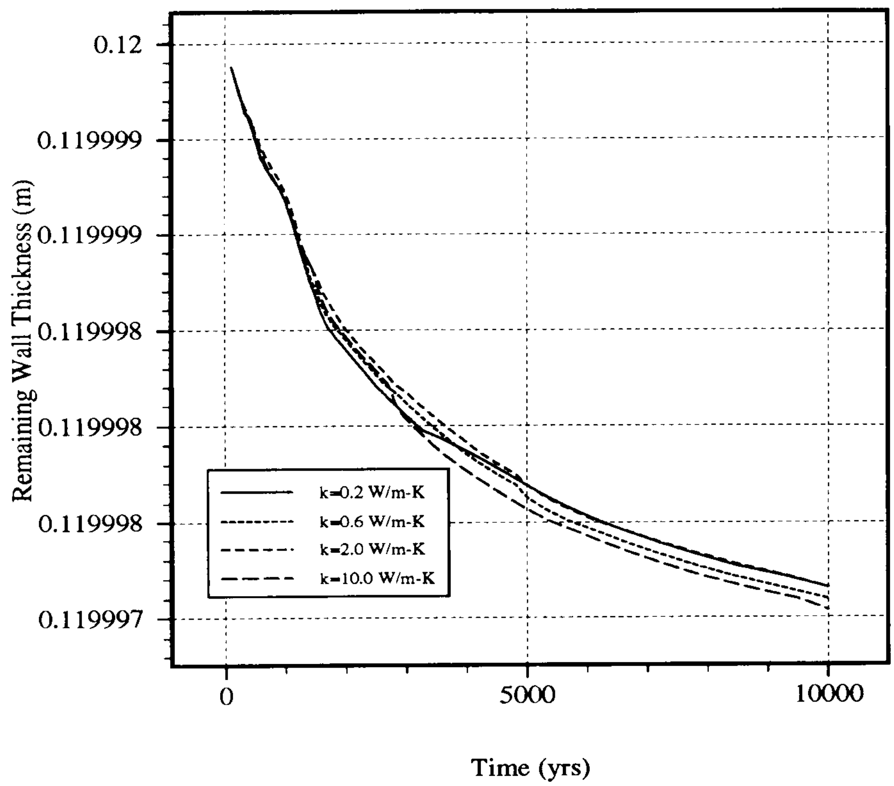

Figure 2-2 Time history of remaining WP wall thickness with backfill thermal conductivity ranging from 0.2 W/m-K to 10 W/m-K.

2.2. Selection of Parameters for TEF Dose-Sensitivity Analyses

2.2.1. Parameters for TEF dose sensitivity analyses using Multiflo and TPA30
2.2.2. Parameters for the base case multiflo calculation
2.2.3. Parameters for dose-sensitivity analyses and data ranges
2.2.4. Parameters and their statistic information from TSPA-93
2.2.5. Parameters used in TSPA-95
2.2.6. Other parameters as input for TPA30
2.2.7. References

2.2.1 Parameters for TEF dose sensitivity analyses using Multiflo and TPA30

2.2.1.1 Parameters used in Multiflo Calculations

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

e. Backfill properties (same as a through c)

2.2.1.2 Parameters to be considered for TEF sensitivity analyses using Multiflo

- Heat load
- With and without backfill
- Matrix permeability
- Matrix van Genuchten α
- Fracture permeability
- Fracture van Genuchten α
- Matrix porosity (?)

2.2.2. Parameters for the base case

(Parameters are taken as TSPA-93 mean values as documented in Section 4, unless noted otherwise)

2.2.2.1 Matrix hydrologic properties

Table 2.2.2-1. Matrix hydrologic properties

Parameters		TCw	PTn	TSw	TSv	CHnv	CHuz
Porosity		0.087	0.421	0.139	0.065	0.331	0.306
Ksat (m/s) [Permeability (m^2)]		2.042e-11 (2.083e-18)	3.802e-7 (3.879e-14)	2.089e-11 (2.131e-18)	9.772e-12 (9.967e-19)	1.096e-9 (1.118e-16)	1.585e-11 (1.617e-18)
Residual Saturation		0.021	0.154	0.045	0.118	0.097	0.121
van Genuchten Parameter	α (m^{-1}) (Pa^{-1})	7.907e-3 (7.907e-7)	5.559e-1 (5.559e-5)	1.355e-2 (1.355e-6)	2.193e-3 (2.193e-7)	2.786e-2 (2..786e-6)	5.943e-3 (5.943e-7)
	β	1.622	2.371	1.799	2.228	2.460	1.706
	$\lambda = 1 - 1/\beta$	0.383	0.578	0.444	0.551	0.593	0.414

2.2.2.2 Fracture hydrologic properties

Table 2.2.2-2. Fracture hydrologic properties

Parameters		TCw	PTn	TSw	TSv	CHnv	CHuz
Porosity*		1.800e-3	1.800e-3	1.800e-3	1.800e-3	1.800e-3	1.800e-3
Ksat (m/s) [Permeability (m^2)]**		3.900e-12	3.900e-13	3.900e-12	3.900e-12	3.900e-13	3.900e-12
Residual Saturation1		0.04	0.04	0.04	0.04	0.04	0.04
van Genuchten Parameter	α (m^{-1}) (Pa^{-1})	12.3 (1.23e-3)	14.0 (1.40e-3)	12.2 (1.22e-3)	13.1 (1.31e-3)	12.2 (1.22e-3)	7.3 (7.3e-4)
	β ***	4.23	4.23	4.23	4.23	4.23	4.23
	$\lambda = 1 - 1/\beta$	0.764	0.764	0.764	0.764	0.764	0.764

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

** TSPA-93 values lead to excessive computer time. THerefore, these values were taken from TSPA-95 Table 4-2-2

*** Parameter statistics not available in TSPA-93. Values are from TSPA-95 Table 4.2-2

2.2.2.3 Matrix Thermal Properties

Table 2.2.2-3 Matrix thermal (dry) properties*

Unit	Thermal Conductivity [W/(m-K)]		Density (kg/m^3)	Specific Heat [J/(kg-K)]
	Dry	Wet**		
TCw	1.69	2.23	2580	728
PTn	0.61	0.81	2580	422
TSw	2.10	2.78	2580	840
TSv	1.28	1.69	2580	948
CHnv	0.84	1.11	2580	488
CHnz	1.42	1.88	2580	526

* TSPA-95 p 4-19 Table 4.2-3
** Higher values are assigned for wet thermal conductivity to be more realistic

2.2.2.4 Others

- Thermal load (83 MTU/acre, TPA30 data)
- Infiltration (0.05 mm/yr, previous multiflo calculation) (See Ron Green's Memo dated 05/27/97) .
- maximum cut off value for capillary pressure (50, previous multiflo calculation)
- residual gas saturation (0, previous multiflo calculation)

2.2.2.5 Backfill hydrologic and thermal properties

Table 2.2.2-4 Backfill hydrologic and thermal properties*

Parameters			Unit	Values
Porosity	Matrix		-	0.500
	Fracture***			1.8e-3
Permeability	Matrix		m^2	3.9e-14
	Fracture			3.9e-12
van Genuchten Parameter	α	Matrix	m^{-1} (Pa^{-1})	0.111 (1.106e-5)
		Fracture		0.131 (1.305e-5)
	β	Matrix	-	3.333
		Fracture		4.230
	$\lambda = 1 - 1/\beta$	Matrix	-	0.700
		Fracture		0.764
Residual Saturation	Matrix		-	0.010
	Fracture			0.040
Thermal Conductivity**	Unsaturated		W/(m-K)	0.260
	Saturated			0.490
Density			kg/m^3	2580
Specific Heat			J/(kg-K)	840

* According to TSPA-95, Tables 4-2.1 through 4-2.3.
** According to Green et al. (1997)
*** Previous Multiflo input file

Memo from Ron Green 5/27/97

A refined 3D basecase MULTIFLO model has been formulated for process-level TEF calculations (i.e., temperature, relative humidity, liquid flux). The refined model has the same six layers as in TSPA-95 but with property values taken from TSPA-93, with the following exceptions. The thermal conductivity is assigned the same dry values as in TSPA-93 but with higher values for wet thermal conductivity. TSPA-93 had unrealistically assigned the same value to both dry and wet conditions.

The fractures are assigned permeabilities of e-12 and e-13 m^2, similar to TSPA-95, but much lower than the e-9 m^2 assigned in TSPA-93. Using the TSPA-93 values results in excessively long computation times (i.e., several days or weeks). I suspect that is the same reason TSPA-95 assigned the lower permeabilities to fractures.

An infiltration rate of 0.05 mm/yr was selected, even though much recent work suggests that Yucca Mt infiltration rates may be significantly higher (i.e., greater than 10 mm/yr). The lower infiltration rate was chosen because of modeling limitations due to the ECM formulation. An infiltration rate of 0.05 mm/yr results in TSw saturations of about 0.92-0.97, somewhat higher than the values observed in the TSw at Yucca Mt. However, an infiltration rates of 0.3 mm/yr or greater result in TSw saturations that approach unity, certainly an unrealistic estimation of the site. These excessively high saturations from the higher infiltration rates are due to the inability of the ECM to replicate infiltration by fracture flow. (Note: This result supports the premise that the majority of infiltration at Yucca Mt occurs as fracture rather than matrix flow). The higher saturations have a significant effect on depressing temperatures and increasing humidity and liquid flux rates. It is important to maintain realistic saturation values in the simulations. Therefore, a 0.05 mm/yr infiltration is assigned to the basecase because it approximates the matrix infiltration rate, not because it is close to the total infiltration rate.

This basecase requires about 0.5 to 0.6 days to run on a sparc 20. This time requirement should not be a limitation to the process-level sensitivity runs. Please provide any comments or questions regarding these basecase property assignments.

2.2.3 Parameters for dose-sensitivity analyses and data ranges

2.2.3.1 Scooping analyses on effect of matrix porosity

[TSw: E(x)=0.139, Emin=0.082, Emax=0.196]

2.2.3.2 Selection of parameters and data range

Parameters to be studied

1. Heat load
2. With or without backfill
3. Matrix permeability
4. Matrix van Genuchten α
5. Fracture permeability
6. Fracture van Genuchten α

Table 2.2.3-1. Statistical data

Rock Units	Parameters	E[x]	Low	High	Source
-	Heat Load (mtu/acre)	-	25	85	TSPA-95
	Backfill		No	Yes	-
TSw	Matrix Ksat (m/s) [Permeability (m^2)]	2.089e-11 2.131e-18	2.884e-13 2.942e-20	1.072e-8 1.093e-15	TSPA-93
	Matrix van Genuchten α (m^{-1})	1.355e-2	2.099e-3	5..000e-1	TSPA-93
	Fracture Ksat (m/s) [Permeability (m^2)]	1.566e-2 1.598e-9	3.303e-5 3.369e-12	1.159 1.182e-7	TSPA-93
	Fracture van Genuchten α (m^{-1})	12.2	0.4	81.0	TSPA-93

2.2.4 Parameters and their statistic information from TSPA-93

2.2.4.1 Matrix statistics from TSPA-93

Table 2.2.4-1. Matrix saturated hydraulic conductivity (m/s) [permeability (m^2)]*

Unit	E(x)	min [E(x)-SD}	max [E(x)+SD]
TCw	2.042e-11 (2.083e-18)	6.310e-13 (6.436e-20)	6.1663e-9 (6.290e-16)
PTn	3.802e-7 (3.879e-14)	1.175e-9 (1.199e[16])	1.738e-4 (1.773e-11)
TSw	2.089e-11 (2.131e-18)	2.884e-13 (2.942e-20)	1.072e-8 (1.093e-15)
TSv	9.772e-12 (9.967e-19)	2.692e-13 (2.746e-20)	2.239e-10 (2.284e-17)
CHnv	1.096e-9 (1.118e-16)	3.981e-12 (4.061e-19)	1.047e-6 (1.068e-13)
CHnz	1.585e-11 (1.617e-18)	6.761e-15 (6.896e-22)	1.072e-8 (1.093e-15)

* TSPA-93 p 7-14 Table 7-5b (Entropy-fit beta distribution parameters)

Table 2.2.4-2. Matrix porosity (-)*

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	0.087	0.032	0.142
PTn	0.421	0.317	0.525
TSw	0.139	0.082	0.196
TSv	0.065	0.022	0.108
CHnv	0.331	0.241	0.421
CHnz	0.306	0.242	0.370

* TSPA-93 p 7-11 Table 7-3 (basic statistics)

Table 2.2.4-3. Matrix α (m^{-1})*

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	7.907e-3	2.588e-4	1.384e-1
PTn	5.559e-1	1.803e-1	1.718
TSw	1.355e-2	2.099e-3	5.000e-1
TSv	2.193e-3	1.758e-4	7.691e-3
CHnv	2.786e-2	1.718e-3	1.109
CHnz	5.943e-3	3.936e-4	3.133e-1
* TSPA-93 p 7-14 Table 7-6b (Entropy-fit beta distribution parameters)			

Table 2.2.4-4. Matrix β *

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	1.622	1.453	1.811
PTn	2.371	1.465	3.839
TSw	1.799	1.337	2.421
TSv	2.228	1.617	3.070
CHnv	2.460	1.554	3.894
CHnz	1.706	1.287	2.261
* TSPA-93 p 7-14 Table 7-6b (Entrop-fit beta distribution parameters)			

Table 2.2.4-5 Matrix residual degree of saturation*

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	0.021	0**	0.076
PTn	0.154	0**	0.325
TSw	0.045	0**	0.106
TSv	0.118	0**	0.285
CHnv	0.097	0**	0.233
CHnz	0.121	0**	0.292
* TSPA-93 p 7-17 Table 7-8 (basic statistics) ** [E(x)-SD] less than zero, set at zero			

2.2.4.2 Fracture statistics from TSPA-93

Table 2.2.4-6 Fracture hydraulic conductivity* (m/s) [permeability (m^2)]

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	1.849e-2 (1.886e-9)	5.211e-4 (5.315e-11)	7.851e-1 (8.008e-8)
PTn	1.883e-2 (1.921e-9)	4.886e-4 (4.983e-11)	2.202 (2.246e-7)
TSw	1.566e-2 (1.598e-9)	3.303e-5 (3.369e-12)	1.159 (1.182e-7)
TSv	1.762e-2 (1.797e-9)	4.064e-5 (4.145e-12)	1.422 (1.450e-7)
CHnv	1.169e-2 (1.193e-9)	1.117e-4 (1.139e-11)	2.535 (2.585e-7)
CHnz	5.022e-3 (5.123e-10)	3.184e-5 (3.247e-12)	6.010e-1 (6.131e-8)
* TSPA-93 p 7-30 Table 7-20 (log_{10} statistics)			

Table 2.2.4-7 Fracture Porosity (-)*

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	8.650e-4	3.200e-4	2.322e-3
PTn	2.339e-4	8.088e-5	6.763e-4
TSw	1.002e-2	2.699e-4	3.722e-3
TSv	8.851e-4	2.377e-4	3.295e-3
CHnv	3.648e-4	9.571e-5	1.390e-3
CHnz	1.884e-4	5.159e-5	6.878e-4
* TSPA-93 p 7-3 Table 7-19 (log_{10} statistics)			

Table 2.2.4-8 Fracture alpha (m^{-1})*

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	12.3	1.7	66.7
PTn	14.0	1.7	111.6
TSw	12.2	0.4	81.0
TSv	13.1	0.5	89.8
CHnv	12.2	0.8	119.8
CHnz	7.3	0.4	58.4
* TSPA-93 p 7-3 Table 7-21 (basic statistics)			

2.2.5 Parameter values form TSPA-95 etc.
(not used for TEF sensitivity analyses, only listed for references)

2.2.5.1 Matrix properties

Table 2.2.5-1 Matrix properties from TSPA-95

Parameters		TCw	Ptn	TSw	Tsv	CHnv	CHuz
Porosity		0.087	0.421	0.139	0.065	0.331	0.306
Ksat (m/s)		9.7×10^{-12}	3.9×10^{-7}	1.9×10^{-11}	1.9×10^{-11}	2.7×10^{-7}	2.0×10^{-11}
Residual Saturation		0.002	0.100	0.080	0.080	0.041	0.110
van Genuchten Parameter	α (m^{-1})	0.0084	0.0153	0.0058	0.0058	0.0163	0.0031
	β	1.558	6.872	1.798	1.798	3.861	1.602
	$\lambda=1-1/\beta$	0.36	0.85	0.44	0.44	0.74	0.38

2.2.5.2 Fracture properties

Table 2.2.5-2 Fracture properties from TSPA-95

Parameters		TCw	Ptn	TSw	Tsv	CHnv	CHuz
Porosity*		1.8×10^{-3}	1.8×10^{-3}	1.8×10^{-3}	1.8×10^{-3}	1.8×10^{-3}	1.8×10^{-3}
Ksat (m/s)		3.9×10^{-5}	3.9×10^{-6}	3.9×10^{-5}	3.9×10^{-5}	3.9×10^{-6}	3.9×10^{-5}
Residual Saturation		0.004	0.004	0.004	0.004	0.004	0.004
van Genuchten Parameter	α (m^{-1})	0.1305	0.1305	0.1305	0.1305	0.1305	0.1305
	β	4.230	4.230	4.230	4.230	4.230	4.230
	$\lambda=1-1/\beta$	0.7636	0.7636	0.7636	0.7636	0.7636	0.7636
*Note: Not from TSPA-95, but from previous Multiflo input file							

2.2.6 Other Parameters as Input to TPA30 (NFENV/THERMAL)
(These parameters are provide to TPA30 for input, most of them are not used in TEF analyses)

2.2.6.1 Mass Density of YM Rock

Table 2.2.6-1 Matrix bulk density (kg/m^3)*

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	2285	2171	2399
PTn	1419	1140	1699
TSw	2247	2112	2381
TSv	2308	2248	2368
CHnv	1737	1447	2027
CHnz	1746	1554	1938
* TSPA-95 p 2-13 Table 2.4-1			

Also see Table 2-3 for approximate value

2.2.6.2 Others

Specific Heat of YM Rock: see Table 2-3 (according to TSPA-95)
Thermal Conductivity of YM Rock: see Table 2-3 (according to TSPA-95)
Effective thermal conductivity of backfill: see Table 2-5 (according to Green et al. 1997)

2.2.7. References

Andrews, R.W., T.F. Dale, and J.A. McNeish. 1994. Total System Performance Assessment-1993: An Evaluation of the Potential Yucca Mountain Repository. B00000000-01717-2200-00099-Rev. 01, Civilian Radioactive Waste Management System, Management and Operating Contractor, Las Vegas, Nevada.

Green, R., J. Prikryl, and M. Hill. 1997. Assessment of Heat Flow Through Bulk Geological Materials. CNWRA Milestone No. 20-5708-661-720. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses.

TRW Environmental Safety Systems Inc. 1995. Total System Performance Assessment - 1995: An Evaluation of the Potential Yucca Mountain Repository. B00000000-01717-2200-00136-Rev. 01, Civilian Radioactive Waste Management System, Management and Operating Contractor, Las Vegas, Nevada.

2.3 Metra Base Case Analyses for TEF Dose-Sensitivity Study

Continued from Mikko's Scientific Notebook #216

2.3.1 Test of Mikko's 3D Metra Base Case

Mikko's 3D Metra base case include 2 geometries and 4 input files:

A. 3D Full Model
- extends from the ground surface (z=0) to the water table (z=-660 m)
- all properties are TSw2 properties (single layer)
- no heater properter, no air or backfill in the draft
- initial gas saturation in the heater region for the second run (c3big_th2.dat) was changed to 0.99 by editing and reformating the Cut and Paste from from *c3big_1_out* using *format.f*
- input files:

c3big_1.dat	full model initial hydrological equilibrium
c3big_th2.dat	full model thermal run

Run #1:

- change properties to base case properties as documented in Section 2.2 2 of this Notebook
- c3big_th2.dat run to about only 300 yrs over more than 24 hrs
- it was speculated that permf is probably causing the problem, so permf (frature permeability) was changed back to the TSPA-95 (3.9e-12) value from base case value (1.598e-9)

Run #2:

- changed permf from 1.598e-9 back to 3.9e-12
- appear to be successful

B. 3D Submodel
- extends from z=-240 m to z=-440 m (i.e., 100 m above and below the repository, respectivly)
- boundary conditions at z=-240 m and z=-440 m are obtained as results at the equivalent depth from the 3D full model (c3big_th2.dat)

3. REFERENCES

Green, R.T. 1996. The effect of media properties on prediction of moisture redistribution at a high-level nuclear waste repository. *Proceedings of the Seventh Annual International Conference on High-Level Radioactive Waste Management.* La Grange, Park, IL: American Nuclear Society.

Manteufel, R.D. 1996. Effects on ventilation and backfill on a mined waste disposal facility. *Nuclear Engineering and Design.* Submitted for publication (ask Randy for a copy)

Sothoff, S.A. 1996. Sensitivity of Long-Term Bare-Soil Infiltration Simulations to Hydraulic Properties in an Arid Environment. *Water Resource Research.* Submitted for publication (ask Stuart for a copy)

Stothoff, R.D., H. Castellaw, and A. Bagtzoglou. 1996. Simulating the Spatial Distribution of Infiltration at Yucca Mountain. *Water Resource Research.* Submitted for publication (ask Stuart for a copy)

Andrews, R.W., T.F. Dale, and J.A. McNeish. 1994. Total System Performance Assessment-1993: An Evaluation of the Potential Yucca Mountain Repository. B00000000-01717-2200-00099-Rev. 01, Civilian Radioactive Waste Management System, Management and Operating Contractor, Las Vegas, Nevada.

Green, R., J. Prikryl, and M. Hill. 1997. Assessment of Heat Flow Through Bulk Geological Materials. CNWRA Milestone No. 20-5708-661-720. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses.

TRW Environmental Safety Systems Inc. 1995. Total System Performance Assessment - 1995: An Evaluation of the Potential Yucca Mountain Repository. B00000000-01717-2200-00136-Rev. 01, Civilian Radioactive Waste Management System, Management and Operating Contractor, Las Vegas, Nevada.

Appendix A

Fortran source code for changing format of temperature and relative humidity data

Filename: /export/home/rchen/TEFKTI/BK_cond/temphumd.f

```
      PROGRAM FORMAT
C ***********************************************************************
C This program converts the format of temperature and relative humidity
C data files from MULTIFLO analyses (jobname_tmp.xyp & jobname_rh.xyp)
C to the format required by EBSPAC analyses (tefkti.inp). Twp is waste
C package temperature, Tw is drift wall temperature, and RH represents
C relative humidity.
C
C Developed by: Rui Chen
C January 8, 1997
C ***********************************************************************
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      CHARACTER LINE*180,FNAME*80
      REAL*8 Time(2000,12),Twp(2000,12),Tw(2000,12),RH(2000,12)
      REAL*8 VAR1(2000,12),VAR2(2000,12)
      INTEGER nset,nrow1_t,nrow1_r,nrow2_t,nrow2_r,nrow_t,nrow_r
      INTEGER flag_t,flag_r
      INTEGER row(12)
C
      PRINT*, 'ENTER Number of Data Set (nset):'
      READ(*,*) nset
C
C Open output file
C
      PRINT*,'ENTER OUTPUT FILENAME'
      READ(*,'(A80)') FNAME
      OPEN(UNIT=3,FILE=FNAME, STATUS='UNKNOWN',FORM='FORMATTED')
C
C Open files and read in data for pre-closre
C
C       PRINT*,'ENTER TEMPERATURE DATA FILENAME FOR PRECLOSURE ANALYSES'
C       READ(*,'(A80)') FNAME
      FNAME='bk1_precls_tmp.xyp'
      OPEN(UNIT=1,FILE=FNAME, STATUS='UNKNOWN',FORM='FORMATTED')
      nrow1_t=0
      DO 11 j=1,1000000
       READ(1,'(A)',END=22) LINE
       IF (LINE(1:1) .NE. '!') then
         nrow1_t=nrow1_t+1
         READ(LINE,*) (VAR1(nrow1_t,k),k=1,5)
         DO 33 i=1,nset
          Time(nrow1_t,i)=VAR1(nrow1_t,1)
          Twp(nrow1_t,i)=VAR1(nrow1_t,2)
          Tw(nrow1_t,i)=VAR1(nrow1_t,4)
   33    CONTINUE
       ENDIF
   11 CONTINUE
   22 CONTINUE
C       PRINT*,'ENTER RH DATA FILENAME FOR PRECLOSURE ANALYSES'
C       READ(*,'(A80)') FNAME
       FNAME='bk1_precls_rh.xyp'
       OPEN(UNIT=1,FILE=FNAME,STATUS='UNKNOWN',FORM='FORMATTED')
       nrow1_r=0
```

```
      DO 44 J=1,1000000
       READ(1,'(A)',END=55) LINE
       IF (LINE(1:1) .NE. '!') THEN
         nrow1_r=nrow1_r+1
         READ(LINE,*) (VAR2(nrow1_r,k),k=1,5)
         do 66 i=1,nset
           RH(nrow1_r,i)=VAR2(nrow1_r,2)
  66       CONTINUE
       ENDIF
  44  CONTINUE
  55  CONTINUE
      print*,'nrow1_t=',nrow1_t
      print*,'nrow1_r=',nrow1_r
      nrow1=nrow1_t
C
C Open files and read in data for post-closure
C
      flag_t=0
      flag_r=0
      do 5 i=1,nset
       row(i)=0
   5  continue
      DO 99 I=1,nset
C        PRINT*,'ENTER POSTCLOSURE TEMP DATA FILENAME FOR DATA SET #',i
C        READ(*,'(A80)') FNAME
       if(i .EQ. 1) then
        FNAME='bk1_poscls_tmp.xyp'
       elseif (i .EQ. 2) then
        FNAME='bk2_poscls_tmp.xyp'
       elseif(i .EQ. 3) then
        FNAME='bk3_poscls_tmp.xyp'
       elseif(i .EQ. 4) then
        FNAME='bk4_poscls_tmp.xyp'
       endif
       OPEN(UNIT=1,FILE=FNAME, STATUS='UNKNOWN',FORM='FORMATTED')
       nrow2_t=0
       DO 88 J=1,1000000
        READ(1,'(A)',END=77) LINE
        IF (LINE(1:1) .NE. '!') then
          nrow2_t=nrow2_t+1
          nrow_t=nrow2_t+nrow1
          READ(LINE,*) (VAR1(nrow_t,k),k=1,5)
          Time(nrow_t,i)=VAR1(nrow_t,1)+100
          Twp(nrow_t,i)=VAR1(nrow_t,2)
          Tw(nrow_t,i)=VAR1(nrow_t,4)
        ENDIF
  88   CONTINUE
  77   CONTINUE
       if (flag_t .LT. nrow_t) then
         flag_t=nrow_t
       endif
       row(i)=nrow_t
       print*, 'nrow_t=',nrow_t,' after nset# ',i
       print*, 'flag_t=',flag_t,' after nset# ',i
C        PRINT*,'ENTER POSTCLOSURE RH DATA FILENAME FOR DATA SET #',i
C        READ(*,'(A80)') FNAME
       if(i .EQ. 1) then
```

```
       FNAME='bk1_poscls_rh.xyp'
      elseif (i .EQ. 2) then
       FNAME='bk2_poscls_rh.xyp'
      elseif(i .EQ. 3) then
       FNAME='bk3_poscls_rh.xyp'
      elseif(i .EQ. 4) then
       FNAME='bk4_poscls_rh.xyp'
      endif
      OPEN(UNIT=1,FILE=FNAME,STATUS='UNKNOWN',FORM='FORMATTED')
      nrow2_r=0
      DO 1 J=1,1000000
       READ(1,'(A)',END=2) LINE
       IF (LINE(1:1) .NE. '!') THEN
         nrow2_r=nrow2_r+1
         nrow_r=nrow2_r+nrow1_r
         READ(LINE,*) (VAR2(nrow_r,k),k=1,5)
         RH(nrow_r,i)=VAR2(nrow_r,2)
       ENDIF
    1 CONTINUE
    2 CONTINUE
      if (flag_r .LT. nrow_r) then
        flag_r=nrow_r
      endif
      print*, 'nrow_r=',nrow_r,' after nset# ',i
      print*, 'flag_r=',flag_r,' after nset# ',i
   99 CONTINUE
C
C Write Out Data for EBSPAC
C
   98 Do 9 i=1,nset
      write(3,4000)
      if(i .NE. nset) then
       write(3,4400) i,i,i
      else
       write(3,4500) i,i,i
      endif
    9 continue
C
      Do 7 i=1,nset
       if(i .NE. nset) then
        write(3,5000) row(i), 99999.0, 99999.0, 99999.0
       else
        write(3,6000) row(i), 99999.0, 99999.0, 99999.0
       endif
    7 continue
C
      DO 3 I=1,flag_t
       do 4 j=1,nset
        if (j .ne. nset) then
         WRITE(3,2000) Time(i,j),Twp(i,j),Tw(i,j),RH(i,j)
        else
         WRITE(3,3000) Time(i,j),Twp(i,j),Tw(i,j),RH(i,j)
        endif
    4 CONTINUE
    3 CONTINUE
C
      print*, 'flag_t=',flag_t
```

```
      print*, 'flag_r=',flag_r
C
 2000 FORMAT(4E16.6, $)
 3000 FORMAT(4E16.6)
 4000 FORMAT(12x, 'Time', $)
 4400 FORMAT(5x,'Twp nset#',I2,6x,'Tw nset#',I2,6x,'RH nset#',I2, $)
 4500 FORMAT(5x,'Twp nset#',I2,6x,'Tw nset#',I2,6x,'RH nset#',I2)
 5000 FORMAT(I16,3E16.6,$)
 6000 FORMAT(I16,3E16.6)
      END
```

Appendix B

EBSPAC input file for analyzing the effect of backfill thermal conductivity

Filename: /export/home/rchen/TEFKTI/BK_cond/bk_cond_fail.inp

```
\example input file for ebspac_fail
!
\simulation time
10000.                   ! tend: simulation time length [yr]
\                    ! when iflag=1 (defined later)
\
5.682, 1.802             ! wplen,wpdia: wp length and diameter [m]
0.1, 0.02            ! cthick1,cthick2: wp layers 1&2 thicknesses [m]
!
\choose source of temperature data
2                    ! iflag 1: emp. equation, 2: tab.data
1                    ! nset (temp.-rel hum. relationship to use
49.9999999           ! timintv (used when iflag=2)
!
\other temperature parameters
0.                   ! age of fuel (not used in this version)
!
\Dry oxidation of wp outer overpack
5.                   ! grainr: metal grain radius [micrometer]
25                   ! nseries (terms in the infinite series)
0.7e-3                   ! gbthick [micrometer]
1.e-2                ! constant: used in the dry oxidation equn.
!
\evaporation-condensation
0.65                 ! humdc: critical relative humidity
2.e-3                    ! filmthk: thickness of water film [m]
97.                  ! ctemp: boiling point of water [C]
!
\Corrosion Parameters(Ep: pitting potential [mV]; Erp: repassivation potential [mV])
-584.8                   ! xipto: outer overpack Ep intercept
3.92                 ! pttemo: temp. coef. of outer overpack Ep intercept
-24.5                    ! slpto: outer overpack Ep slope
-1.1                 ! slpttemo: temp. coef. of outer overpack Ep slope
-620.3                   ! xirpo: outer overpack Erp intercept
0.47                 ! rptemo: temp. coef. of outer overpack Erp intercept
-95.2                    ! slrpo: outer overpack Erp slope
0.88                 ! slrptemo: temp. coef. of outer overpack Erp slope
200.                 ! xipti: inner overpack Ep intercept
0.                   ! pttemi: temp. coef. of inner overpack Ep intercept
-240.                    ! slpti: inner overpack Ep slope
0.                   ! slpttemi: temp. coef. of inner overpack Ep slope
422.8                    ! xirpi: inner overpack Erp intercept
-4.1                 ! rptemi: temp. coef. of inner overpack Erp intercept
-64.                 ! slrpi: inner overpack Erp slope
-0.80                    ! slrptemi: temp. coef. of inner overpack Erp slope
0.75, 0.5            ! betaox1, betahy1: beta kinetics parameters
\                      for oxygen and water for WP outer overpack
0.75, 0.5            ! betaox2, betahy2: beta kinetics parameters for
\                      oxygen and water for WP inner overpack
3.80e12, 1.6e-1                  ! rkox1 [c*m/y/mol], rkhy1 [c/m2/yr]
37300., 25000.                   ! gox1 [J/mol], ghy1 [J/mol]
3.0e10, 3.2              ! rkox2 [c*m/y/m], rkhy2 [c/m2/yr]
40000., 25000.                   ! gox2 [J/mol], ghy2 [J/mol]
3.15e5, 0.0, 0.0         ! aa(1,1) [C/m2/yr], aa(1,2), aa(1,3)
6.30e4, 0.0, 0.0         ! aa(2,1) [C/m2/yr], aa(2,2), aa(2,3)
```

```
-0.46               ! eexpt: in Vshe
8.66e-3             ! rcoef:
0.45                ! rexpont:
2.05e-4             ! crate2: m/yr corrosion rate
0.0                 ! xcouple, a fractional coupling strength
0.0                 ! xread
3.e-1               ! clconc: chloride concentration [mol/L]
3.e-4               ! clcrit1: crit. chloride conc. for 1st layer [mol/L]
2.e-3               ! clcrit2: crit. chloride conc. for 2nd layer [mol/L]
100.                ! cfactor: chloride dilution factor
9.0                 ! refph: reference pH
1.0, 1.0            ! taus:deposit tortuosity,spor:deposit porosity
|
\Runge-kutta control parameters
1.e-3, 1.e0         ! dtini, dtmax
1.e-2, 1.e-30       ! errrel (same as eps), errabs (same as tiny)
|
\end
////2000            ! nhista (used when iflag=1)
```

SCIENTIFIC NOTEBOOK

by

Rui Chen

Southwest Research Institute
Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

January 12, 1998

1/16/97

Bruce: 1/16/98

Work described in this scientific Notebook has been completed. No further entries will be made. Please close the Scientific Notebook # 204

Rui Chen

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1. INITIAL ENTRIES

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1.1. Objectives

The objectives of this task are two folds: 1. establish procedures for TEF KTI implementation of EBSPAC and TPA codes for sensitivity analyses; and 2. carry out analyses to develop estimates of sensitivity of dose to gravity-driven refluxing and to thermally-induced perturbations in water flux through the repository.

1.2. Technical Approaches

Estimation of sensitivity of dose to gravity-driven refluxing and thermally-induced perturbations in water flux through the repository is to be accomplished using TPA code through EBSPAC module. While TPA code controls the probabilistic aspects of the input parameters and spatial discretization of the repository, EBSPAC evaluates the actual, deterministic effects of input parameters on various EBSPAC output parameters for each TPA sub-area. At the present stage, only EBSPAC will be used to analyze one particular sub-area witch corresponds to one basic unit consisting a column from ground surface to water table with cross section equals to a drift spacing and a waste package (WP) spacing. Following is a list of specific steps to be taken:

Determine cases to be considered

Baseline cases will be those listed in Table 1-1 which consider the effects of (1) three thermal loading (or two, the high and the low); (2) with and without ventilation; (3) with and without backfill. Additional cases may include:

<u>Backfill properties:</u>

backfill thermal conductivity (0.2, 0.6 2.0, 10.0 W/m-K)
backfill initial saturation (0.01, 0.5, 0.99)

<u>Effect of media properties (??):</u>

evaluate the hydraulic conditions at Yucca Mountain (YM) for different, yet reasonable, homogeneous

Table 1-1. Cases for Parameter Sensitivity Analyses Using EBSPAC (Modified Based on Manteufel, 1996)

Set	AML (MTU/Acre)	Ventilation (up to 100 yr)	Backfill at 100 yr
1	80	N	N
2	80	N	Y
3	80	Y	N
4	80	Y	Y
5	40	N	N
6	40	N	Y
7	40	Y	N
8	40	Y	Y
9	20	N	N
10	20	N	Y
11	20	Y	N
12	20	Y	Y
y: yes N: no			

hydraulic property values assigned to the Paintbrush Tuff (PTn) and Calico Hills (CHnv) units located above and below the proposed repository horizon, respectively, in the presence of heat-generating HLW (Green 1996).

geologic structure and features on the evolution of perched water body (??):

perched water (? Goodluck and Ross)

geologic structure and media hydrologic properties on temperature and saturation

Effect of a zone of higher permeability (width) intersecting the drift on thermohydrology of the drift (temperature, saturation, and relative humidity within the drift and at the drift wall).

Evaluation of baseline cases

The results of baseline cases listed in Table 1-1 from thermal model (Manteufel 1996, figure 5-1 in EBSPAC manual) will be used in EBSPAC to look at the effects of thermal load, ventilation, and backfill on various EBSPAC output parameters.

Effect of other cases

(Need more consideration as how to incorporate them)
[The effect of various factors on importance of various factors will be examined, including baseline factors list in Table 1. The sensitivities will be examined through comparisons of the statistical properties of the CCDFs. (Use of TPA??)]

1.3. Data Sources

To implement EBSPAC, TEF KTI will provide parameter estimates and the technical basis for those estimates. The primary parameters include:

Temperature and Relative Humidity Data (5.1.1 in EBSPAC report)

- WP temperature as a function of time
- WP relative humidity (RH) as a function of time
- drift wall temperature as a function of time (no longer used?)

These parameters are implemented in EBSPAC through tabular data files *tefkti.inp* and *floebs.dat*. Most of these parameters are obtained through the so called **Thermal Model**, which is a set of external calculations to EBSPAC developed within the TEF KTI. An example of such calculation is described in detail by Manteufel (1996).

Some basic cases to be studied for sensitivities using EBSPAC are listed in Table 1-1. Others may include variations of these basic cases considering other factors studied by TEF KTI in FY96 and FY97 sensibility study, namely:

<u>Effect of backfill on temperature and saturation:</u>

a. backfill thermal conductivity (0.2, 0.6 2.0, 10.0 W/m-K)
b. backfill initial saturation (0.01, 0.5, 0.99)

<u>Effect of media properties on prediction of moisture redistribution:</u> (?)

evaluate the hydraulic conditions at YM for different, yet reasonable, homogeneous hydraulic property values assigned to the Paintbrush Tuff (PTn) and Calico Hills (CHnv) units located above and below the proposed repository horizon, respectively, in the presence of heat-generating HLW (Green 1996).

<u>geologic structure and features on the evolution of perched water body</u> (?)

perched water (? Goodluck and Ross)

<u>geologic structure and media hydrologic properties on temperature and saturation</u> (?)

Effect of a zone of higher permeability (width) intersecting the drift on thermohydrology of the drift (temperature, saturation, and relative humidity within the drift and at the drift wall).

Water Flow Data (5.2.2 in EBSPAC report)

- rate of flow into EBS.

The infiltration of meteoric water and its arrival at the WP is a function of the hydro-stratigraphic conditions above and below the repository horizon. The carrying capacity of the fractures and matrix above the repository, as well as horizontal diversion depending on the dip of fractures and matrix above the repository, as well as horizontal diversion depending on the dip of the bedding planes, and thermal conditions will dictate the rate of infiltration into the EBS. In some instances the infiltrating water may reach the EBS by matrix-only flow. EBSPAC uses the funnel flow concept adopted in SOTEC to represent flow into the EBS. The funnel flow concept assumes that flow through fractures over a wide area will converge to focused spots on the drift and will result in dripping of water on the WP. The average fracture infiltration rate can be specified as a function of time for more realistic input of infiltration data. Detailed calculation of infiltration performed elsewhere (Stothoff, 1996, Stothoff et al, 1996) will provide average fracture infiltration rate.

Other input for EBSPAC (??)

- critical RH above which the water vapor condenses
- thickness of water film on the WP surface (a uniform thickness all around the WP is assumed)
- backfill porosity corresponding to zone 1
- funnel factor or fractional area for capture of darcy flow onto WP
- water level inside the WP expressed as a fraction of WP internal diameter

1.4. Computers, Computer Codes, and Data Files

Table 1-2. Computing Equipment

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

Table 1-2 lists computer equipment and computer codes. Table 1-3 provides names, type, and content of data files for EBSPAC analyses.

Table 1-3. Names, Type, and Content of Relative EBSPAC Files

File Name	Type	Content
ebspac_fail.x	executable of EBSPAC code	executable of EBSPAC code
TEFKTI.inp	text	input temperature and RH data file for EBSPAC from TEF KTI
Example_fail.inp	text	EBSPAC input data file
temphumd.dat chloride.dat	text	EBSPAC output data files

2. IN-PROGRESS ENTRIES

2.1. Establishment of EBSPAC and TPA Implementation Procedures

Result from four cases of MULTIFLO analyses on the effect of thermal conductivity of backfill materials were used to establish EBSPAC and TPA implementation procedures for TEF KTI.

2.1.1 Thermal-Hydrological Model - Effect of Thermal Conductivity of Backfill Materials

The six-layer ECM hydro-stratigraphic model of YM taken from TSPA-95 was used in analyses of the effect of backfill thermal conductivity. The analyses considered two-phase, nonisothermal flow using computer code MULTIFLO. The numerical model extended from ground surface to water table (at 654 m depth) and included one half of an "unit cell" width (from the center of emplacement drift to the center of the pillar). The model was discretized into 19 elements along the horizontal direction and 43 elements along the vertical direction. The vertical boundaries were modeled as symmetric boundaries (i.e., no heat and no fluid flow). The upper boundary was assigned a uniform, steady infiltration of 0.3 mm/yr.

The modeling started with an initial simulation to achieve steady-state conditions under 0.3 mm/yr infiltration at the top boundary. A 5x5 m^2 emplacement draft was, then, "excavated" by changing the corresponding material properties to "air" properties and a decay heater source with initial heat load of about 84 kW/acre was emplaced. The simulation continued to 100 years with "air" filling the emplacement drift before backfill was emplaced.

Figure 1 shows the time history of WP temperature with backfill thermal conductivities ranging from 0.2 W/m-K to 10 W/m-K. This figure shows that lower backfill thermal conductivity resulted in higher WP temperature. This effect is most pronounced immediately after the emplacement of backfill and gradually becomes insignificant with time. It is interesting to notice that although backfill thermal conductivity affects temperature at the WP, it has little effect on temperature at the drift wall.

2.1.2 EBSPAC Analyses

Output data files from MULTIFLO that contain time history of temperature and relative humidity (RH) at the WP and temperature at drift wall for all four cases described in the previous section were used as input for EBSPAC analyses. A fortran program was developed to read data from MULTIFLO output history files for each of the analysis cases and write out in the format required by EBSPAC. The fortran program is included in Appendix A. EBSPAC input file is included in Appendix B. Table 2-1 lists names and contents of all data files in those analyses.

EBSPAC analyses for all four cases show that no WP failure occur during the simulation time period (10000 yr). Also, backfill thermal conductivity does not appear to significantly affect other EBSPAC output parameters neither. For example, Figure 2-2 depicts the remaining WP overpack thickness as a function of time for all four cases. Although the curves appear to diverge as time increases, there is no significant difference.

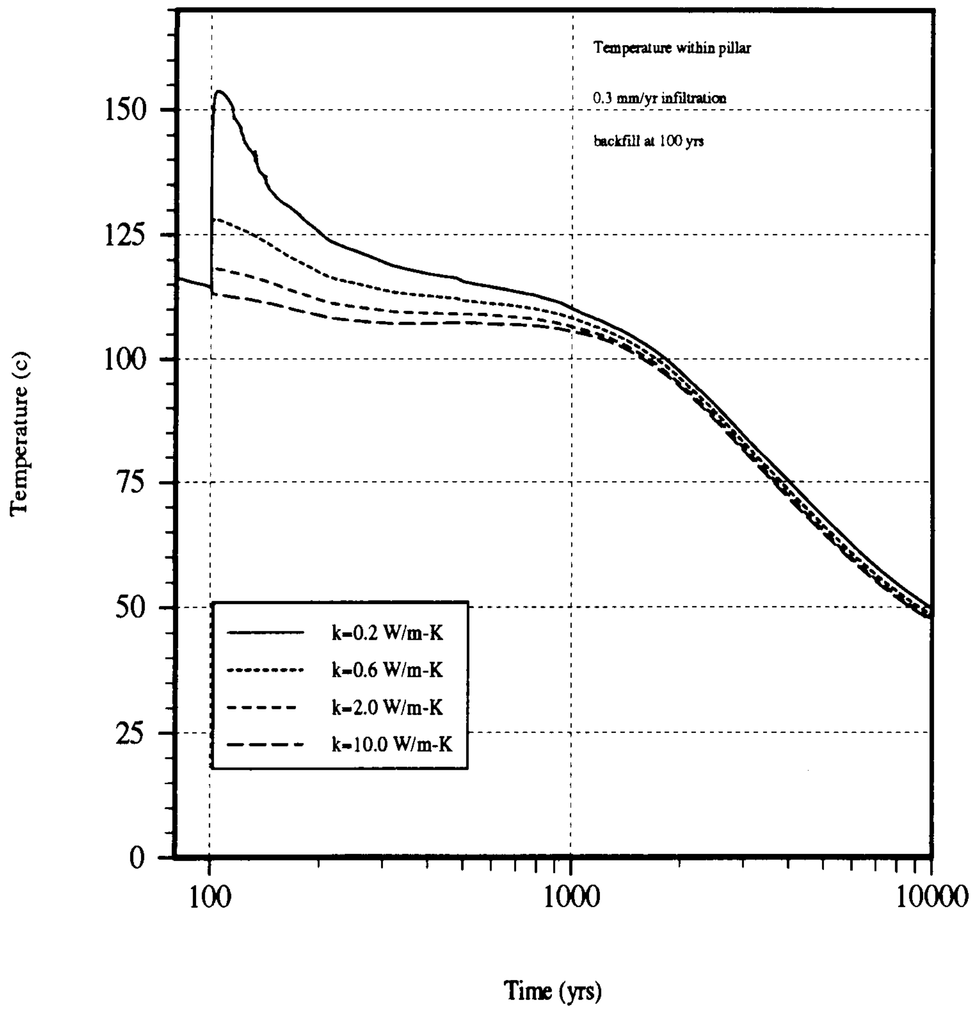

Figure 2-1 Time history of temperature at the WP with backfill thermal conductivity ranging from 0.2 W/m-K to 10 W/m-K.

Table 2-1: Names and Content of Data files for EBSPAC analyses of the Effect of Backfill Thermal Conductivity

File Name	Content
bk1_precls_tmp.xyp bk1_poscls_tmp.xyp bk2_poscls_tmp.xyp bk3_poscls_tmp.xyp bk4_poscls_tmp.xyp	Temperature at waste package and drift wall as functions of time from MULTIFLO analyses
bk1_precls_rh.xyp bk1_poscls_rh.xyp bk2_poscls_rh.xyp bk3_poscls_rh.xyp bk4_poscls_rh.xyp	Relative humidity at waste package as a function of time from MULTIFLO analyses
temphumd.f	Fortran file for reading MULTIFLO output data and writing the data for EBSPAC input
bk_cond.inp	Temperature and humidity history data in EBSPAC specified format for all four cases of backfill thermal conductivity
bk_cond_fail.inp	EBSPAC input file
rthick_his_comb.xpb tmp_his_comb.xpb	Xplot batch files for plotting analysis results
temphumd_bk1.dat temphumd_bk2.dat temphumd_bk3.dat temphumd_bk4.dat	EBSPAC output data file containing temperature and humidity data for corrosion analyses, and WP failure time
chloride_bk1.dat chloride_bk2.dat chloride_bk3.dat chloride_bk4.dat	EBSPAC output data file containing remaining WP thickness

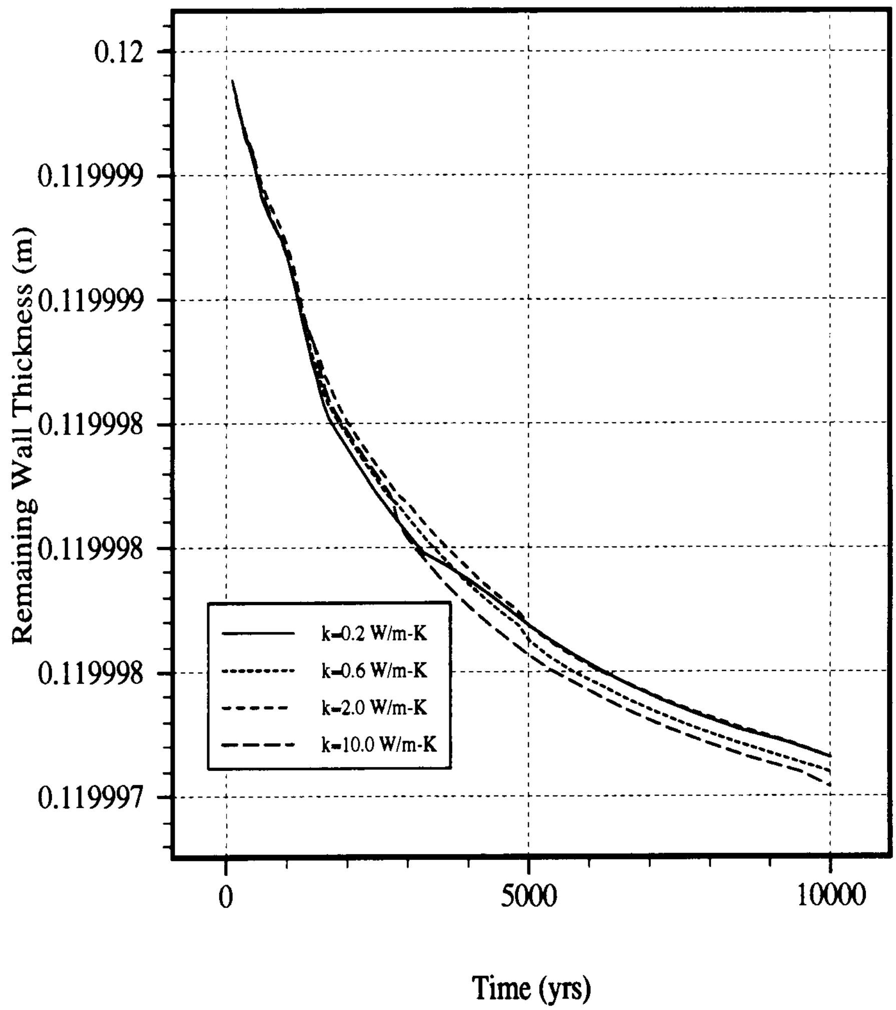

Figure 2-2 Time history of remaining WP wall thickness with backfill thermal conductivity ranging from 0.2 W/m-K to 10 W/m-K.

2. 2 Selection of Parameters for TEF Dose-Sensitivity Analyses

2.2.1 Parameters for TEF dose sensitivity analyses using Multiflo and TPA30

2.2.1.1 Parameters used in Multiflo Calculations

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

e. Backfill properties (same as a through c)

2.2.1.2 Parameters to be considered for TEF sensitivity analyses using Multiflo

- Heat load
- With and without backfill
- Matrix permeability
- Matrix van Genuchten α
- Fracture permeability
- Fracture van Genuchten α
- Matrix porosity (?)

2.2.2. Parameters for the base case

(Parameters are taken as TSPA-93 mean values as documented in Section 4, unless noted otherwise)

2.2.2.1 Matrix hydrologic properties

Table 2.2.2-1. Matrix hydrologic properties

Parameters		TCw	PTn	TSw	TSv	CHnv	CHuz
Porosity		0.087	0.421	0.139	0.065	0.331	0.306
Ksat (m/s) [Permeability (m^2)]		2.042e-11 (2.083e-18)	3.802e-7 (3.879e-14)	2.089e-11 (2.131e-18)	9.772e-12 (9.967e-19)	1.096e-9 (1.118e-16)	1.585e-11 (1.617e-18)
Residual Saturation		0.021	0.154	0.045	0.118	0.097	0.121
van Genuchten Parameter	α (m^{-1}) (Pa^{-1})	7.907e-3 (7.907e-7)	5.559e-1 (5.559e-5)	1.355e-2 (1.355e-6)	2.193e-3 (2.193e-7)	2.786e-2 (2..786e-6)	5.943e-3 (5.943e-7)
	β	1.622	2.371	1.799	2.228	2.460	1.706
	$\lambda=1-1/\beta$	0.383	0.578	0.444	0.551	0.593	0.414

2.2.2.2 Fracture hydrologic properties

Table 2.2.2-2. Fracture hydrologic properties

Parameters		TCw	PTn	TSw	TSv	CHnv	CHuz
Porosity*		1.800e-3	1.800e-3	1.800e-3	1.800e-3	1.800e-3	1.800e-3
Ksat (m/s) [Permeability (m^2)]**		3.900e-12	3.900e-13	3.900e-12	3.900e-12	3.900e-13	3.900e-12
Residual Saturation		0.04	0.04	0.04	0.04	0.04	0.04
van Genuchten Parameter	α (m^{-1}) (Pa^{-1})	12.3 (1.23e-3)	14.0 (1.40e-3)	12.2 (1.22e-3)	13.1 (1.31e-3)	12.2 (1.22e-3)	7.3 (7.3e-4)
	β***	4.23	4.23	4.23	4.23	4.23	4.23
	$\lambda=1-1/\beta$	0.764	0.764	0.764	0.764	0.764	0.764

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

** TSPA-93 values lead to excessive computer time. Therefore, these values were taken from TSPA-95 Table 4-2-2

*** Parameter statistics not available in TSPA-93. Values are from TSPA-95 Table 4.2-2

2.2.2.3 Matrix Thermal Properties

Table 2.2.2-3 Matrix thermal (dry) properties*

Unit	Thermal Conductivity [W/(m-K)]		Density (kg/m^3)	Specific Heat [J/(kg-K)]
	Dry	Wet**		
TCw	1.69	2.23	2580	728
PTn	0.61	0.81	2580	422
TSw	2.10	2.78	2580	840
TSv	1.28	1.69	2580	948
CHnv	0.84	1.11	2580	488
CHnz	1.42	1.88	2580	526

* TSPA-95 p 4-19 Table 4.2-3

** Higher values are assigned for wet thermal conductivity to be more realistic

2.2.2.4 Others

- Thermal load (83 MTU/acre, TPA30 data)
- Infiltration (0.05 mm/yr, previous multiflo calculation) (See Ron Green's Memo dated 05/27/97)
- maximum cut off value for capillary pressure (50, previous multiflo calculation)
- residual gas saturation (0, previous multiflo calculation)

2.2.2.5 Backfill hydrologic and thermal properties

Table 2.2.2-4 Backfill hydrologic and thermal properties*

Parameters			Unit	Values
Porosity	Matrix		-	0.500
	Fracture***			1.8e-3
Permeability	Matrix		m^2	3.9e-14
	Fracture			3.9e-12
van Genuchten Parameter	α	Matrix	m^{-1} (Pa^{-1})	0.111 (1.106e-5)
		Fracture		0.131 (1.305e-5)
	β	Matrix	-	3.333
		Fracture		4.230
	$\lambda=1-1/\beta$	Matrix	-	0.700
		Fracture		0.764
Residual Saturation	Matrix		-	0.010
	Fracture			0.040
Thermal Conductivity**	Unsaturated		W/(m-K)	0.260
	Saturated			0.490
Density			kg/m^3	2580
Specific Heat			J/(kg-K)	840

* According to TSPA-95, Tables 4-2.1 through 4-2.3.
** According to Green et al. (1997)
*** Previous Multiflo input file

2.2.3 Parameters for dose-sensitivity analyses and data ranges

2.2.3.1 Scooping analyses on effect of matrix porosity

[TSw: E(x)=0.139, Emin=0.082, Emax=0.196]

2.2.3.2 Selection of parameters and data range

Parameters to be studied

1. Infiltration (0.36 mm/yr and 3.6 mm/yr)
2. With or without backfill
3. Matrix permeability
4. Matrix van Genuchten α
5. Fracture permeability
6. Fracture van Genuchten α
7. Matrix porosity (?)

Table 2.2.3-1. Statistical data

Rock Units	Parameters	E[x]	Low	High	Source
-	Heat Load (mtu/acre)	-	25	85	TSPA-95
	Backfill		No	Yes	-
TSw	Matrix Ksat (m/s) [Permeability (m^2)]	2.089e-11 2.131e-18	2.884e-13 2.942e-20	1.072e-8 1.093e-15	TSPA-93
	Matrix van Genuchten α (m^{-1})	1.355e-2	2.099e-3	5..000e-1	TSPA-93
	Fracture Ksat (m/s) [Permeability (m^2)]	1.566e-2 1.598e-9	3.303e-5 3.369e-12	1.159 1.182e-7	TSPA-93
	Fracture van Genuchten α (m^{-1})	12.2	0.4	81.0	TSPA-93

2.2.4 Parameters and their statistic information from TSPA-93

2.2.4.1 Matrix statistics from TSPA-93

Table 2.2.4-1. Matrix saturated hydraulic conductivity (m/s) [permeability (m^2)]*

Unit	E(x)	min [E(x)-SD}	max [E(x)+SD]
TCw	2.042e-11 (2.083e-18)	6.310e-13 (6.436e-20)	6.1663e-9 (6.290e-16)
PTn	3.802e-7 (3.879e-14)	1.175e-9 ($1.199e^{16}$)	1.738e-4 (1.773e-11)
TSw	2.089e-11 (2.131e-18)	2.884e-13 (2.942e-20)	1.072e-8 (1.093e-15)
TSv	9.772e-12 (9.967e-19)	2.692e-13 (2.746e-20)	2.239e-10 (2.284e-17)
CHnv	1.096e-9 (1.118e-16)	3.981e-12 (4.061e-19)	1.047e-6 (1.068e-13)
CHnz	1.585e-11 (1.617e-18)	6.761e-15 (6.896e-22)	1.072e-8 (1.093e-15)

* TSPA-93 p 7-14 Table 7-5b (Entropy-fit beta distribution parameters)

Table 2.2.4-2. Matrix porosity (-)*

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	0.087	0.032	0.142
PTn	0.421	0.317	0.525
TSw	0.139	0.082	0.196
TSv	0.065	0.022	0.108
CHnv	0.331	0.241	0.421
CHnz	0.306	0.242	0.370

* TSPA-93 p 7-11 Table 7-3 (basic statistics)

Table 2.2.4-3. Matrix α (m^{-1})*

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	7.907e-3	2.588e-4	1.384e-1
PTn	5.559e-1	1.803e-1	1.718
TSw	1.355e-2	2.099e-3	5.000e-1
TSv	2.193e-3	1.758e-4	7.691e-3
CHnv	2.786e-2	1.718e-3	1.109
CHnz	5.943e-3	3.936e-4	3.133e-1

* TSPA-93 p 7-14 Table 7-6b (Entropy-fit beta distribution parameters)

Table 2.2.4-4. Matrix β *

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	1.622	1.453	1.811
PTn	2.371	1.465	3.839
TSw	1.799	1.337	2.421
TSv	2.228	1.617	3.070
CHnv	2.460	1.554	3.894
CHnz	1.706	1.287	2.261

* TSPA-93 p 7-14 Table 7-6b (Entrop-fit beta distribution parameters)

Table 2.2.4-5 Matrix residual degree of saturation*

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	0.021	0**	0.076
PTn	0.154	0**	0.325
TSw	0.045	0**	0.106
TSv	0.118	0**	0.285
CHnv	0.097	0**	0.233
CHnz	0.121	0**	0.292

* TSPA-93 p 7-17 Table 7-8 (basic statistics)
** [E(x)-SD] less than zero, set at zero

2.2.4.2 Fracture statistics from TSPA-93

Table 2.2.4-6 Fracture hydraulic conductivity* (m/s) [permeability (m^2)]

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	1.849e-2 (1.886e-9)	5.211e-4 (5.315e-11)	7.851e-1 (8.008e-8)
PTn	1.883e-2 (1.921e-9)	4.886e-4 (4.983e-11)	2.202 (2.246e-7)
TSw	1.566e-2 (1.598e-9)	3.303e-5 (3.369e-12)	1.159 (1.182e-7)
TSv	1.762e-2 (1.797e-9)	4.064e-5 (4.145e-12)	1.422 (1.450e-7)
CHnv	1.169e-2 (1.193e-9)	1.117e-4 (1.139e-11)	2.535 (2.585e-7)
CHnz	5.022e-3 (5.123e-10)	3.184e-5 (3.247e-12)	6.010e-1 (6.131e-8)
* TSPA-93 p 7-30 Table 7-20 (log_{10} statistics)			

Table 2.2.4-7 Fracture Porosity (-)*

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	8.650e-4	3.200e-4	2.322e-3
PTn	2.339e-4	8.088e-5	6.763e-4
TSw	1.002e-2	2.699e-4	3.722e-3
TSv	8.851e-4	2.377e-4	3.295e-3
CHnv	3.648e-4	9.571e-5	1.390e-3
CHnz	1.884e-4	5.159e-5	6.878e-4
* TSPA-93 p 7-3 Table 7-19 (log_{10} statistics)			

Table 2.2.4-8 Fracture alpha (m^{-1})*

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	12.3	1.7	66.7
PTn	14.0	1.7	111.6
TSw	12.2	0.4	81.0
TSv	13.1	0.5	89.8
CHnv	12.2	0.8	119.8
CHnz	7.3	0.4	58.4

* TSPA-93 p 7-3 Table 7-21 (basic statistics)

2.2.5 Parameter values form TSPA-95 etc.
(not used for TEF sensitivity analyses, only listed for references)

2.2.5.1 Matrix properties

Table 2.2.5-1 Matrix properties from TSPA-95

Parameters		TCw	Ptn	TSw	Tsv	CHnv	CHuz
Porosity		0.087	0.421	0.139	0.065	0.331	0.306
Ksat (m/s)		9.7×10^{-12}	3.9×10^{-7}	1.9×10^{-11}	1.9×10^{-11}	2.7×10^{-7}	2.0×10^{-11}
Residual Saturation		0.002	0.100	0.080	0.080	0.041	0.110
van Genuchten Parameter	α (m^{-1})	0.0084	0.0153	0.0058	0.0058	0.0163	0.0031
	β	1.558	6.872	1.798	1.798	3.861	1.602
	$\lambda=1-1/\beta$	0.36	0.85	0.44	0.44	0.74	0.38

2.2.5.2 Fracture properties

Table 2.2.5-2 Fracture properties from TSPA-95

Parameters		TCw	Ptn	TSw	Tsv	CHnv	CHuz
Porosity*		1.8×10^{-3}	1.8×10^{-3}	1.8×10^{-3}	1.8×10^{-3}	1.8×10^{-3}	1.8×10^{-3}
Ksat (m/s)		3.9×10^{-5}	3.9×10^{-6}	3.9×10^{-5}	3.9×10^{-5}	3.9×10^{-6}	3.9×10^{-5}
Residual Saturation		0.004	0.004	0.004	0.004	0.004	0.004
van Genuchten Parameter	α (m^{-1})	0.1305	0.1305	0.1305	0.1305	0.1305	0.1305
	β	4.230	4.230	4.230	4.230	4.230	4.230
	$\lambda=1-1/\beta$	0.7636	0.7636	0.7636	0.7636	0.7636	0.7636

*Note: Not from TSPA-95, but from previous Multiflo input file

2.2.6 Other Parameters as Input to TPA30 (NFENV/THERMAL)
(These parameters are provide to TPA30 for input, most of them are not used in TEF analyses)

2.2.6.1 Mass Density of YM Rock

Table 2.2.6-1 Matrix bulk density (kg/m^3)*

Unit	E(x)	min [E(x)-SD]	max [E(x)+SD]
TCw	2285	2171	2399
PTn	1419	1140	1699
TSw	2247	2112	2381
TSv	2308	2248	2368
CHnv	1737	1447	2027
CHnz	1746	1554	1938
* TSPA-95 p 2-13 Table 2.4-1			

Also see Table 2-3 for approximate value

2.2.6.2 Others

Specific Heat of YM Rock: see Table 2-3 (according to TSPA-95)
Thermal Conductivity of YM Rock: see Table 2-3 (according to TSPA-95)
Effective thermal conductivity of backfill: see Table 2-5 (according to Green et al. 1997)

2.3 Metra Base Case Analyses for TEF Dose-Sensitivity Study

Continued from Mikko's Scientific Notebook #216

2.3.1 Test of Mikko's Nested 3D Metra Base Case (First Test)

Mikko's 3D Metra base case include 2 geometries and 4 input files:

A. 3D Full Model
- extends from the ground surface (z=0) to the water table (z=-660 m)
- all properties are TSw2 properties (single layer)
- no heater, no air or backfill in the draft
- initial gas saturation in the heater region for the second run (c3big_th2.dat) was changed to 0.99 by editing and reformatting the Cut and Paste from *c3big_1_out* using *format.f*
- input files:

c3big_1.dat full model initial hydrological equilibrium
c3big_th2.dat full model thermal run

Run #1 (*c3big_1.dat* for initial equilibrium, *c3big_th2.dat* for thermal run):

- change properties to base case properties as documented in Section 2.2 of this Notebook
- c3big_th2.dat run to about only 300 yrs over more than 24 hrs
- it was speculated that permf is probably causing the problem, so permf (fracture permeability) was changed back to the TSPA-95 (3.9e-12) value from base case value (1.598e-9)

Run #2 (*c3big_1.dat* for initial equilibrium, *c3big_th2.dat* for thermal run):

- changed permf from 1.598e-9 back to 3.9e-12
- appear to be successful
- . Figure 2-3-1 shows time required to reach saturation during the initial run for equilibrium
- . Figure 2-3-2 shows saturation along a vertical line passing through (i=1 j=1, heater center).
- . Figure 2-3-3 shows gas pressure along a vertical line passing through (i=1 j=1, heater center).
- . Figure 2-3-4 shows temperature history at the upper and lower surface of the submodel from the big model thermal run
- . Figure 2-3-5 shows saturation as functions of time from big model thermal run
- . Figure 2-3-6 shows gas pressure as functions of time from the big model thermal run.
- Comparing these figures with results obtained by Mikko using a different set of input parameters for TSw shows that temperature, saturation, as well as gas pressure at the lower and upper boundaries of the 3D-sub model varies when the input parameters vary. Therefore, the nested approach is not suitable for sensitivity analyses.

B. 3D Submodel
- extends from z=-240 m to z=-440 m (i.e., 100 m above and below the repository, respectively)
- boundary conditions at z=-240 m and z=-440 m are obtained as results at the equivalent depth from the 3D full model (c3big_th2.dat)
- after running the full 3D model with thermal load and with the base case parameters, it was shown

(This method is not practical for sensitivity analyses, therefore it is discontinued!)

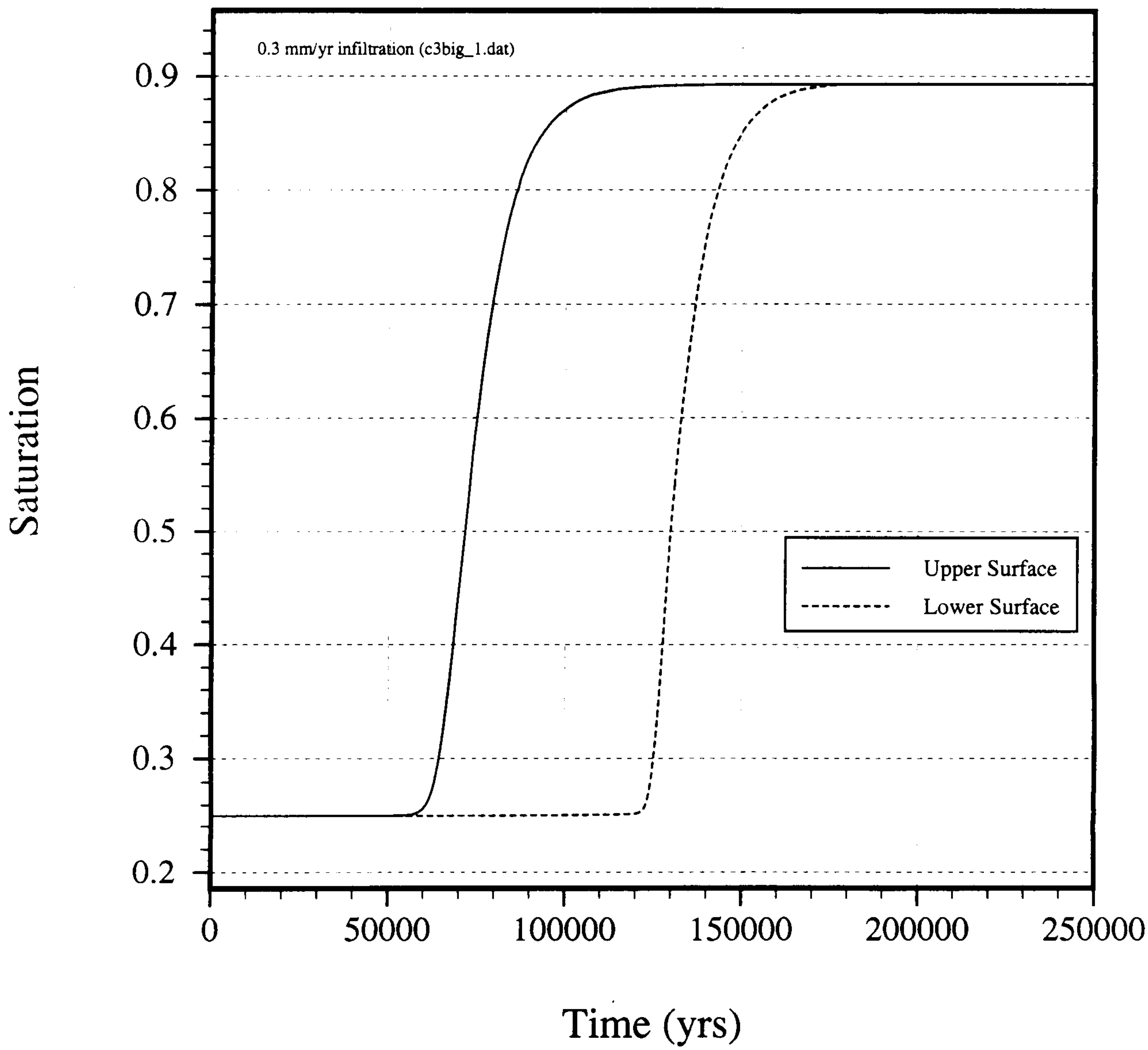

Figure 2.3-1 Time Required to reach equilibrium for the initial run (Time history of saturation and saturation level at the initial equilibrium)

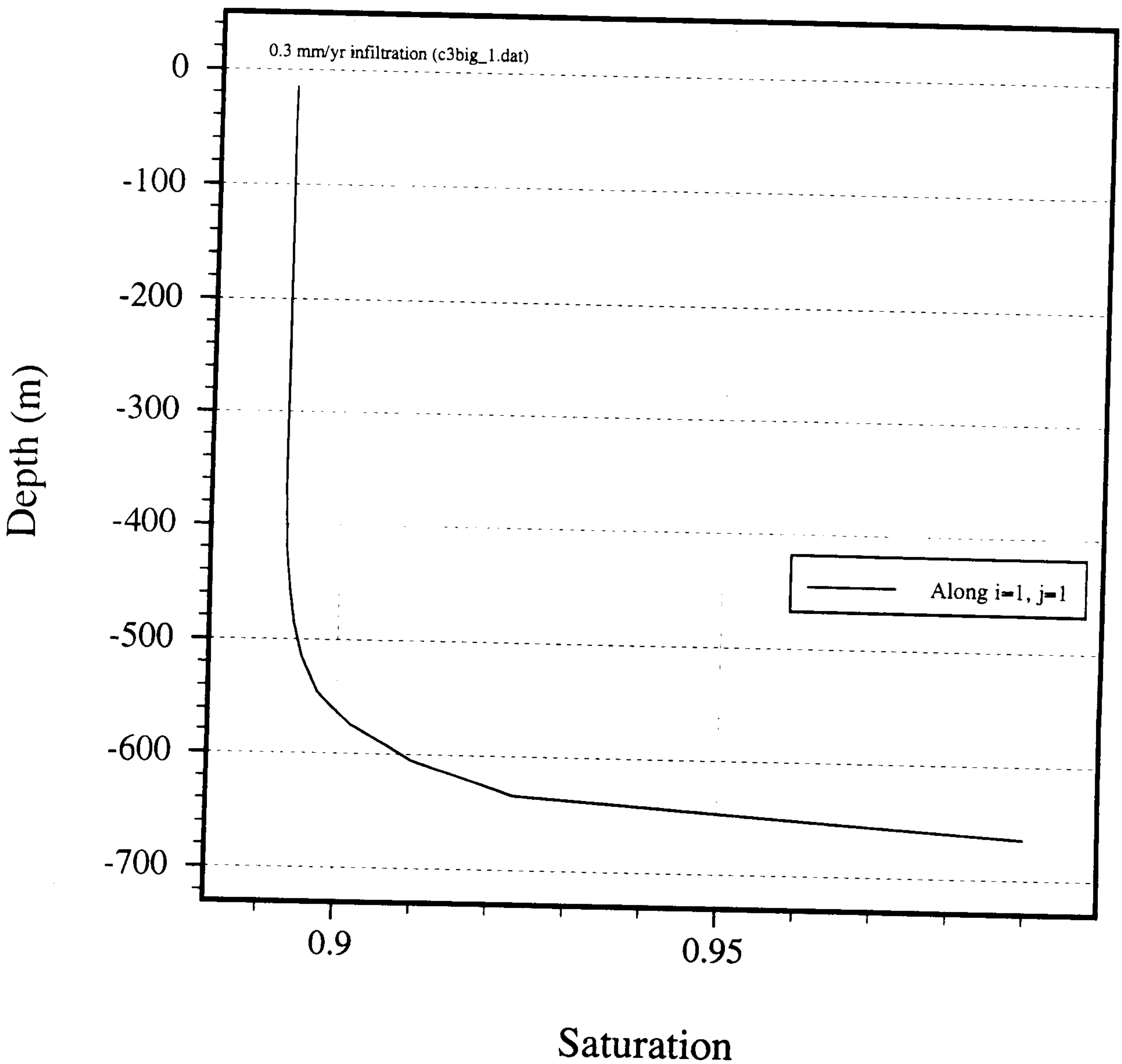

Figure 2.3-2 Saturation distribution along a vertical line through [(i=1,j=1), center of the waste package] at the initial equilibrium.

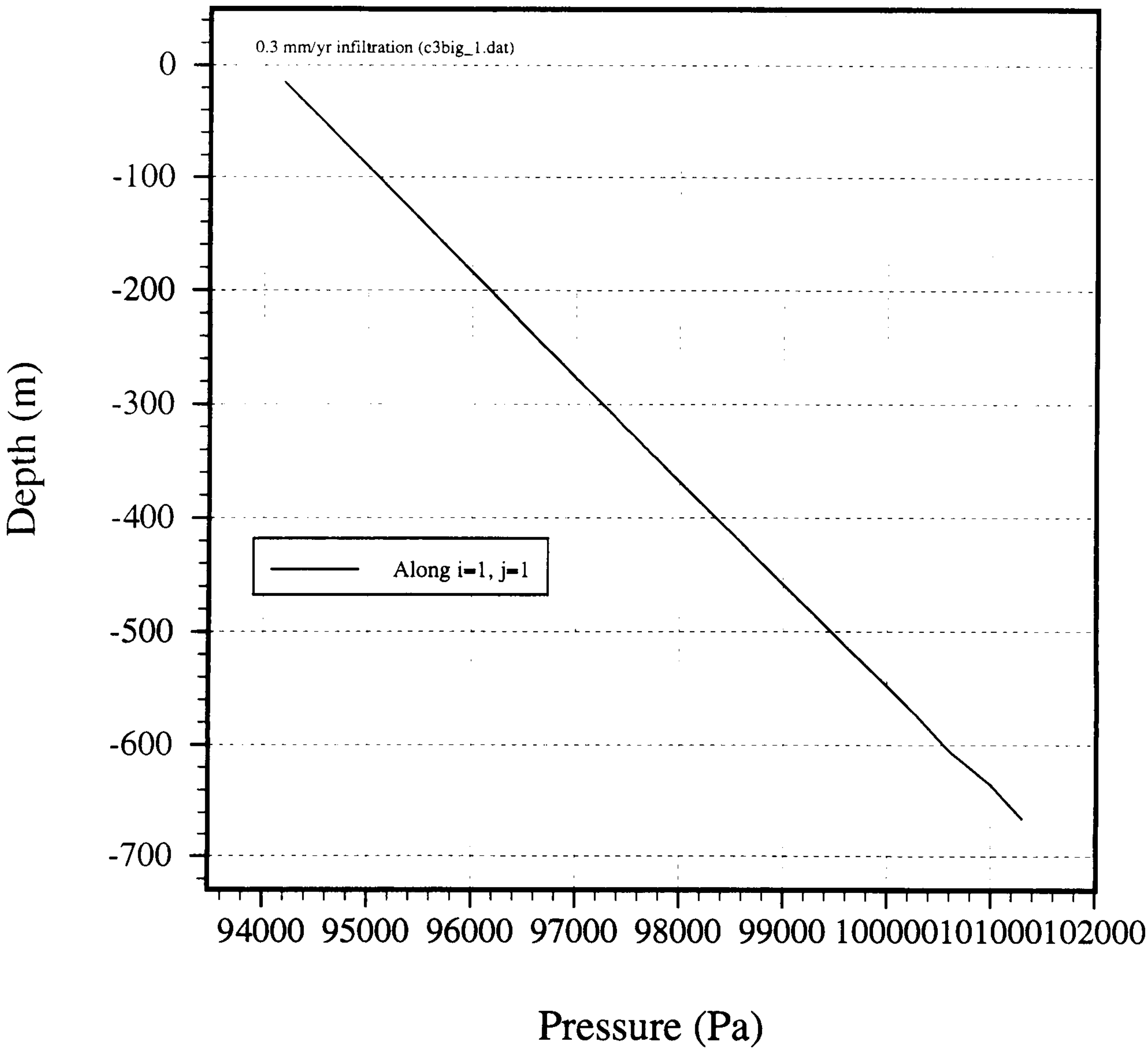

Figure 2.3-3. Gas pressure at the initial equilibrium along a vertical line at (i=1,j=1).

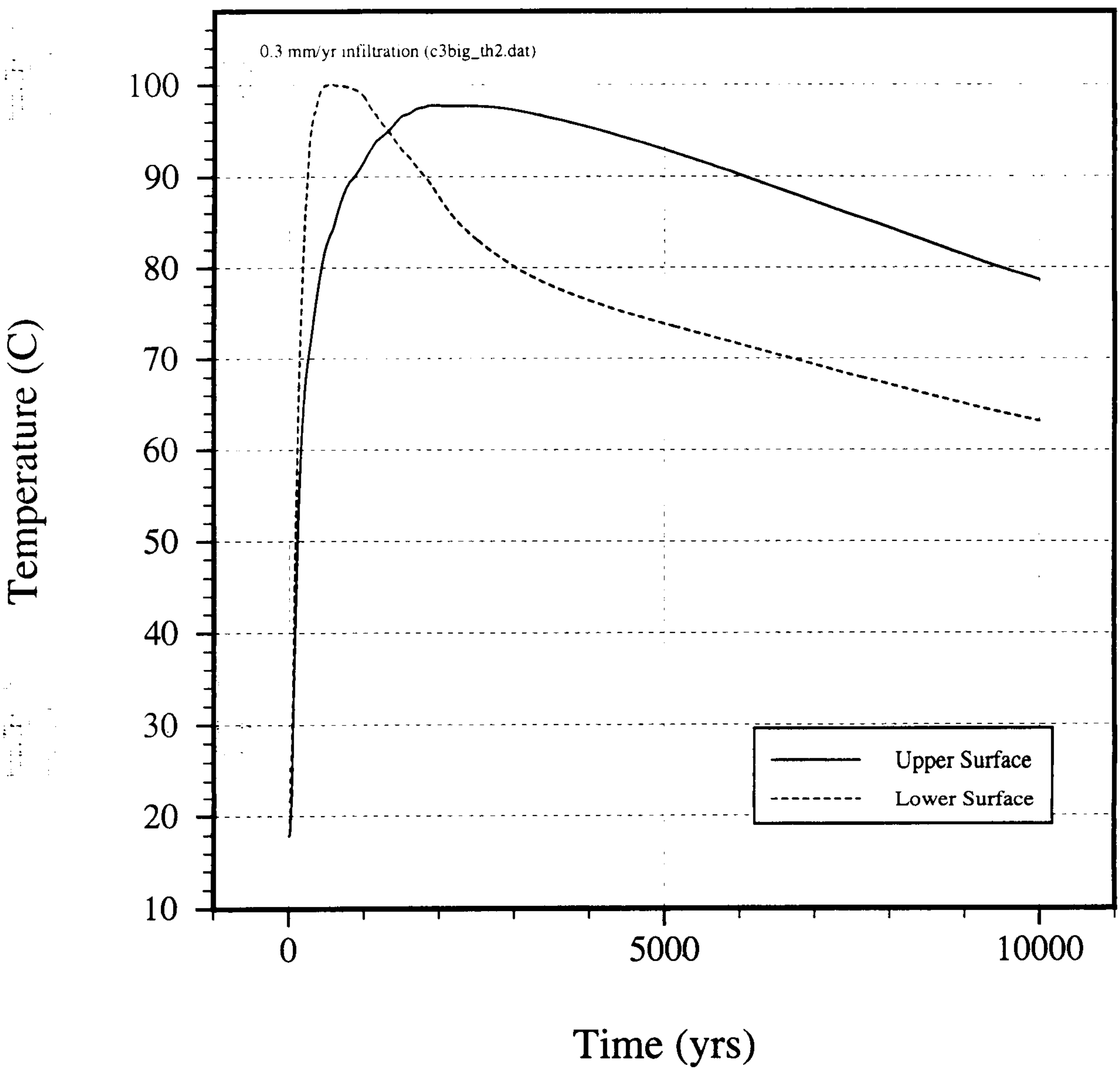

Figure 2.3-4. Temperature time history at the upper and lower surface of the submodel from the big model thermal run.

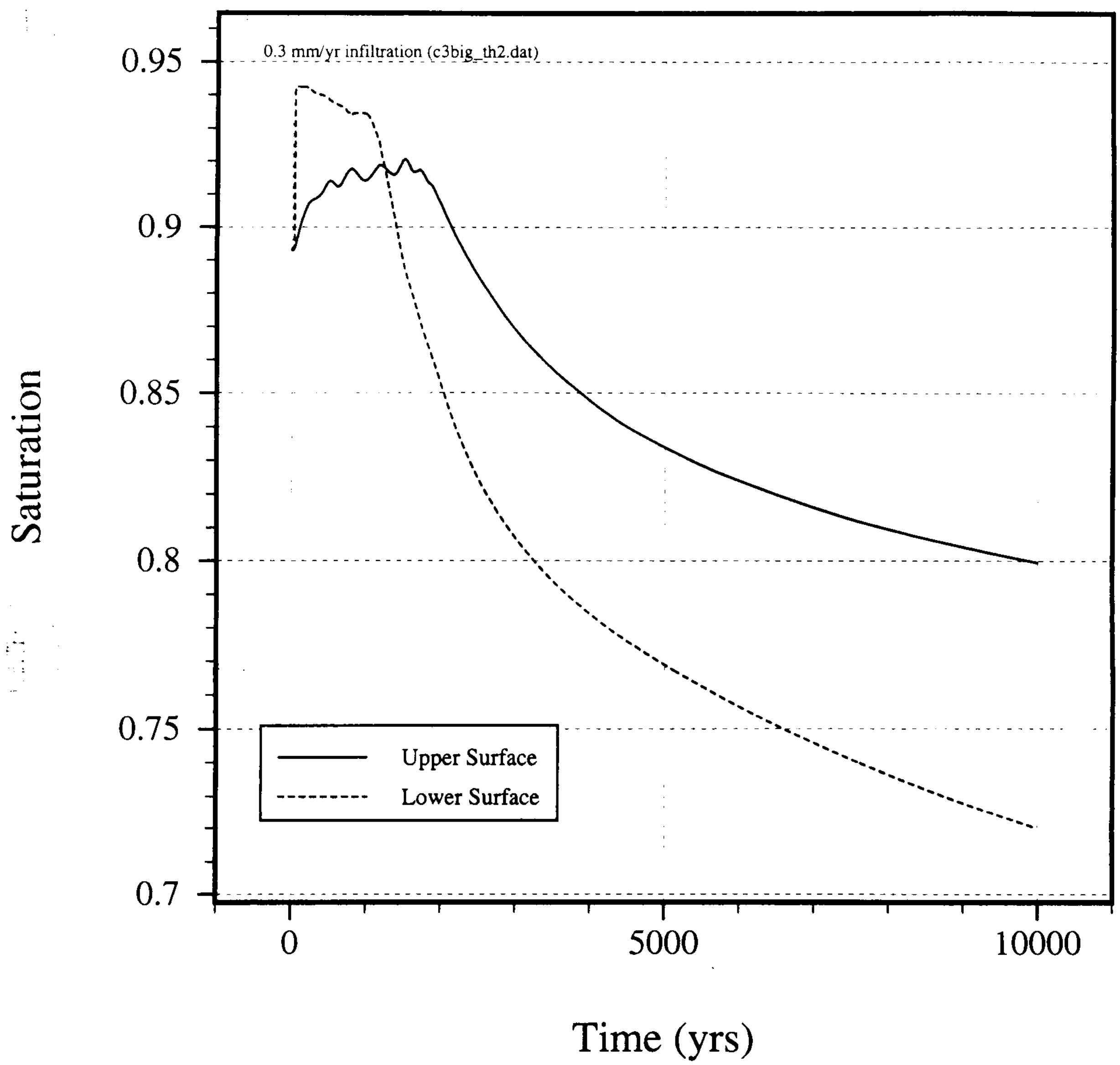

Figure 2.3-5. Saturation as functions of time from the big model thermal run [using TSPA-93 properties, except permf which is kept at original TSPA-95 property].

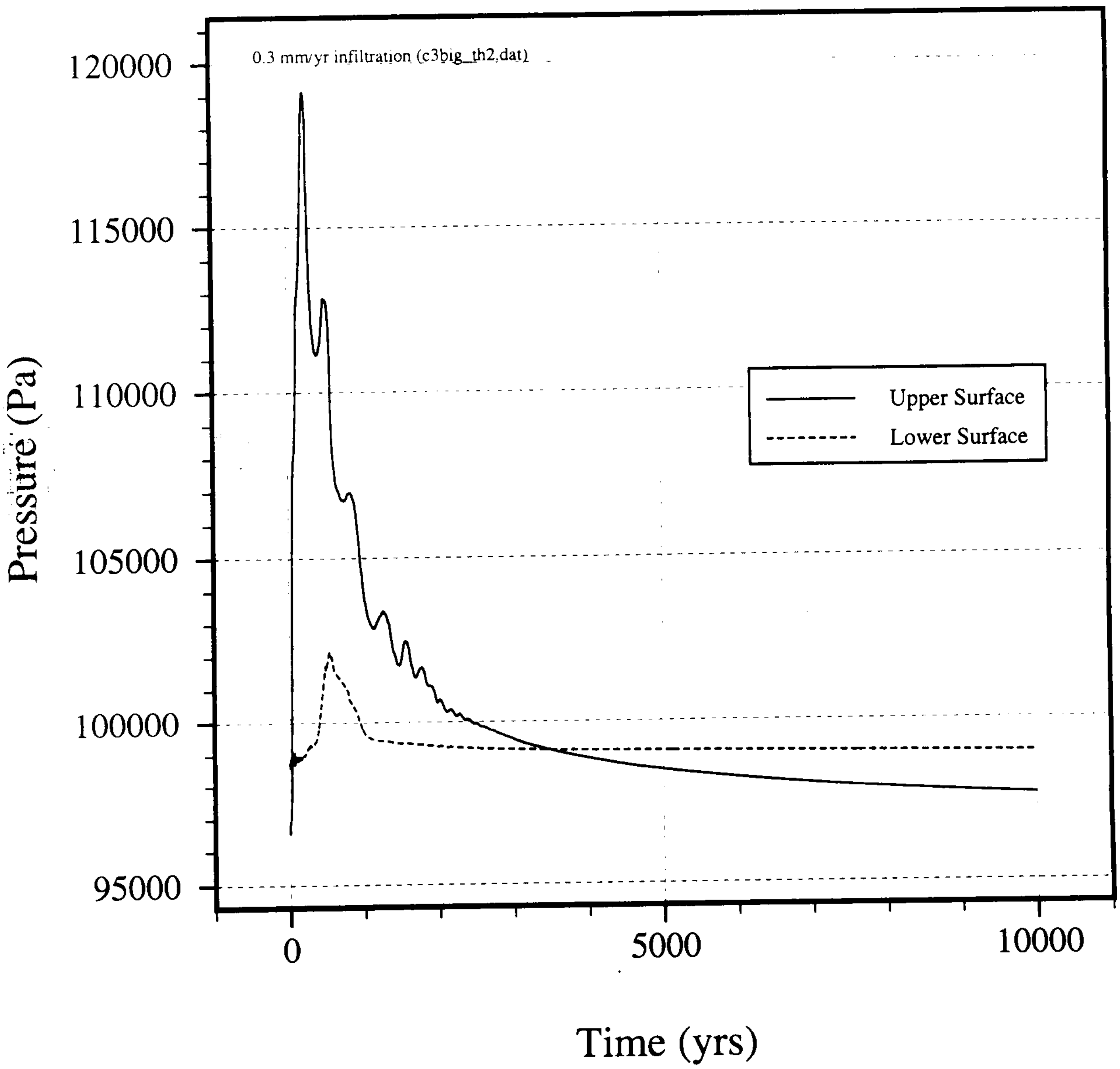

Figure 2.3-6. Gas pressure as functions of time from the big model thermal run.

2.3.2 Test of Mikko's Nested 3D Metra Base Case (Second Test and Scooping Analyses for Matrix Porosity)

2.3.2.1 Scooping Analyses for Matrix Porosity

Case 1 (basecase):	ϕ=0.139	(input file: *c3big2.dat*)
Case 2 (lower ϕ):	ϕ=0.082	(input file: prosity1.dat)
Case 3 (upper ϕ):	ϕ=0.196	(input file: prosity2.dat)

- Figs 2-3-7 through 2-3-9 show temperature time history at various observation points for cases 1 through 3, respectively.
- It was discovered in examining the relative humidity results that RH never changes. The reason is that in order to calculate RH, *ivplwr* in METRA needs to be 1, while basecase input file has 0. Therefore scooping analyses need to be discontinued and basecase needs to be reevaluated.

2.3.2.2 Basecase initial run with *ivplwr*=1

Appear to be working. Figures 2.3-10 through 2-3-12 show time history of saturation, relative humidity, and gas pressure, respectively.

Figures 2.3-13 through 2.3-15 show saturation, temperature, and gas pressure as functions of depth at the initial equilibrium stage before thermal analysis.

2.3.2.3 Basecase thermal run with *ivplwr*=1

Didn't work. Error message: Error in pvtfunc - temperature out of range in block m=1501 tk=0.922264 ???

Mikko will check the problem against George's that seem to work ok.

- After changing ipvtab to 1 (using correlations for calculating water pvt properties rather than using construct tables). The program worked.

- It was decided that the infiltration rate should be 0.36 mm/yr and 3.6 mm/yr. Therefore the basecase need to be recalculated to incorporate these changes.

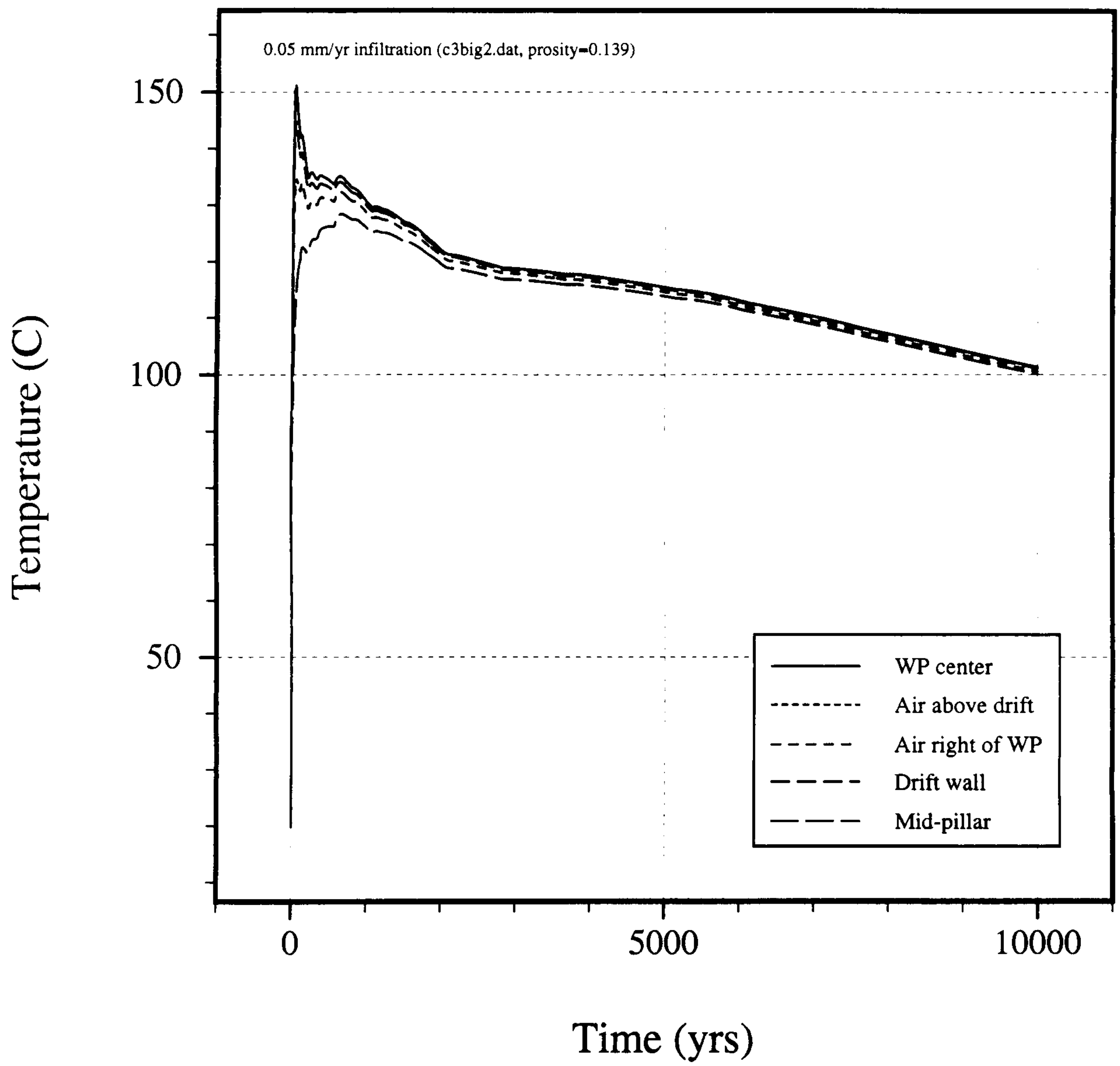

Figure 2.3-7. Temperature time history at various observation points for ϕ = 0.139

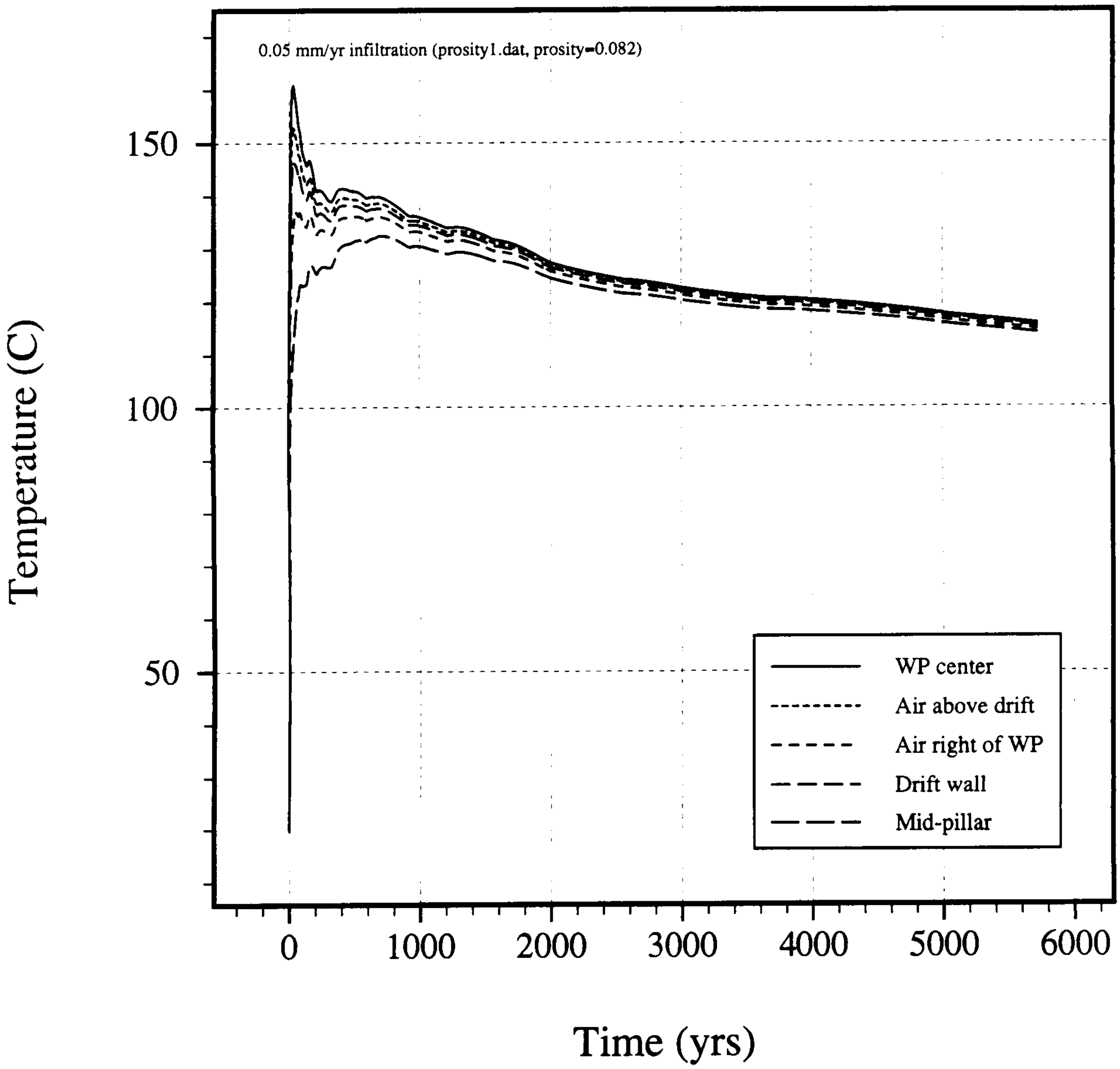

Figure 2.3-8. Temperature time history at various observation points for ϕ = 0.082.

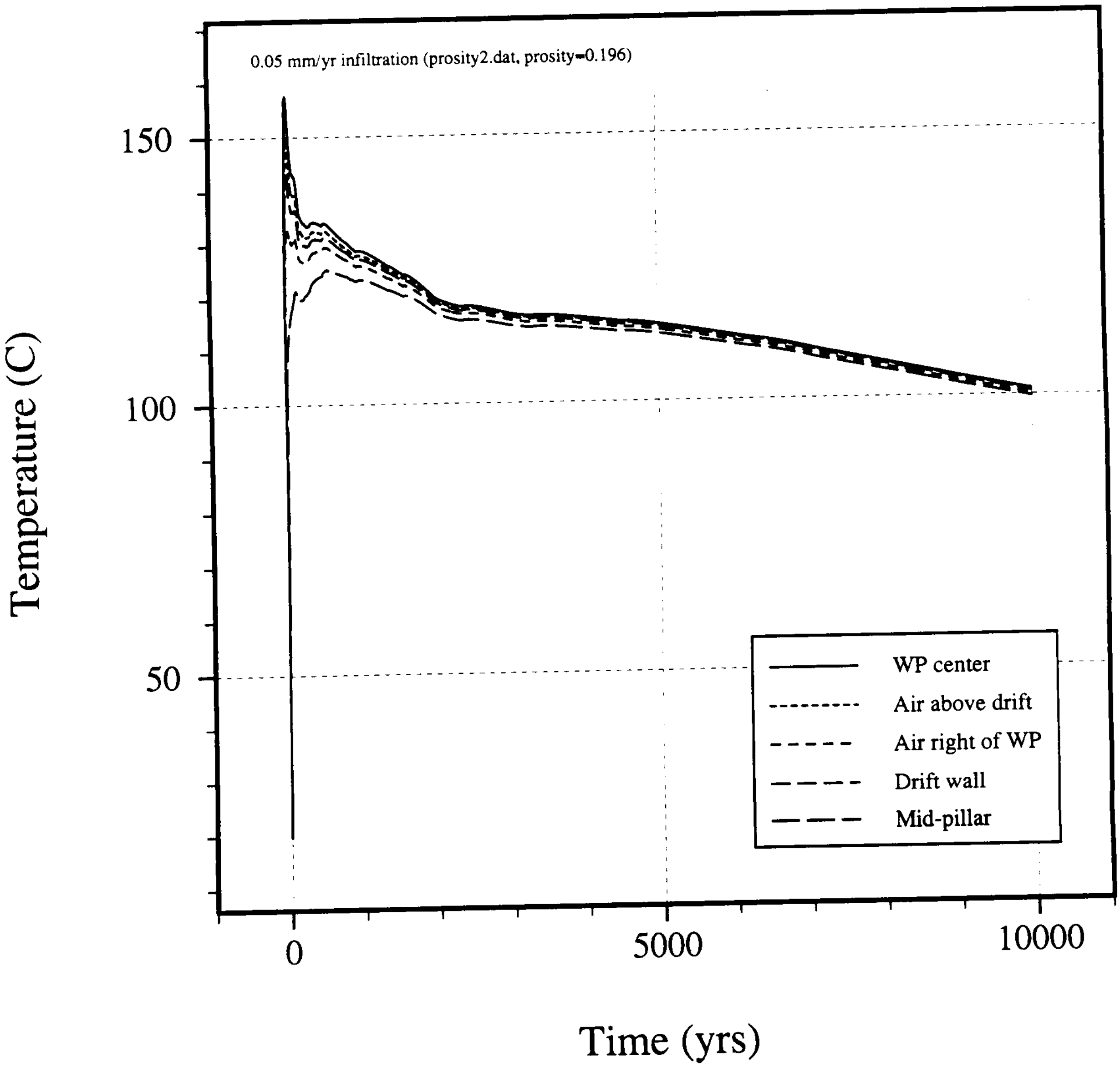

Figure 2.3-9. Temperature time history at various observation points for ϕ = 0.196.

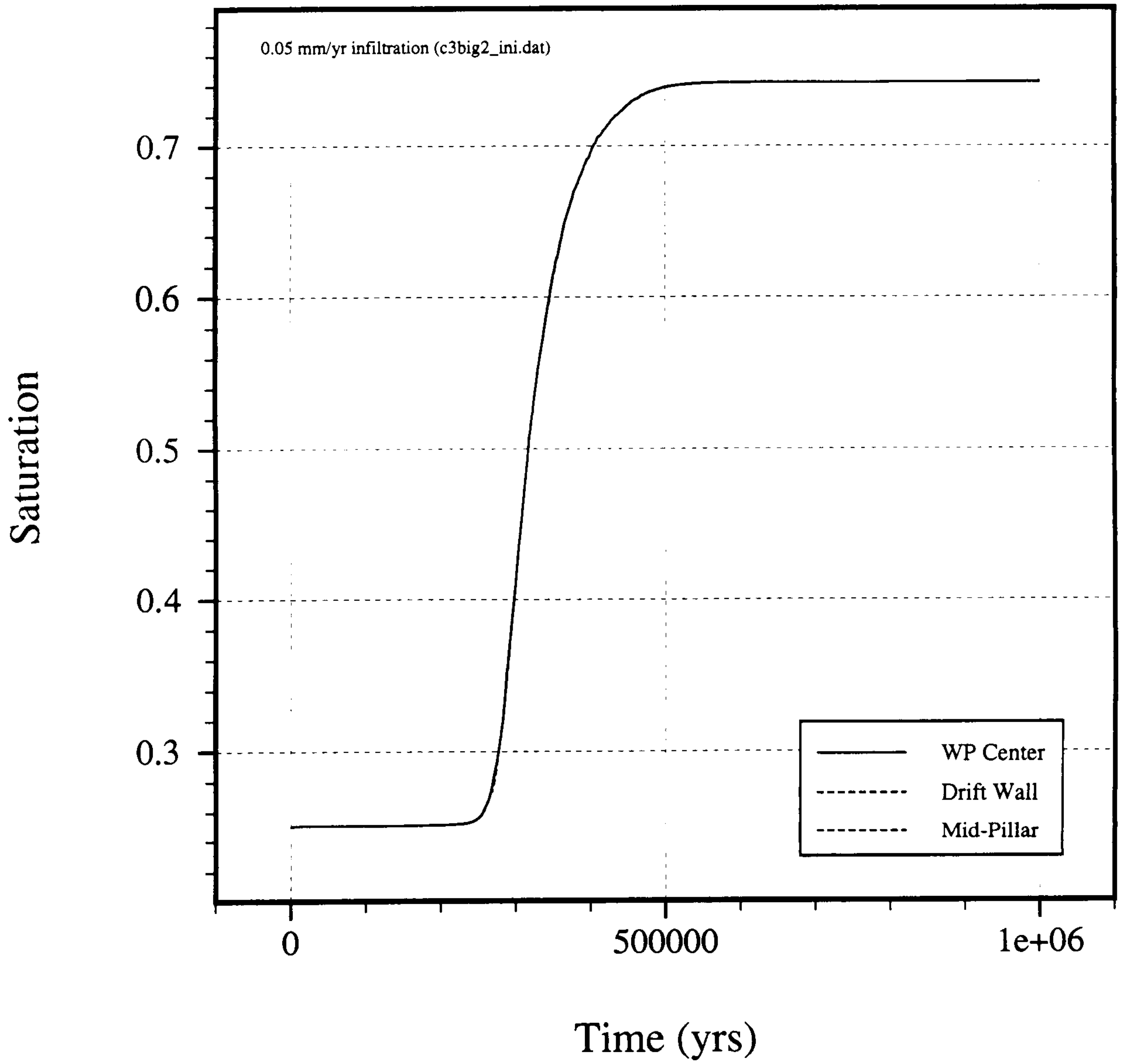

Figure 2.3-10. Time history of saturation for the initial run of the basecase with ivplwr=1, infiltration=0.05 mm/yr.

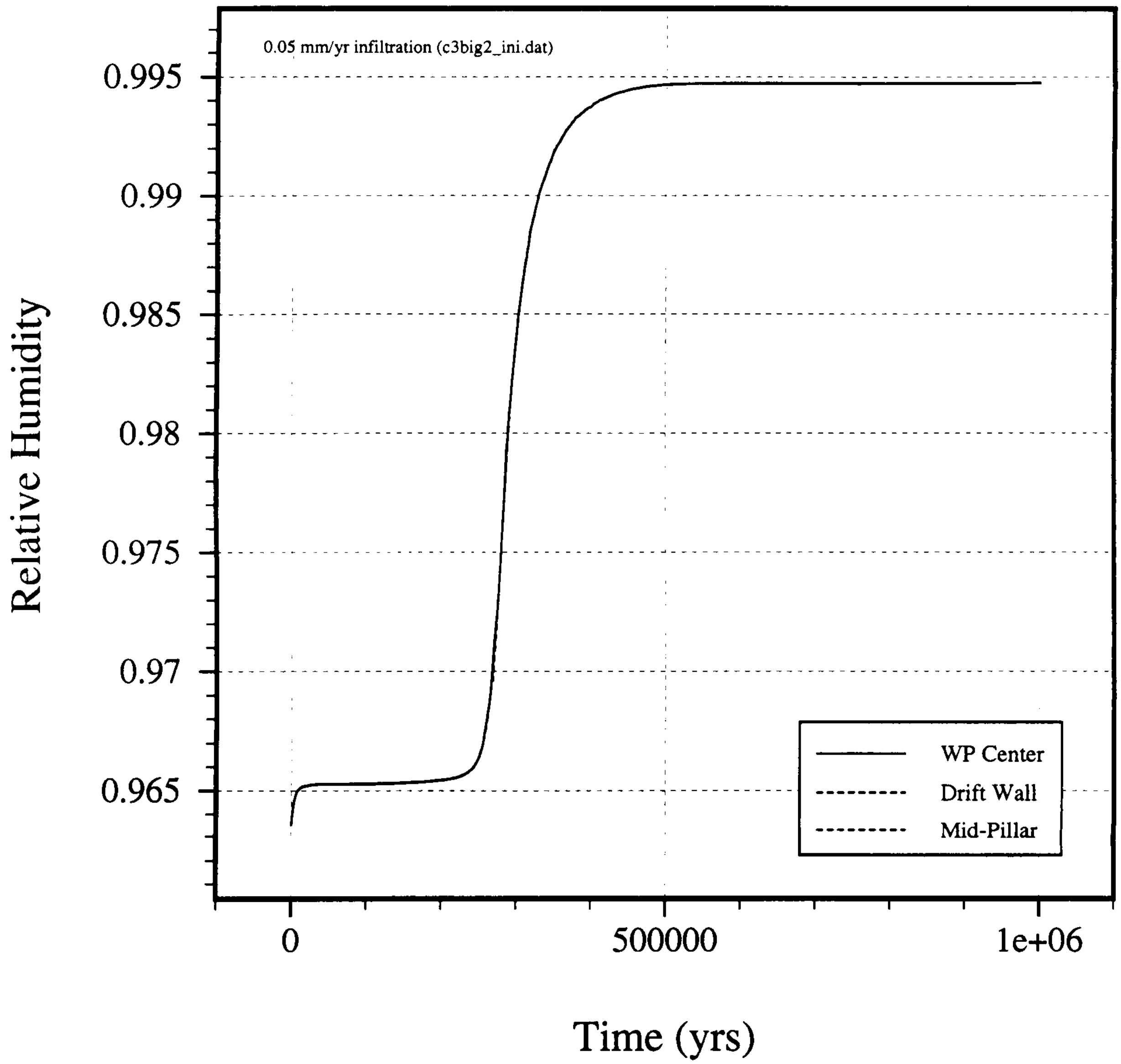

Figure 2.3-11. Time history of the relative humidity from the initial run of the basecase with ivplwr=1, infiltration=0.05 mm/yr.

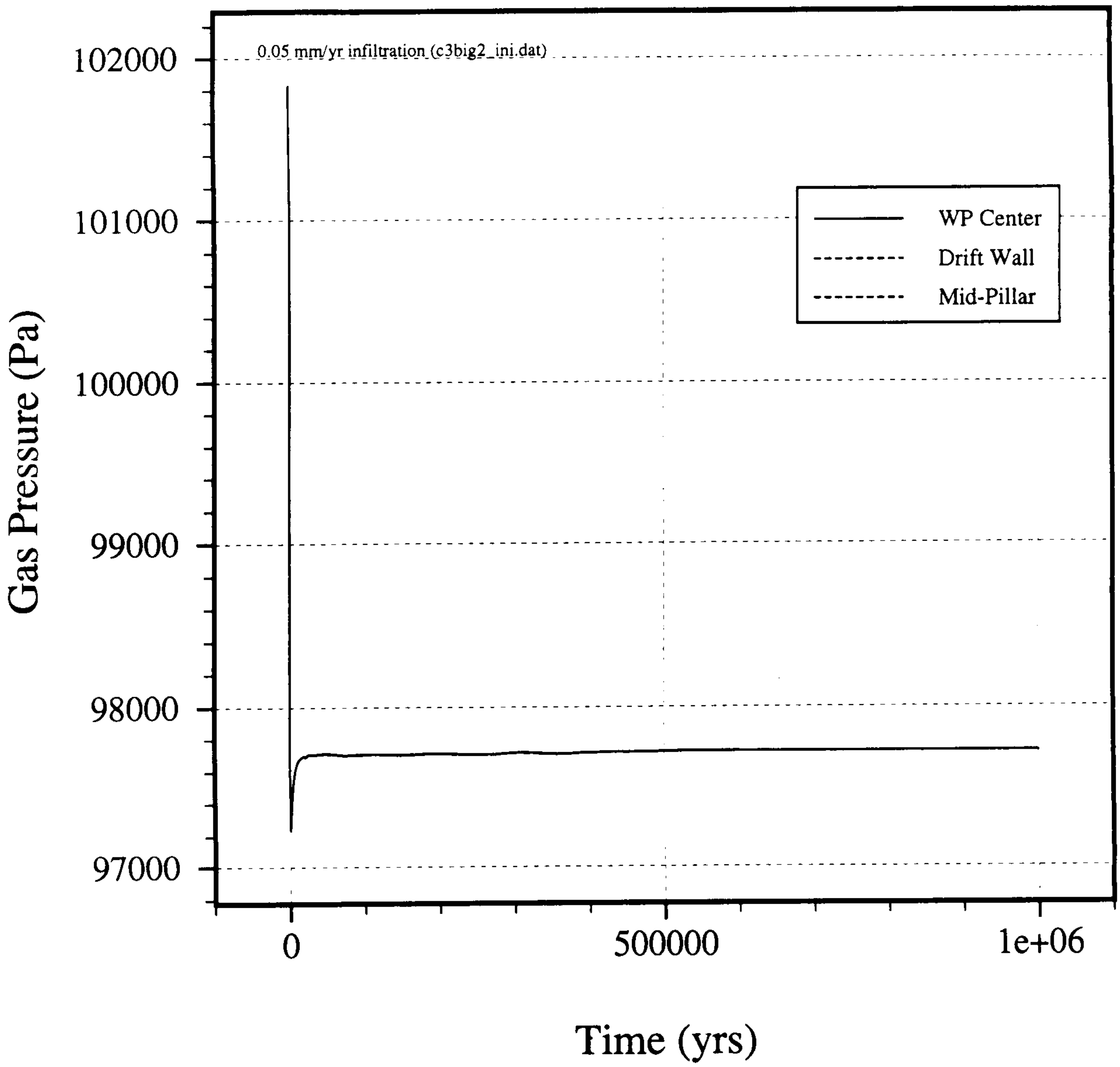

Figure 2.3-12. Time history of gas pressure from the initial run of the basecase with ivplwr=1, infiltration=0.05 mm/yr.

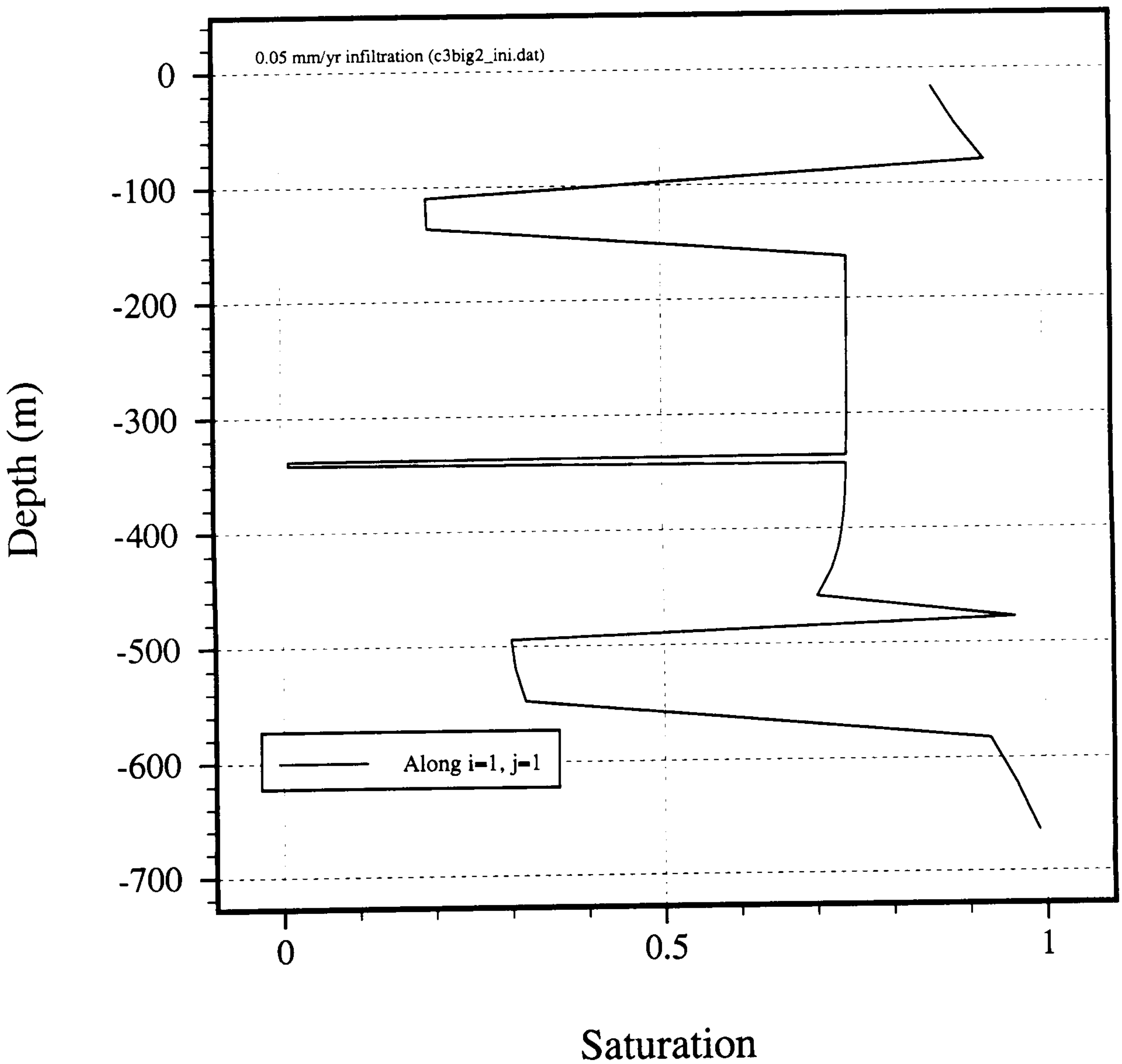

Figure 2.3-13. Saturation distribution along a vertical line through [(i=1,j=1), center of the waste package] at the initial equilibrium for the basecase with ivplwr=1, infiltration=0.05 mm/yr.

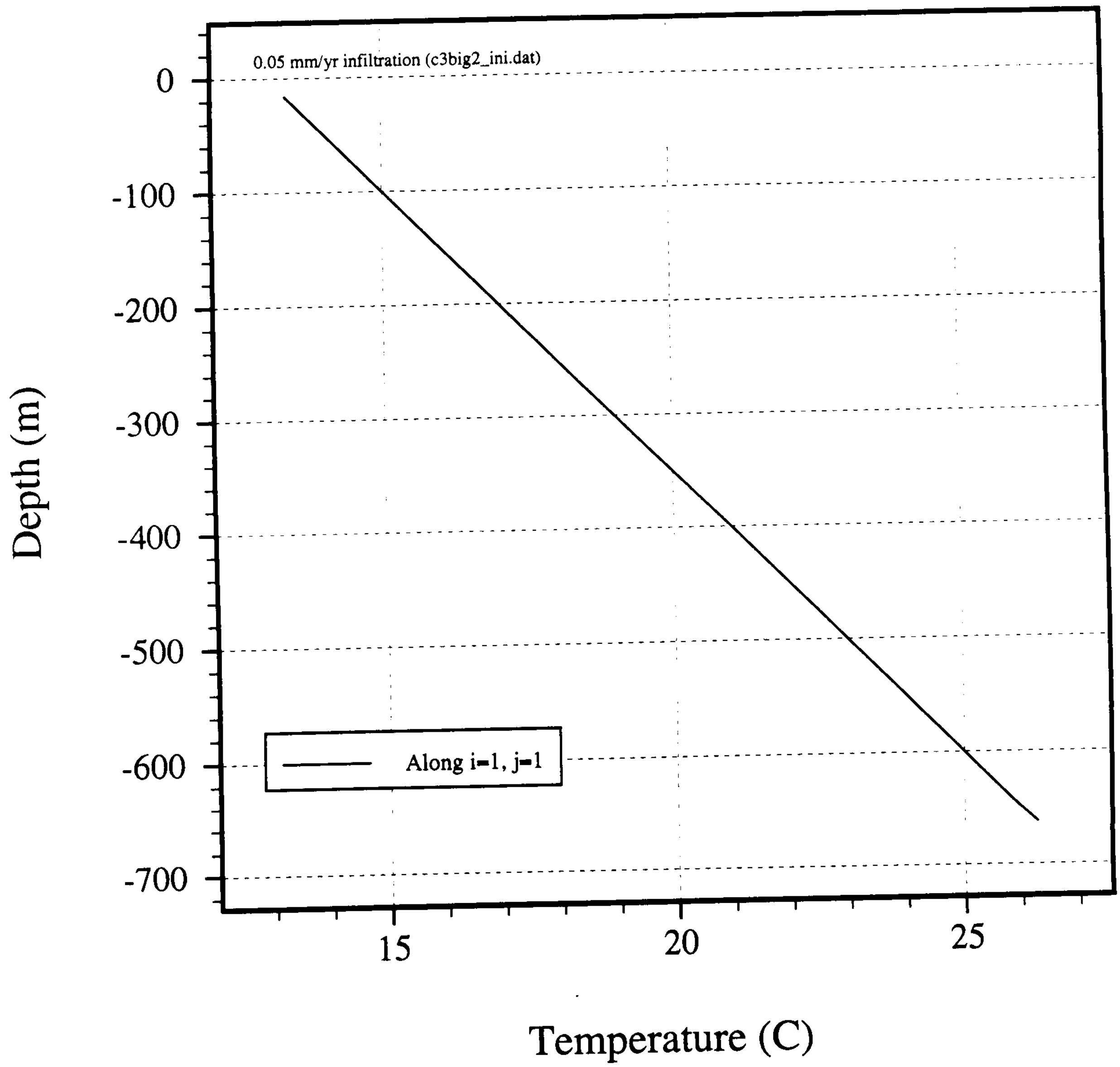

Figure 2.3-14. Temperature distribution along a vertical line through [(i=1,j=1), center of the waste package] at the initial equilibrium for the basecase with ivplwr=1, infiltration=0.05 mm/yr.

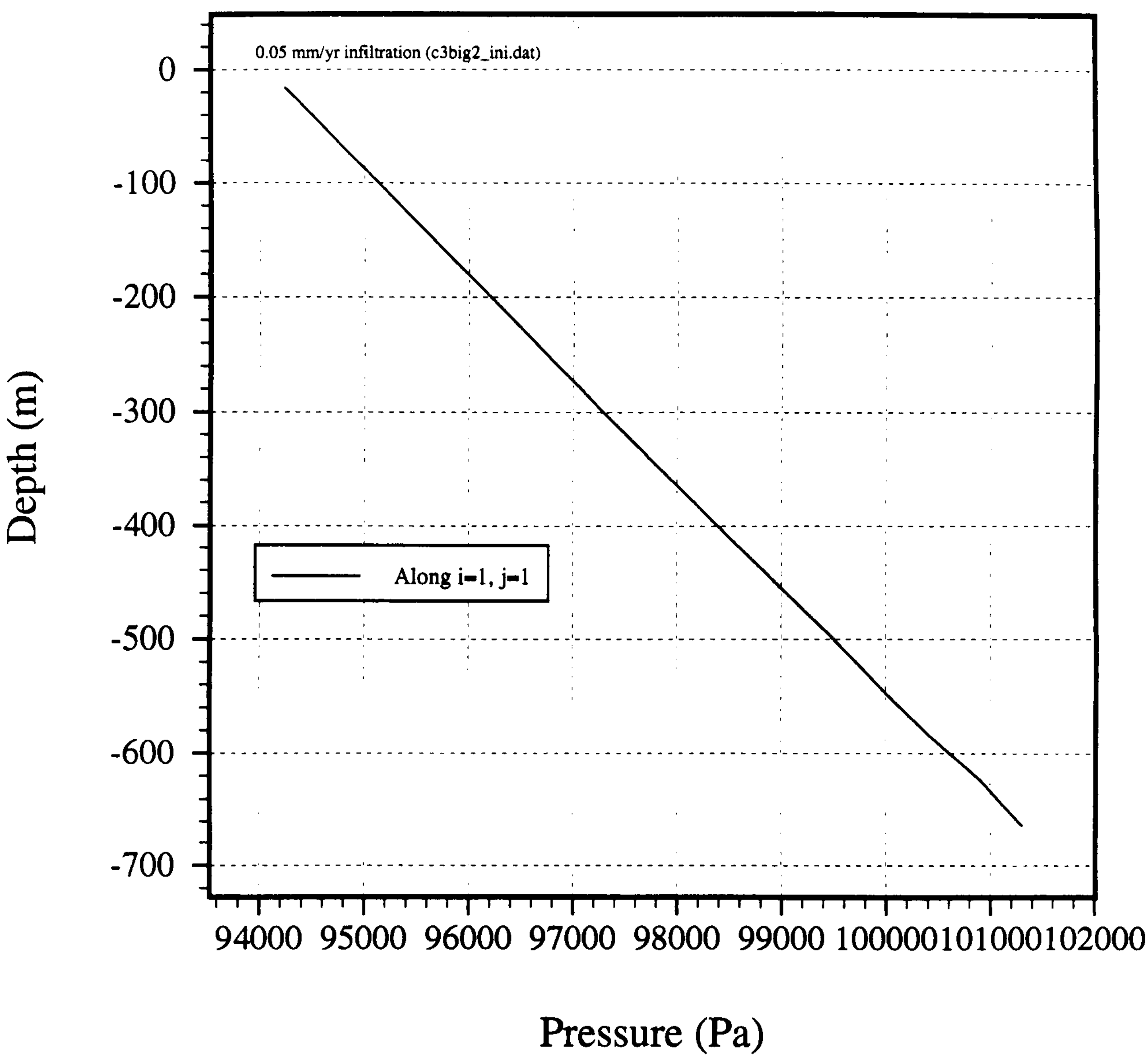

Figure 2.3-15. Gas pressure distribution along a vertical line through [(i=1,j=1), center of the waste package] at the initial equilibrium for the basecase with ivplwr=1, infiltration=0.05 mm/yr.

2.3.3 Test of Mikko's 3D Metra Base Case (Third Test and Scooping Analyses for Matrix Porosity)

New:
- change ivplwr to 1 so that RH is calculated; ipvtab to 1 so that METRA would run
- infiltration rate to high=3.6 mm/yr, low=0.36 mm/yr to using DOE data for surface infiltration

2.3.3.1 Initial Conditions for Low Infiltration:

Figures 2.3-16 through 2.3-18 show saturation, gas pressure, and relative humidity as function of time. Theses figures indicate that equilibrium is well reached before 200000 yrs.

Figures 2.3-19 through 2.3-21 shows distribution of saturation, temperature, and gas pressure along a vertical line through waste package center at the initial equilibrium.

In this calculation, the temperature gradient is not achieved by using Bcon, therefore the temperature distribution shown in Figure 2.3-20 was recalculated according to known geothermal gradient.

2.3.3.2 Thermal Run for Low Infiltration:

- Thermal run at low infiltration (0.36 mm/yr) took about 3 days.

- Figures 2.3-22 through 2.3-25 show time history of temperature, relative humidity, saturation, and gas pressure, respectively. Each of these figures depicts the history at the center of the waste package, air above the drift, air right of the waste package, on the drift wall, and at the middle of the pillar. There is a spike in these figures that is believe to be a numerical abnormal and does not significantly affect the results.

- Figures 2.3-26 through 2.3-28 show distribution of temperature, saturation, and gas pressure along a vertical line through the center of the waste package at 10,000 years. As Figure 2.3-26 shows, the resultant temperature at the ground surface is as high as 100 C, which is obviously not correct. In fact ground was heated up because heat from the WP gradually builds up. The Bcon used in the input file to control ground surface temperature is not effective! In fact, for Type 2 and Type 3 conditions, temperature boundary could not be controlled using "Bcon". The user's manual of Multiflo should make this point clear.

- Because of the wrong temperature, other results (relative humidity, saturation, and gas pressure) are not likely to be correct neither!

2.3.3.3 Re-analyzing the Basecase Model

- Purpose of this rerun and modification to the basecase model is to correct the problem of boundary temperature at the ground surface. In order to hold the temperature constant at the ground surface, a very high heat capacity (1e+4) is specified for the top layer. Also, infiltration is applied using Bcon type 3 boundary (i.e., velocity) instead of type 2 boundary (flux), since velocity is more straight forward.

- Figures 2.3-29 and 2.3-30 shows distribution of temperature and saturation along a vertical line through the waste package. Temperature at the ground surface dropped. However, it is still too high (54 C). It was decided that heat capacity for the top layer should be increased further (1e+20).

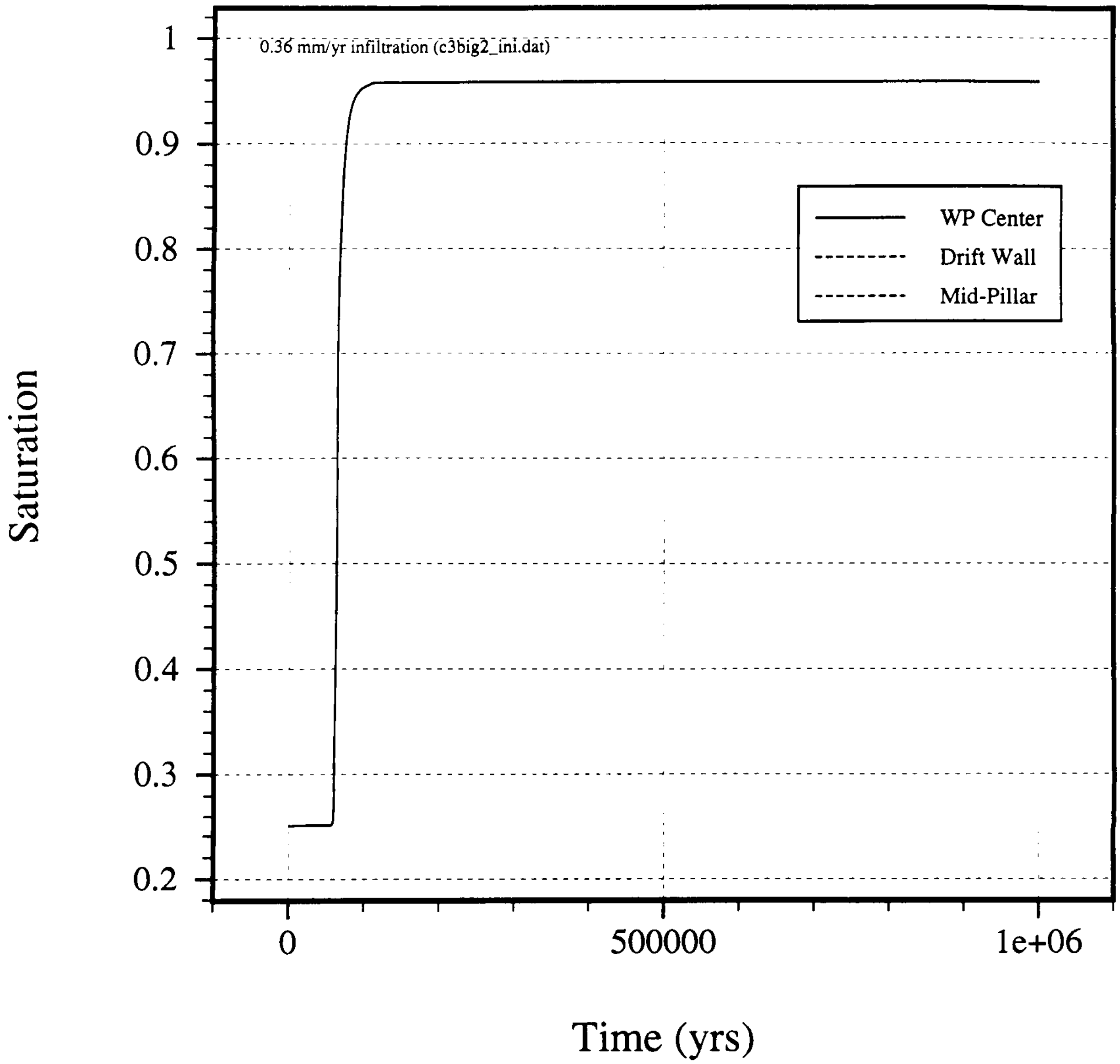

Figure 2.3-16. Saturation history for 0.36 mm/yr infiltration with Bcon, no high heat capacity for the top layer.

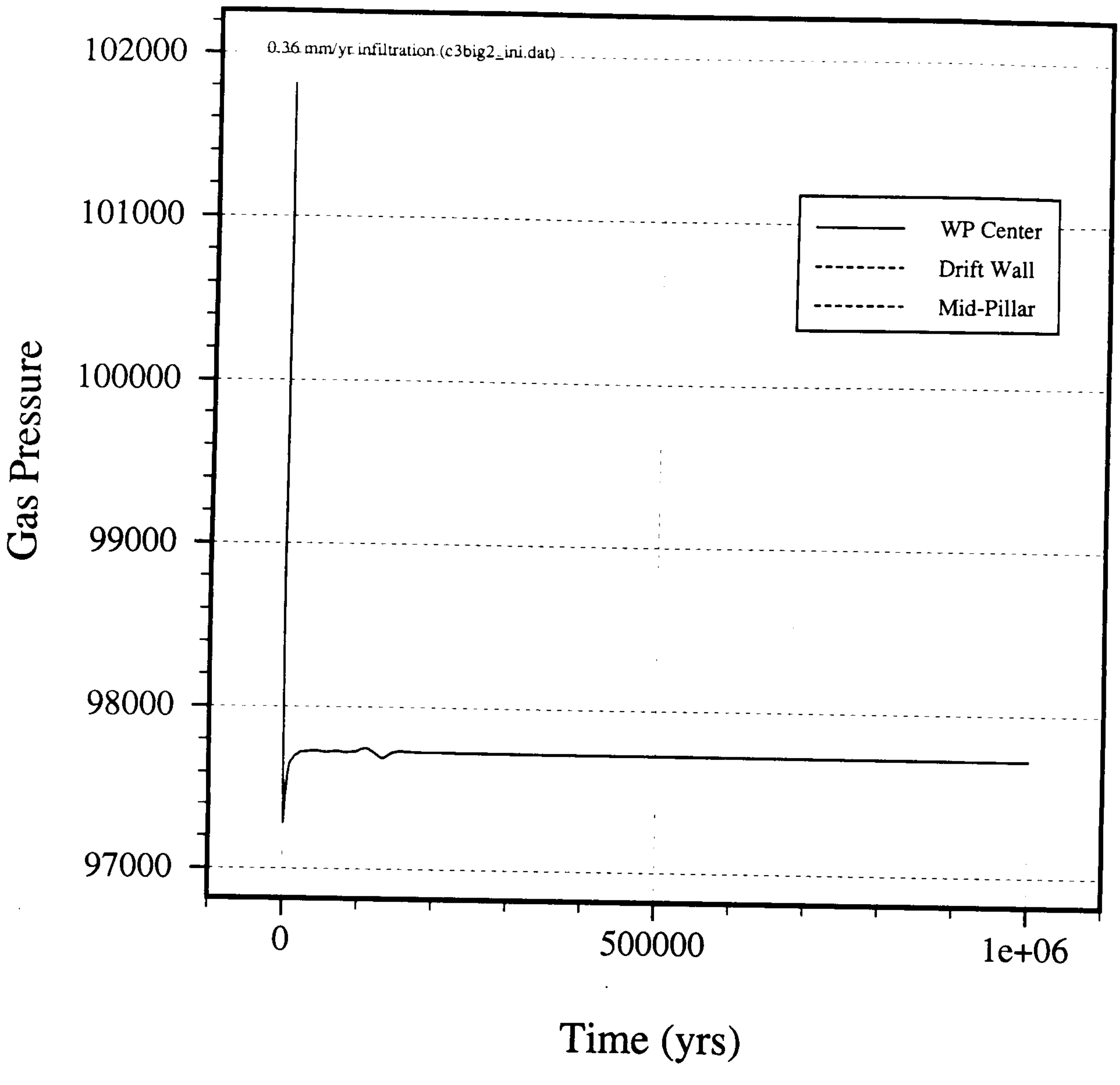

Figure 2.3-17. Gas pressure history for 0.36 mm/yr infiltration with Bcon, no high heat capacity for the top layer.

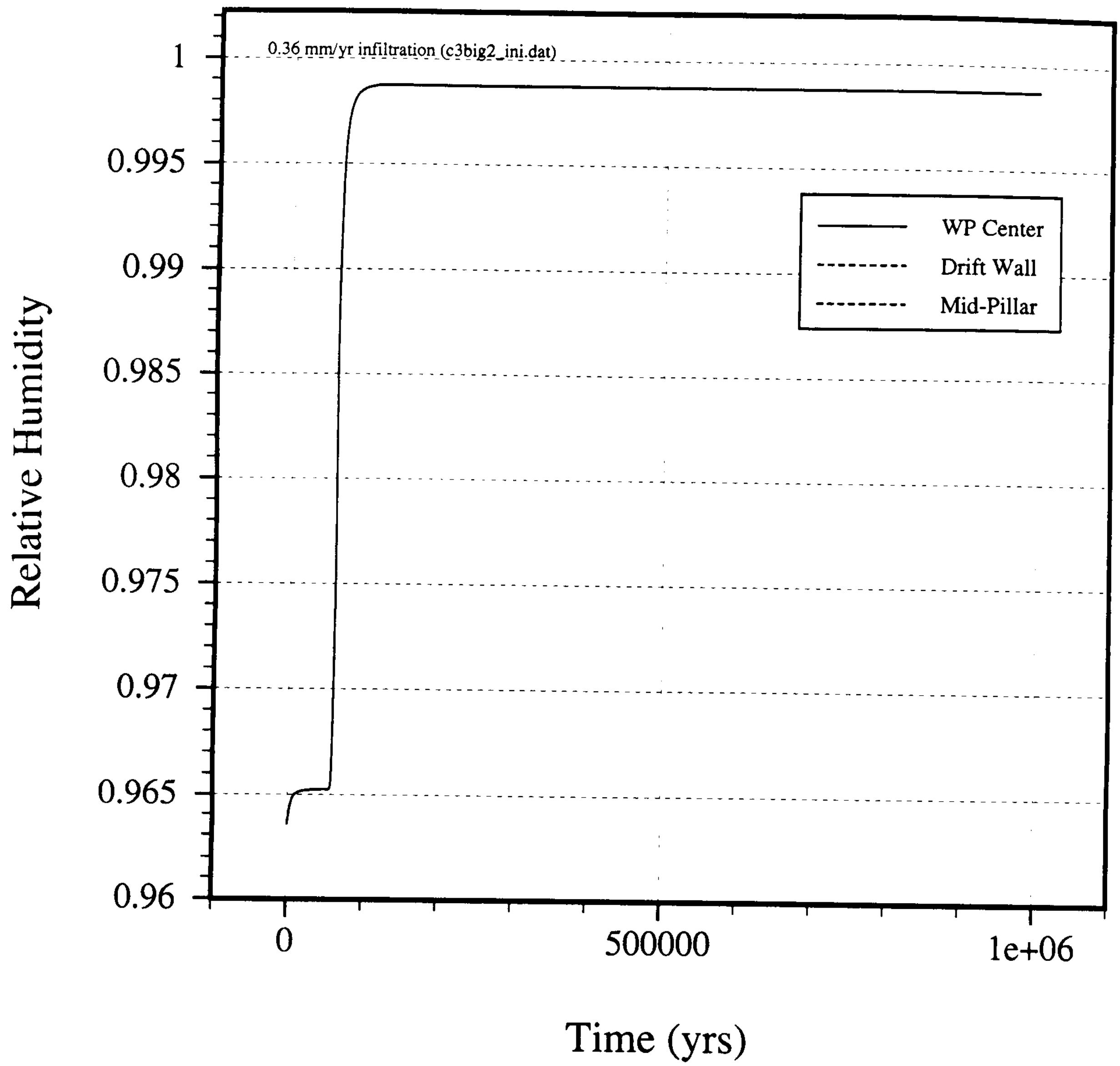

Figure 2.3-18. Relative humidity history for 0.36 mm/yr infiltration with Bcon, no high heat capacity for the top layer.

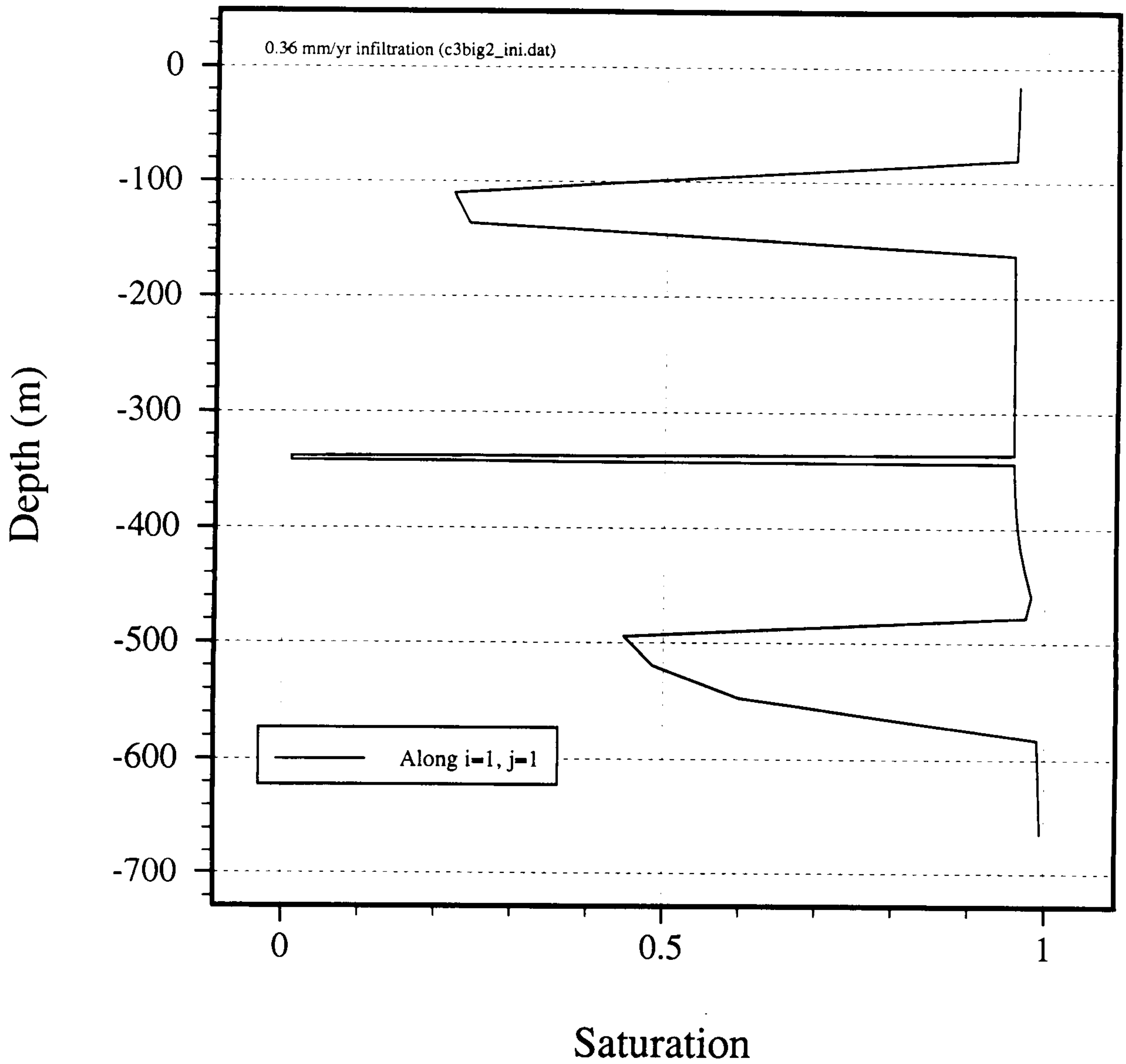

Figure 2.3-19. Distribution of saturation along a vertical line through waste package center (i=1,j=1) at the initial equilibrium.

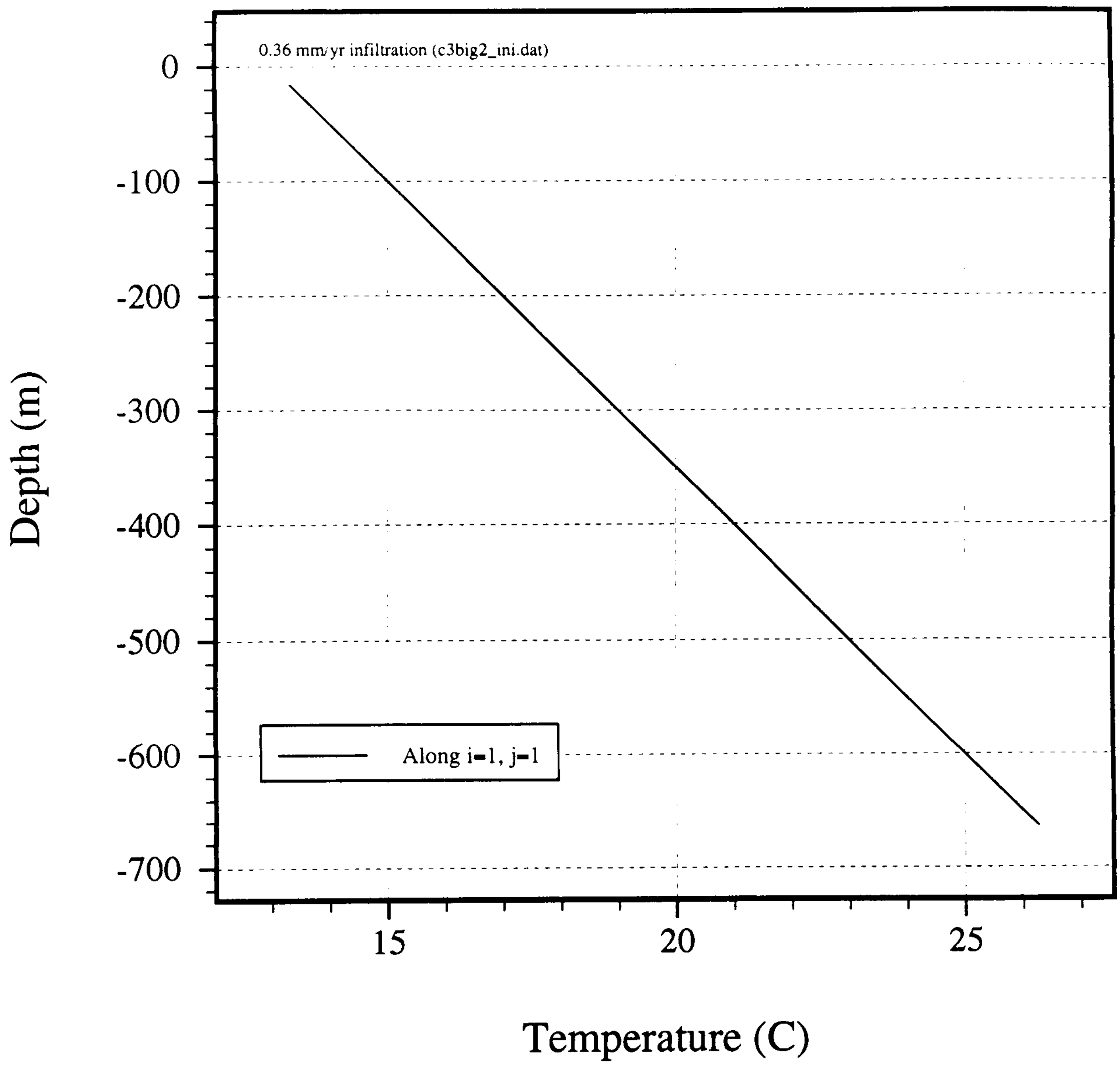

Figure 2.3-20. Distribution of temperature along a vertical line through waste package center (i=1,j=1) at the initial equilibrium.

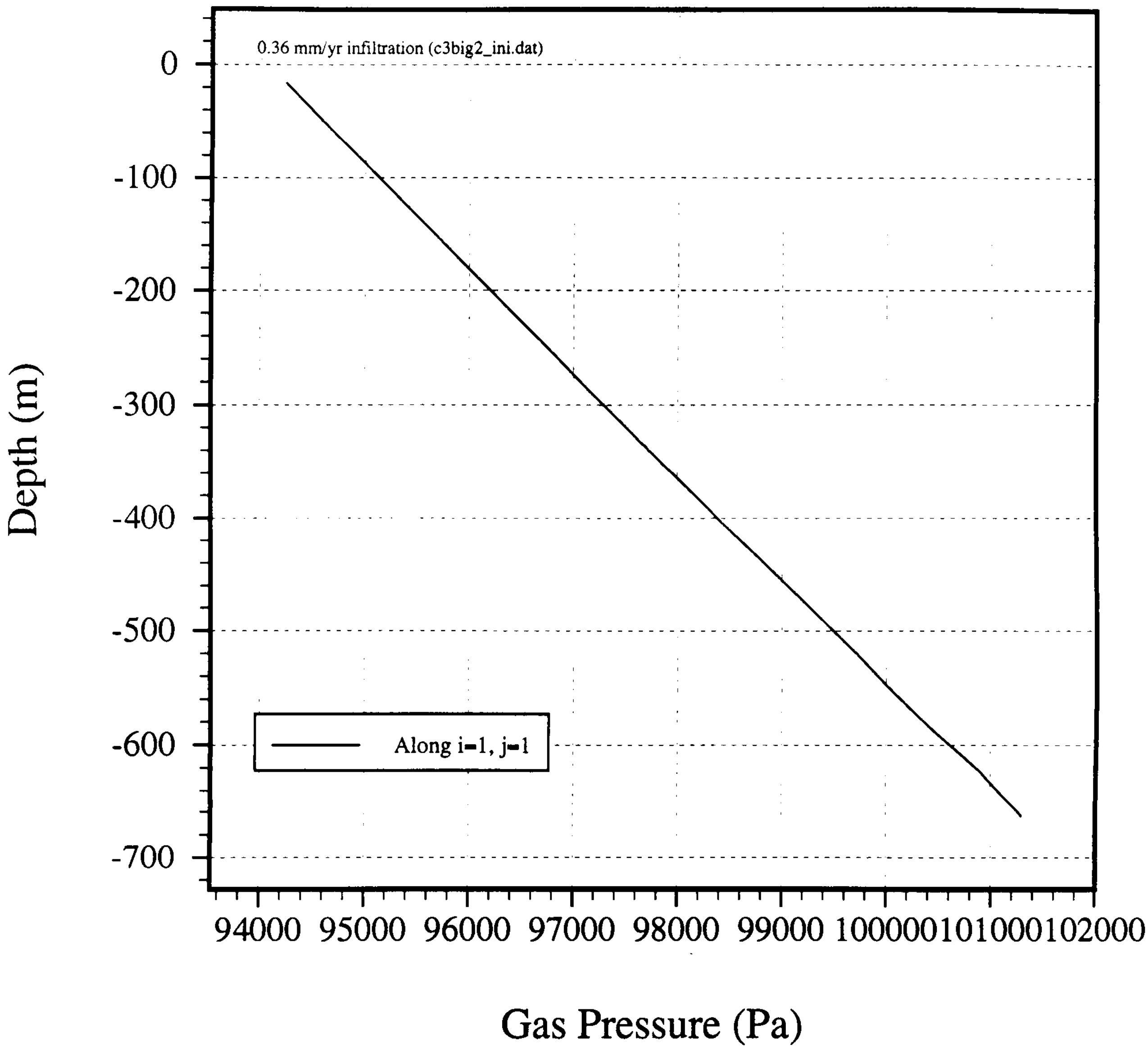

Figure 2.3-21. Distribution of gas pressure along a vertical line through waste package center (i=1,j=1) at the initial equilibrium.

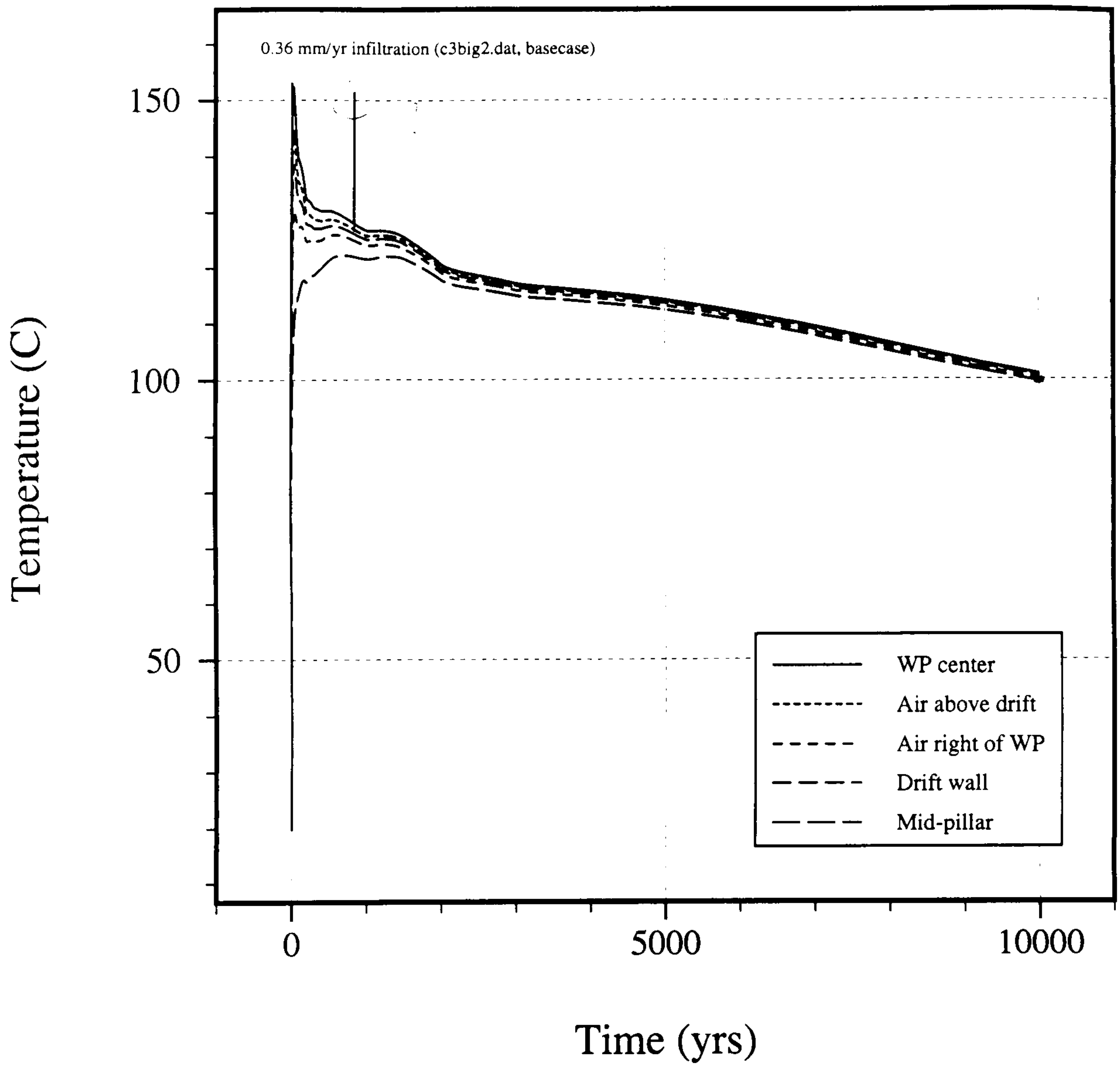

Figure 2.3-22. Time history of temperature for 0.36 mm/yr infiltration.

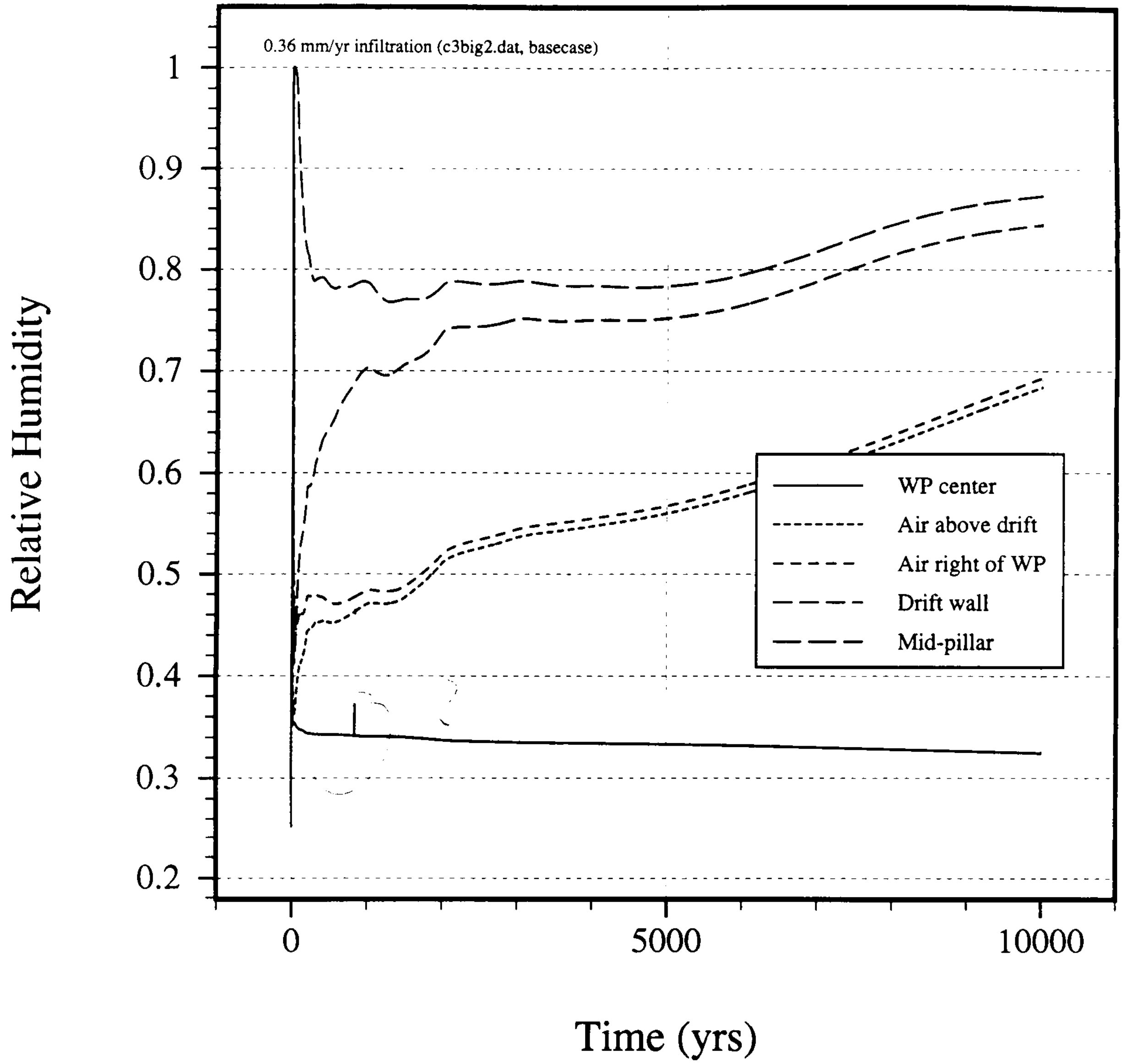

Figure 2.3-23. Time history of relative humidity for 0.36 mm/yr infiltration.

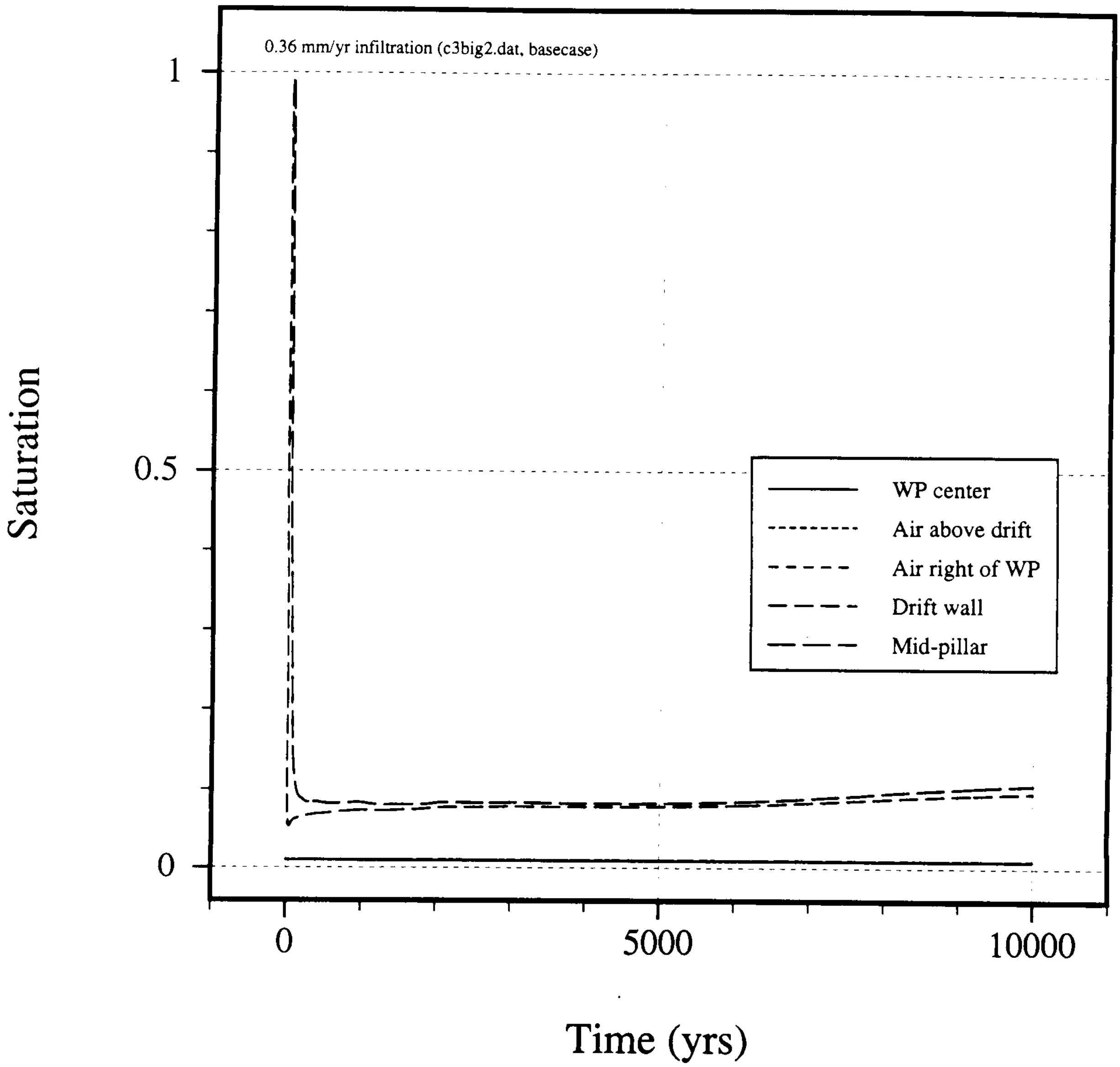

Figure 2.3-24. Time history of saturation for 0.36 mm/yr infiltration.

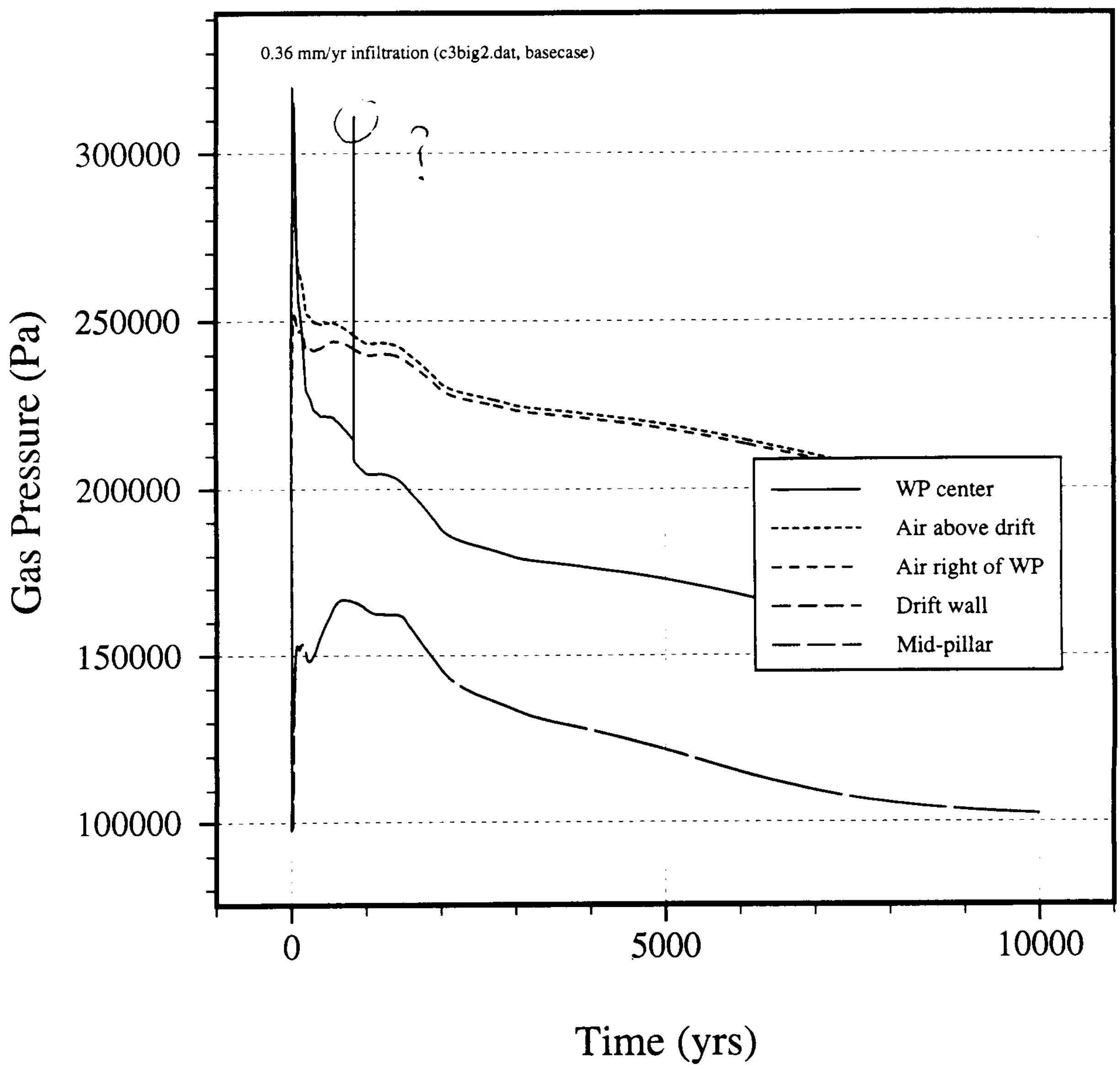

Figure 2.3-25. Time history of gas pressure for 0.36 mm/yr infiltration.

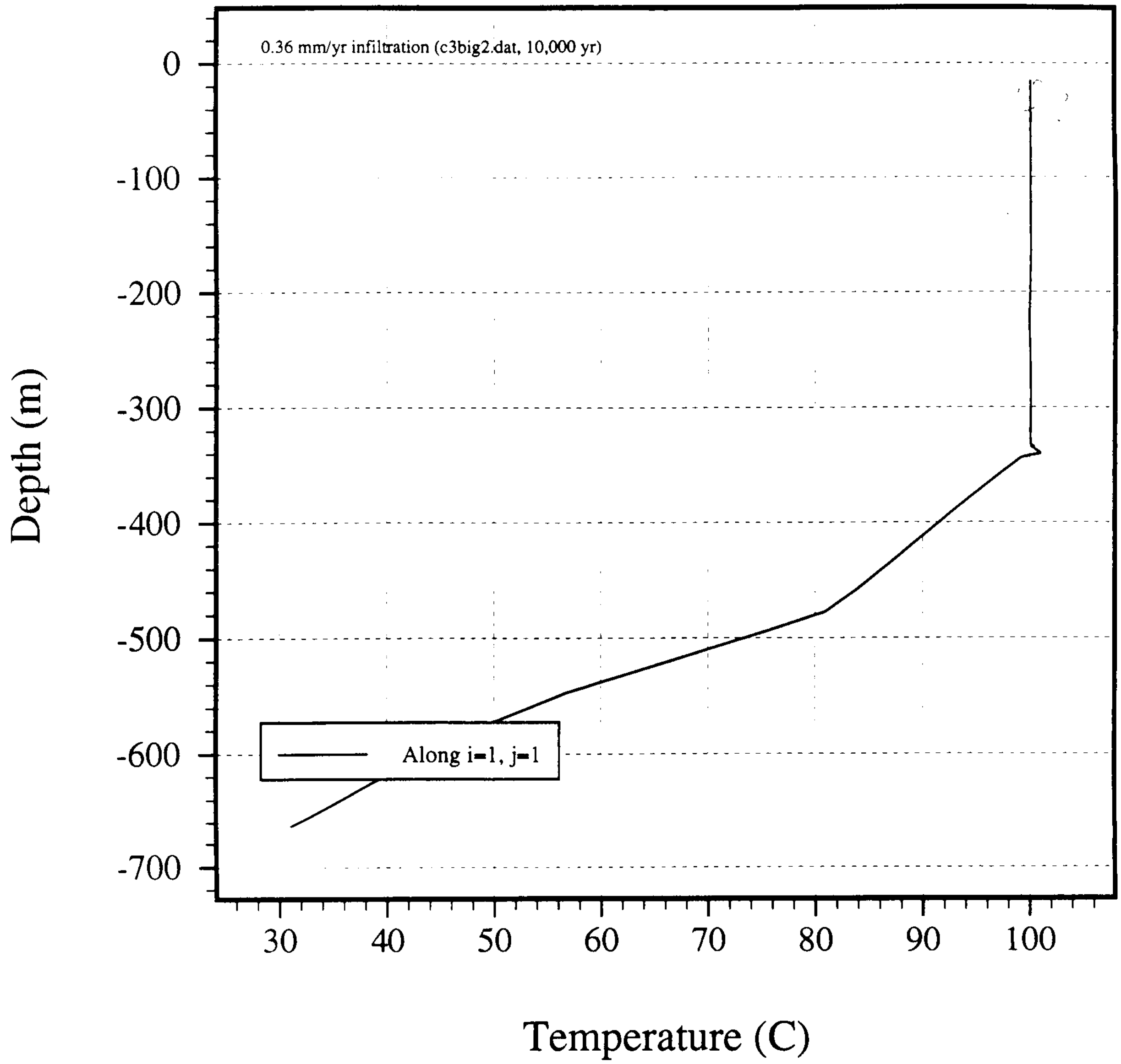

Figure 2.3-26. Distribution of temperature along a vertical line through the center of the waste package (i=1,j=1) at 10,000 yrs for 0.36 mm/yr infiltration.

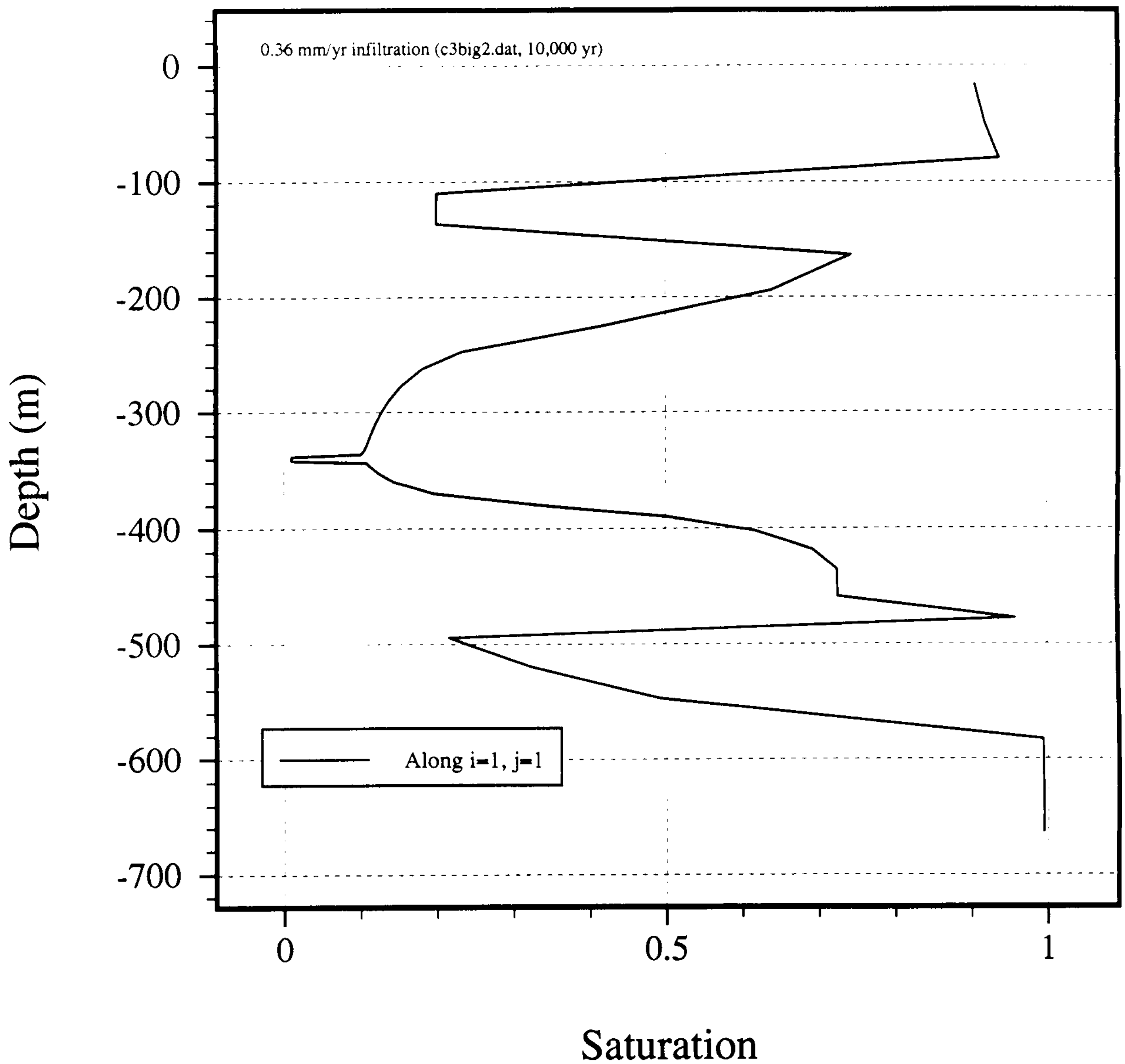

Figure 2.3-27. Distribition of saturation along a vertical line through the center of the waste package (i=1,j=1) at 10,000 yrs for 0.36 mm/yr infiltration.

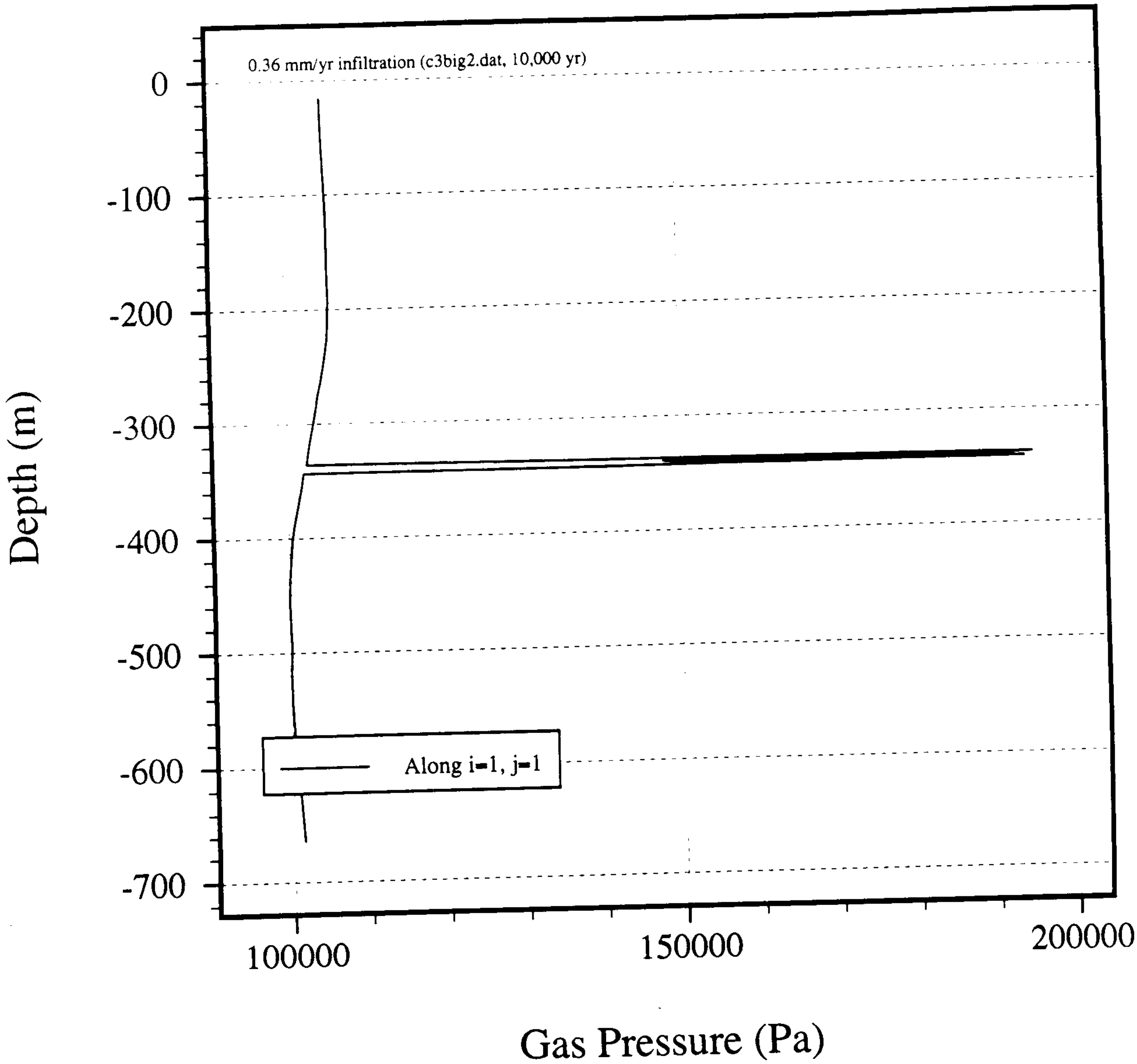

Figure 2.3-28. Distribution of gas pressure along a vertical line through the center of the waste package (i=1,j=1) at 10,000 yrs for 0.36 mm/yr infiltration.

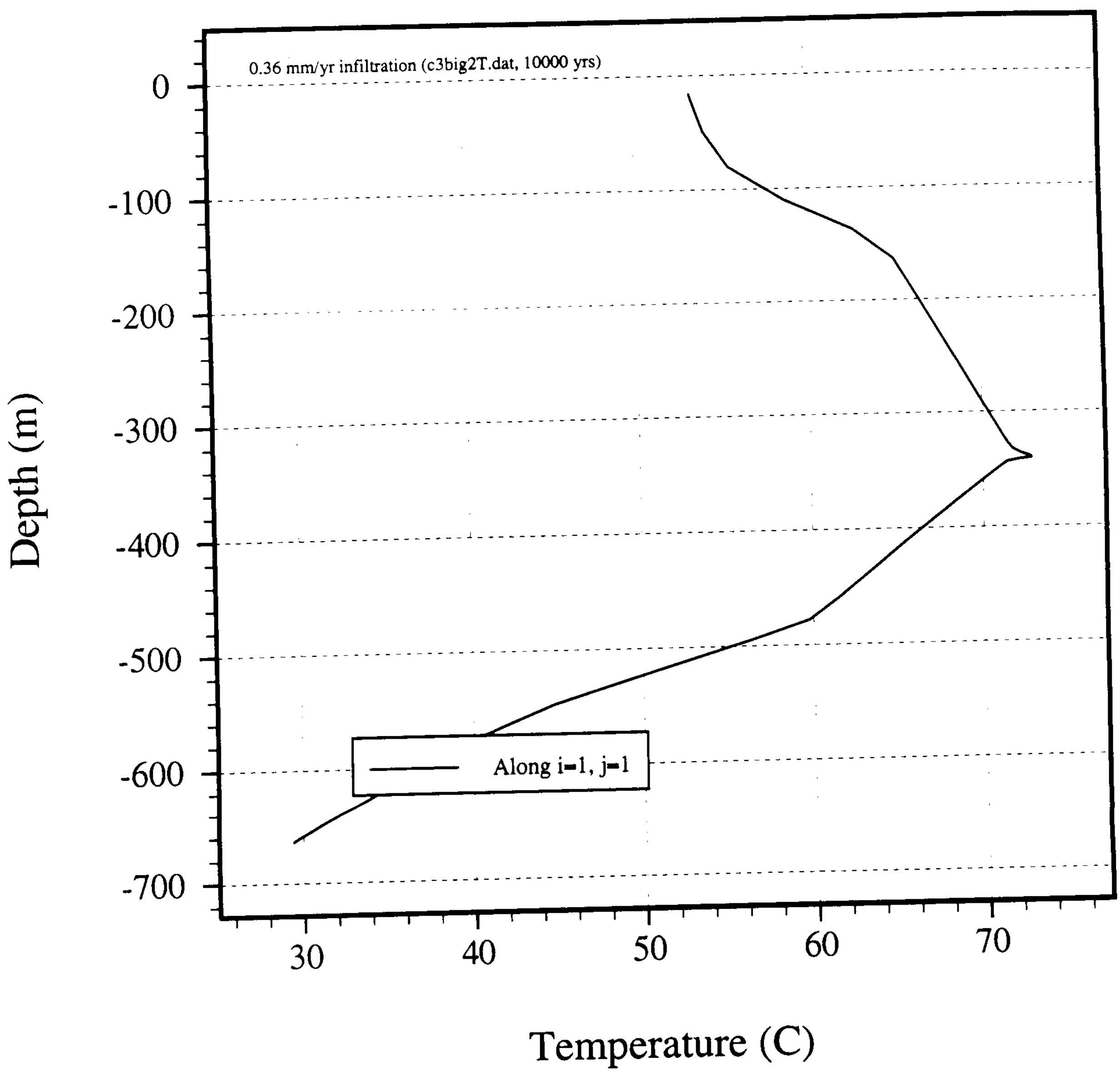

Figure 2.3-29. Distribution of temperature along a vertical line through the center of the waste package (i=1,j=1) at 10,000 yrs for 0.36 mm/yr infiltration and the revised basecase model.

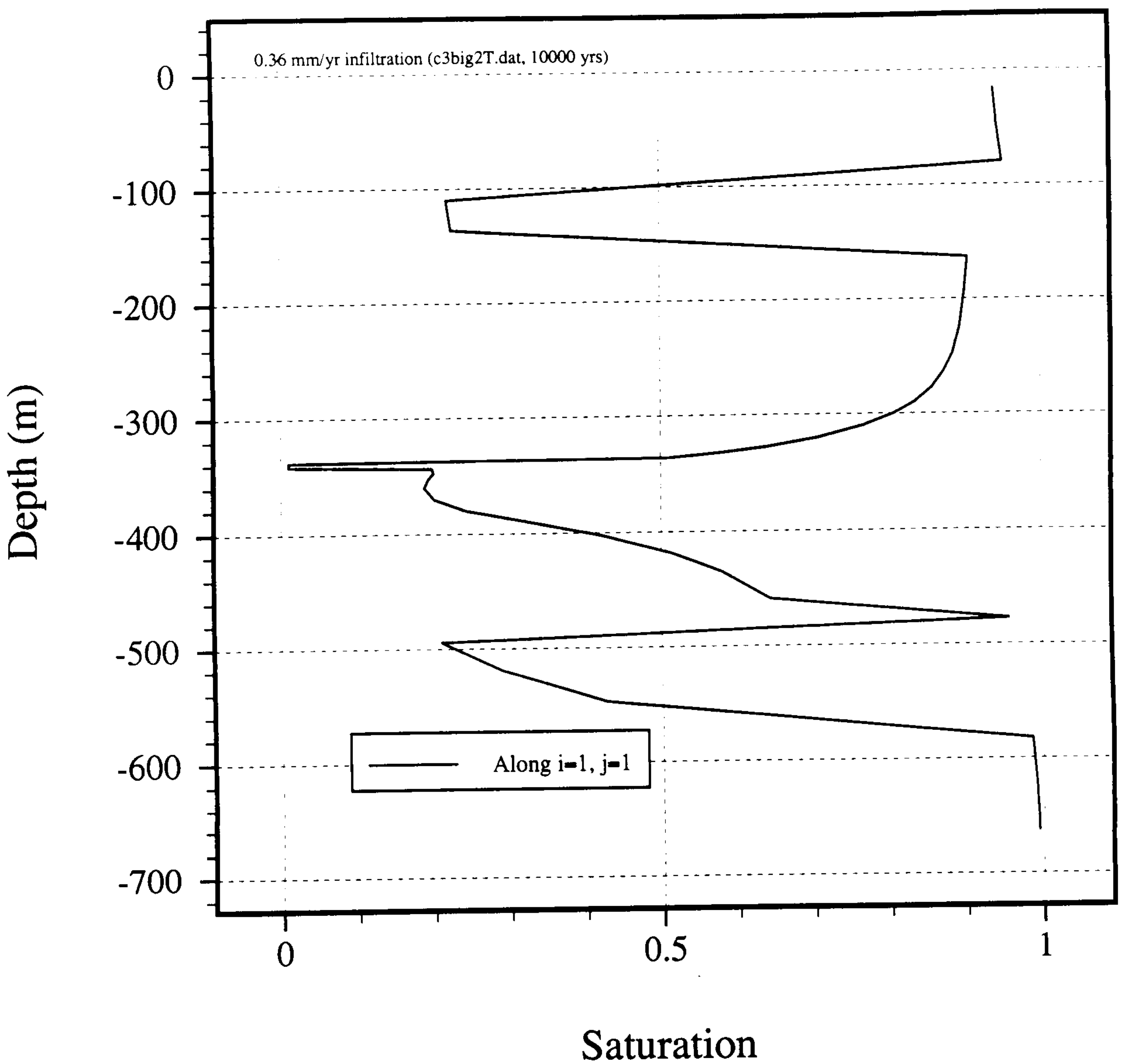

Figure 2.3-30. Distribution of saturation along a vertical line through the center of the waste package (i=1,j=1) at 10,000 yrs for 0.36 mm/yr infiltration and the revised basecase model.

2.3.4 Third Re-analyses of the Basecase Model (Low Infiltration, 0.36 mm/yr)

- To further correct the problem of boundary temperature at the ground surface, the heat capacity at the ground surface (one layer, k=1) was further increased from (1e+4) to (1e+20). However, with this high heat capacity, an error occurred: "error in pvtvp.f- bad vapor press in blk m = 1706". The heat capacity is then decreased to (1e+15) and the problem run successfully.

- Figures 2.3-31 through 2.3-34 show time history of temperature, relative humidity, saturation, and gas pressure, respectively. Figures 2.3-35 through 2.3-37 shows distribution of temperature, saturation, and gas pressure along a vertical line through the center of the waste package. These results look good and reasonable.

2.3.5 Analyses of the Basecase Model with High Infiltration (3.6 mm/yr)

2.3.5.1 Initial Equilibrium

- For the low infiltration run, since temperature boundary condition was not properly maintained, the initial run was only for hydraulic conditions. The temperature was recalculated according to the geothermal gradient. It was decided the artificial high heat capacity strategy be used for the initial calculation of the base case for high infiltration.

- Input file is: c3big1_ini.dat. However, Multiflo bumped at about 600 yrs due to error: "error in pvtvp.f- bad vapor press in blk m = 170". Heat capacity is, therefore, reduced to 1e+10.

*** STUDY CONTINUED BY GEOGY RICE ***

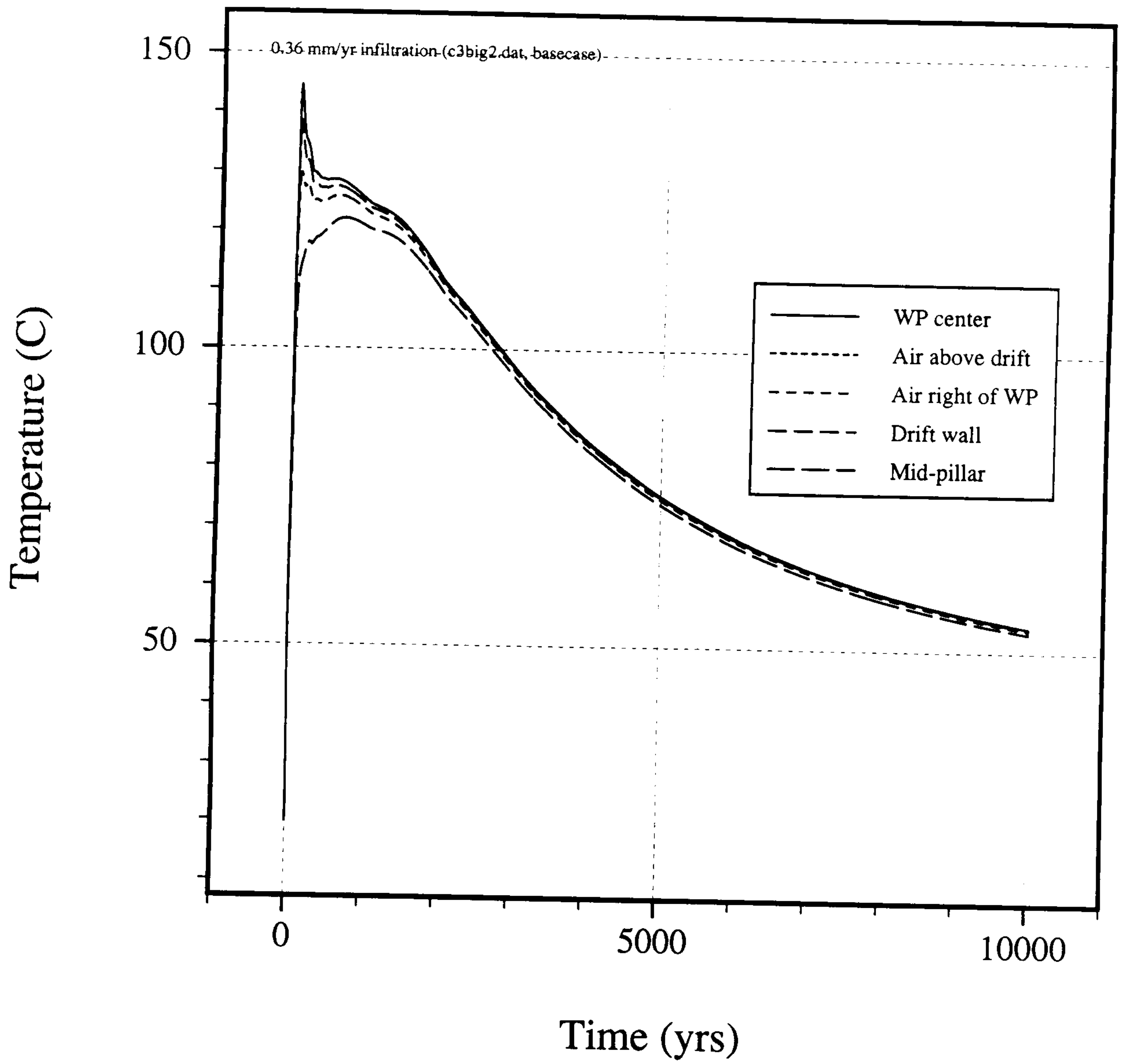

Figure 2.3-31. Time history of termperature for 0.36 mm/yr infiltration and further revised basecase model.

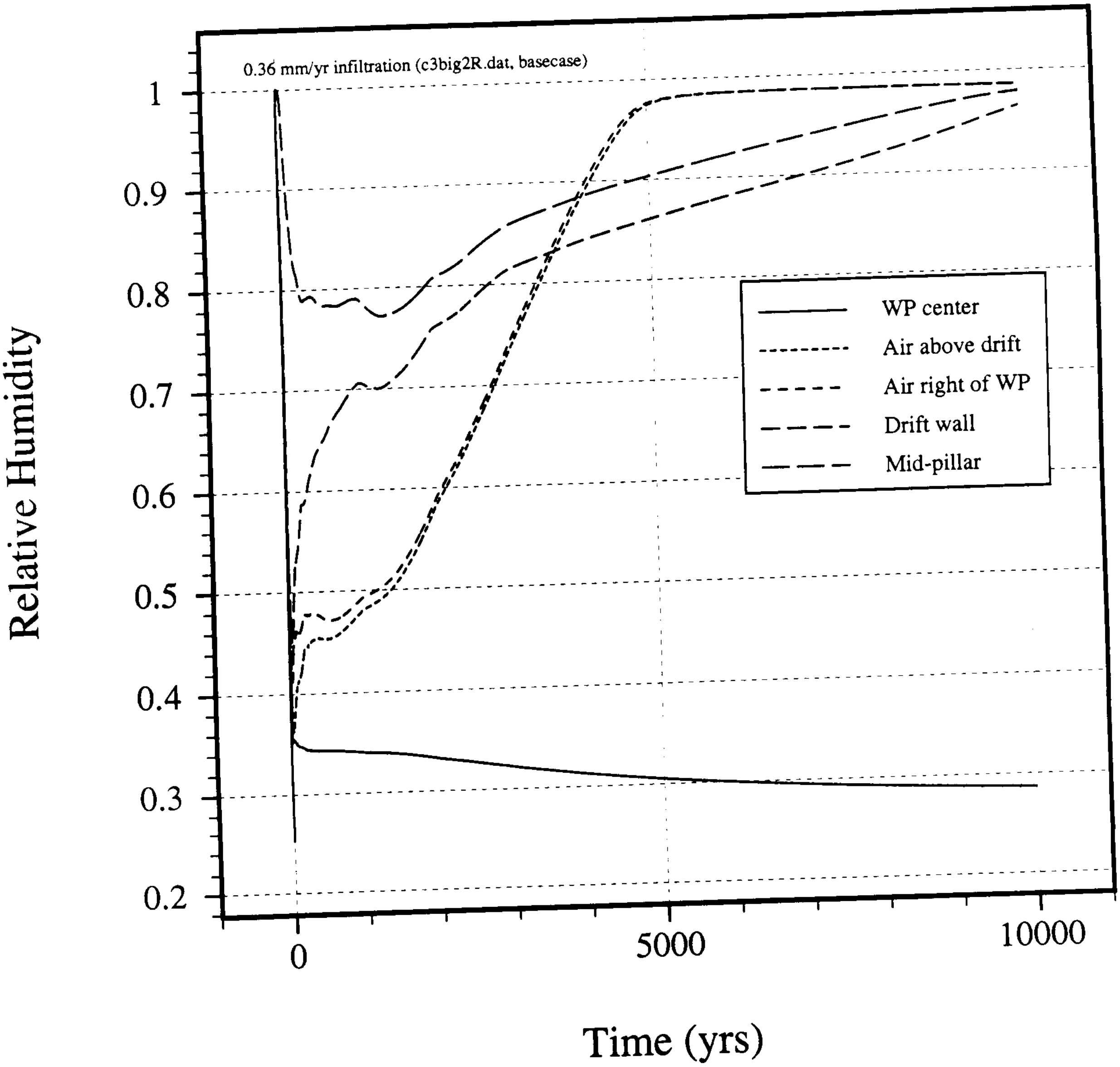

Figure 2.3-32. Time history of relative humidity for 0.36 mm/yr infiltration and further revised basecase model.

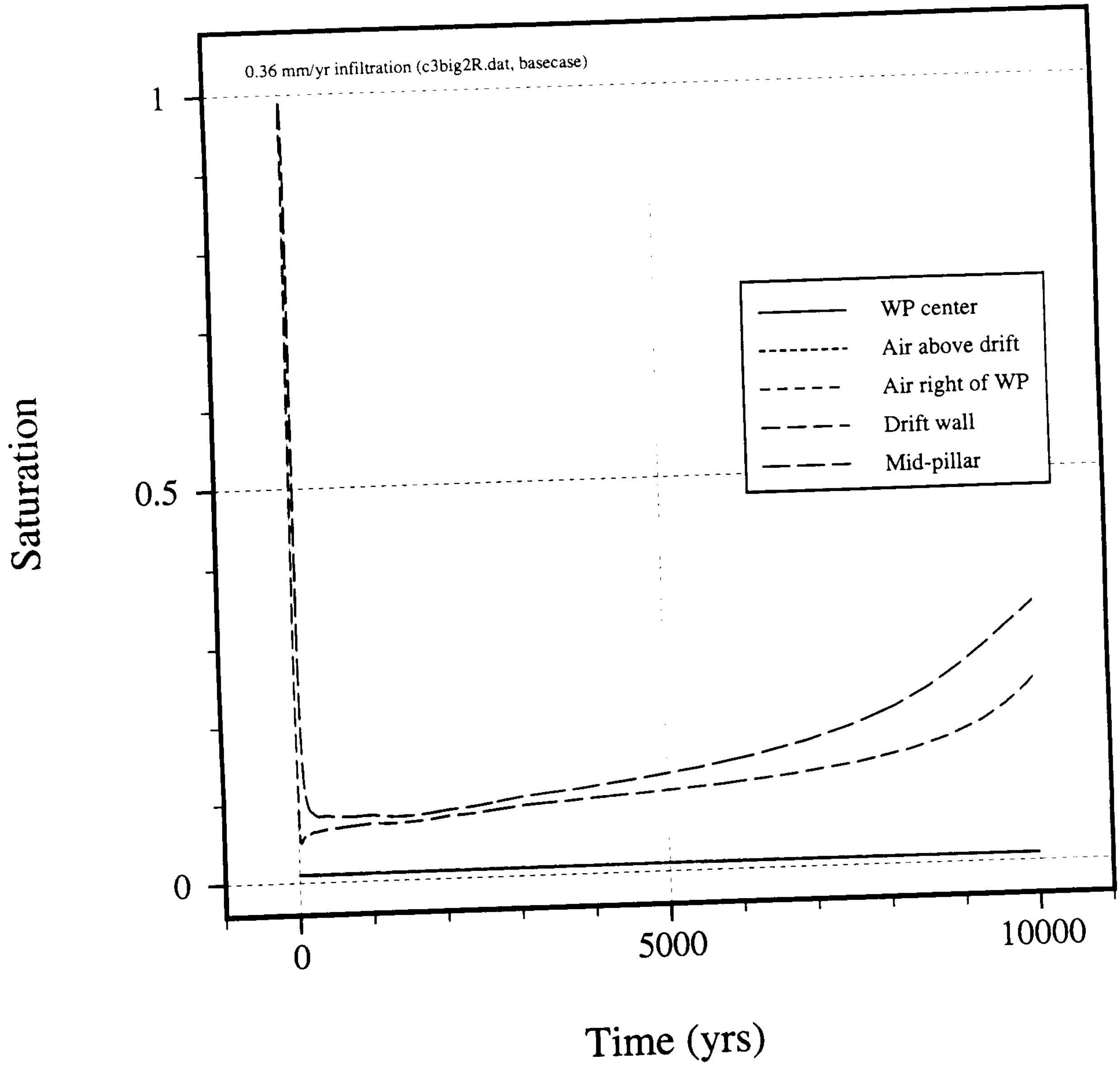

Figure 2.3-33. Time history of saturation for 0.36 mm/yr infiltration and further revised basecase model.

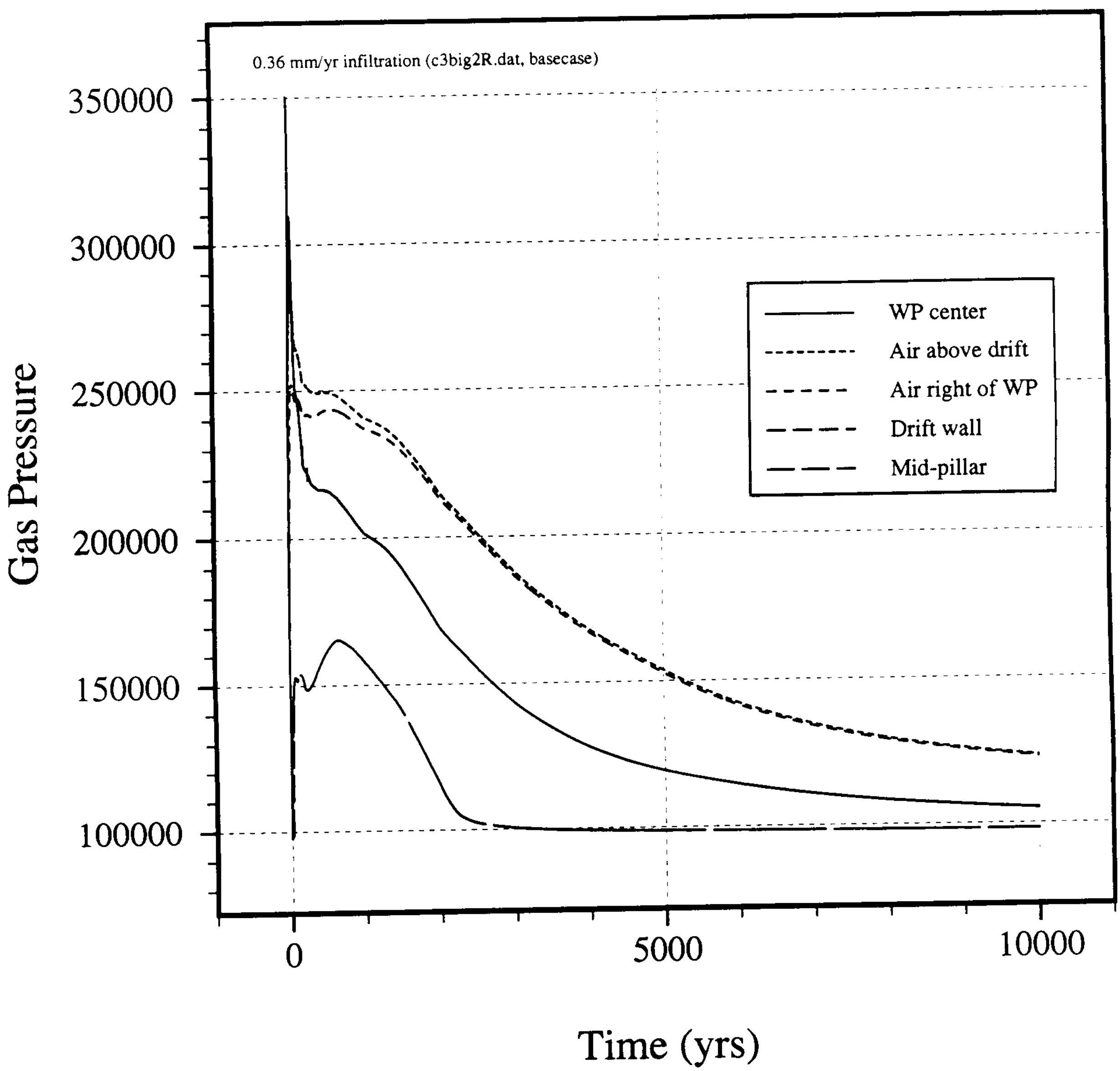

Figure 2.3-34. Time history of gas pressure for 0.36 mm/yr infiltration and further revised basecase model.

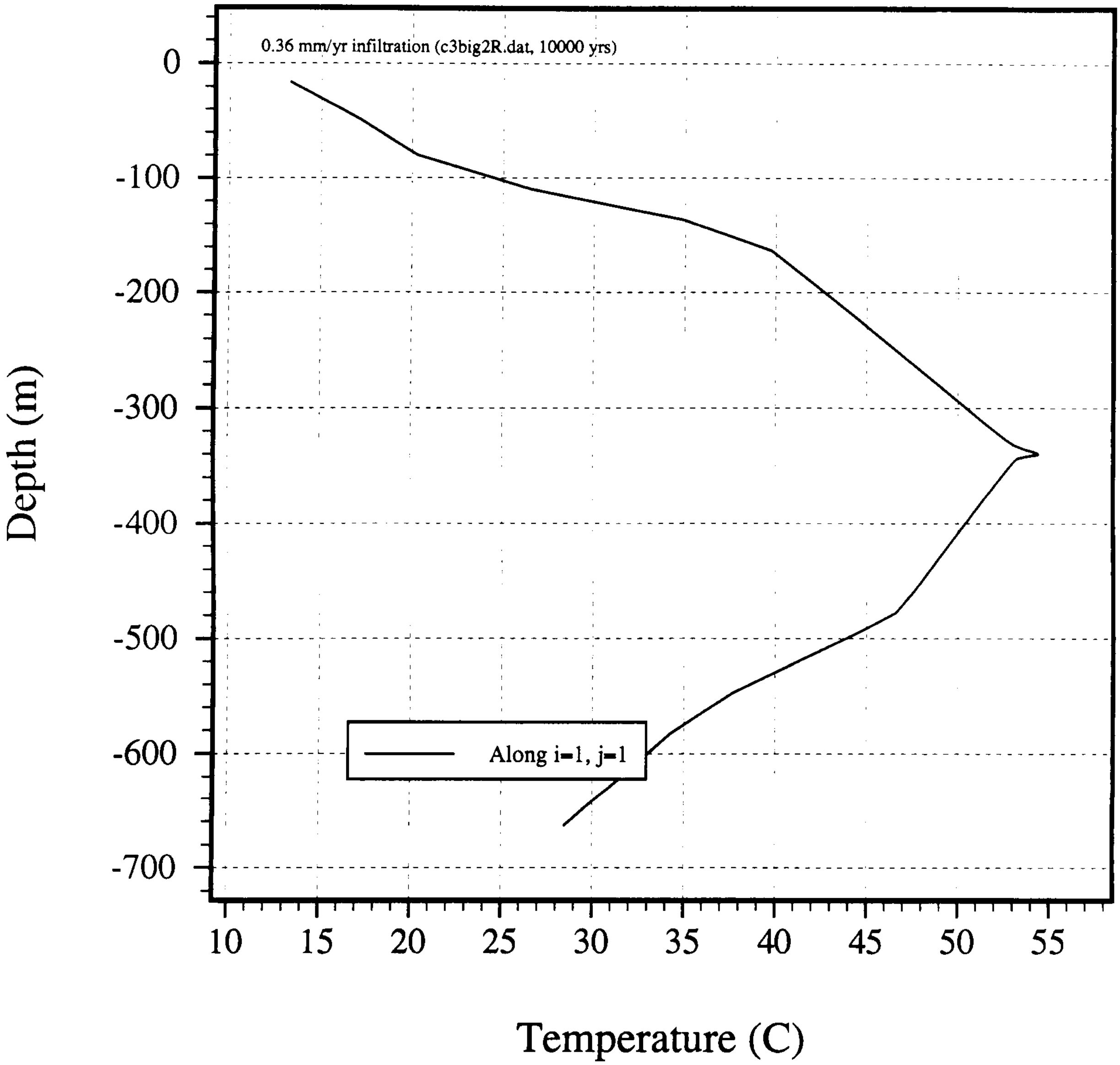

Figure 2.3-35. Distribution of temperature along a vertical line through the center of the waste package (i = 1,j = 1) at 10,000 yrs for 0.36 mm/yr infiltration and the further revised basecase model.

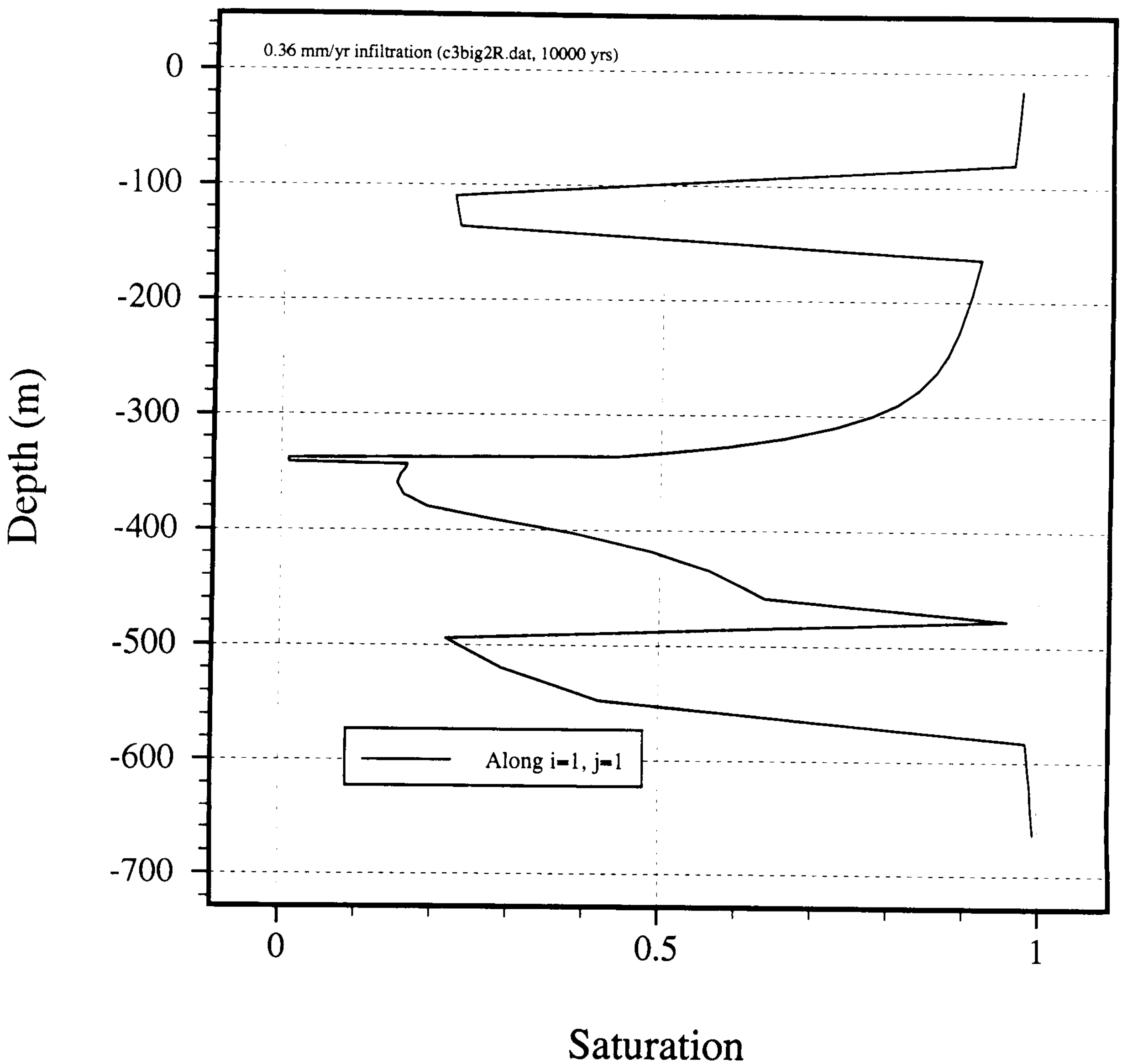

Figure 2.3-36. Distribution of saturation along a vertical line through the center of the waste package (i=1,j=1) at 10,000 yrs for 0.36 mm/yr infiltration and the further revised basecase model.

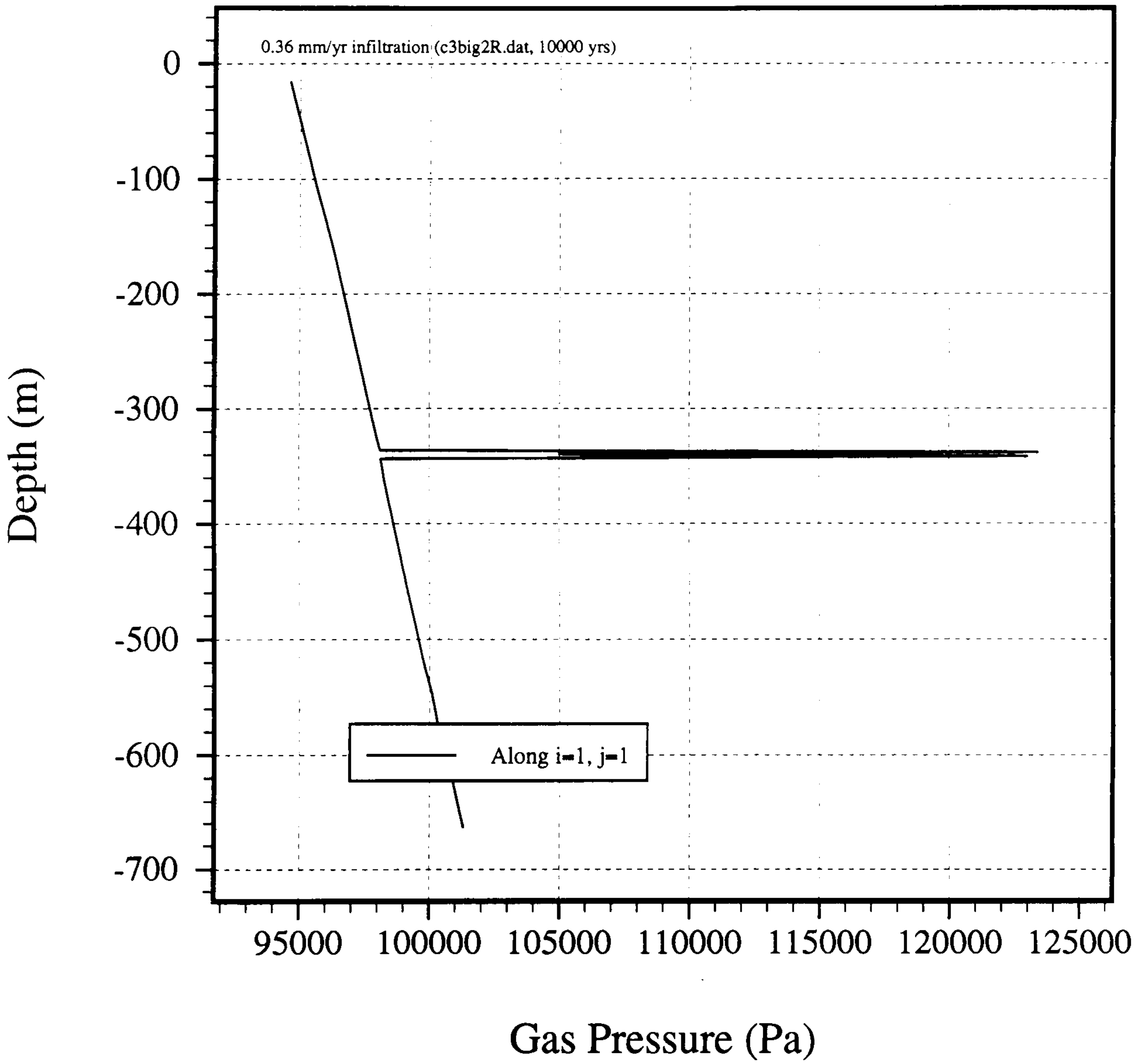

Figure 2.3-37. Distribution of gas pressure along a vertical line through the center of the waste package (i = 1,j = 1) at 10,000 yrs for 0.36 mm/yr infiltration and the further revised basecase model.

3. REFERENCES

Andrews, R.W., T.F. Dale, and J.A. McNeish. 1994. Total System Performance Assessment-1993: An Evaluation of the Potential Yucca Mountain Repository. B00000000-01717-2200-00099-Rev. 01, Civilian Radioactive Waste Management System, Management and Operating Contractor, Las Vegas, Nevada.

Green, R.T. 1996. The effect of media properties on prediction of moisture redistribution at a high-level nuclear waste repository. *Proceedings of the Seventh Annual International Conference on High-Level Radioactive Waste Management.* La Grange, Park, IL: American Nuclear Society.

Green, R., J. Prikryl, and M. Hill. 1997. Assessment of Heat Flow Through Bulk Geological Materials. CNWRA Milestone No. 20-5708-661-720. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses.

Manteufel, R.D. 1996. Effects on ventilation and backfill on a mined waste disposal facility. *Nuclear Engineering and Design.* Submitted for publication (ask Randy for a copy)

Sothoff, S.A. 1996. Sensitivity of Long-Term Bare-Soil Infiltration Simulations to Hydraulic Properties in an Arid Environment. *Water Resource Research.* Submitted for publication (ask Stuart for a copy)

Stothoff, R.D., H. Castellaw, and A. Bagtzoglou. 1996. Simulating the Spatial Distribution of Infiltration at Yucca Mountain. *Water Resource Research.* Submitted for publication (ask Stuart for a copy)

TRW Environmental Safety Systems Inc. 1995. Total System Performance Assessment - 1995: An Evaluation of the Potential Yucca Mountain Repository. B00000000-01717-2200-00136-Rev. 01, Civilian Radioactive Waste Management System, Management and Operating Contractor, Las Vegas, Nevada.

Appendix A

Fortran source code for changing format of temperature and relative humidity data

Filename: /export/home/rchen/TEFKTI/BK_cond/temphumd.f

```
      PROGRAM FORMAT
C ************************************************************************
C This program converts the format of temperature and relative humidity
C data files from MULTIFLO analyses (jobname_tmp.xyp & jobname_rh.xyp)
C to the format required by EBSPAC analyses (tefkti.inp). Twp is waste
C package temperature, Tw is drift wall temperature, and RH represents
C relative humidity.
C
C Developed by: Rui Chen
C January 8, 1997
C ************************************************************************
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      CHARACTER LINE*180,FNAME*80
      REAL*8 Time(2000,12),Twp(2000,12),Tw(2000,12),RH(2000,12)
      REAL*8 VAR1(2000,12),VAR2(2000,12)
      INTEGER nset,nrow1_t,nrow1_r,nrow2_t,nrow2_r,nrow_t,nrow_r
      INTEGER flag_t,flag_r
      INTEGER row(12)
C
      PRINT*, 'ENTER Number of Data Set (nset):'
      READ(*,*) nset
C
C Open output file
C
      PRINT*,'ENTER OUTPUT FILENAME'
      READ(*,'(A80)') FNAME
      OPEN(UNIT=3,FILE=FNAME, STATUS='UNKNOWN',FORM='FORMATTED')
C
C Open files and read in data for pre-closre
C
C       PRINT*,'ENTER TEMPERATURE DATA FILENAME FOR PRECLOSURE ANALYSES'
C       READ(*,'(A80)') FNAME
      FNAME='bk1_precls_tmp.xyp'
      OPEN(UNIT=1,FILE=FNAME, STATUS='UNKNOWN',FORM='FORMATTED')
      nrow1_t=0
      DO 11 j=1,1000000
       READ(1,'(A)',END=22) LINE
       IF (LINE(1:1) .NE. '!') then
         nrow1_t=nrow1_t+1
         READ(LINE,*) (VAR1(nrow1_t,k),k=1,5)
         DO 33 i=1,nset
          Time(nrow1_t,i)=VAR1(nrow1_t,1)
          Twp(nrow1_t,i)=VAR1(nrow1_t,2)
          Tw(nrow1_t,i)=VAR1(nrow1_t,4)
   33     CONTINUE
       ENDIF
   11 CONTINUE
   22 CONTINUE
C        PRINT*,'ENTER RH DATA FILENAME FOR PRECLOSURE ANALYSES'
C        READ(*,'(A80)') FNAME
       FNAME='bk1_precls_rh.xyp'
       OPEN(UNIT=1,FILE=FNAME,STATUS='UNKNOWN',FORM='FORMATTED')
       nrow1_r=0
```

```
      DO 44 J=1,1000000
        READ(1,'(A)',END=55) LINE
        IF (LINE(1:1) .NE. '!') THEN
          nrow1_r=nrow1_r+1
          READ(LINE,*) (VAR2(nrow1_r,k),k=1,5)
          do 66 i=1,nset
            RH(nrow1_r,i)=VAR2(nrow1_r,2)
   66     CONTINUE
        ENDIF
   44 CONTINUE
   55 CONTINUE
      print*,'nrow1_t=',nrow1_t
      print*,'nrow1_r=',nrow1_r
      nrow1=nrow1_t
C
C Open files and read in data for post-closure
C
      flag_t=0
      flag_r=0
      do 5 i=1,nset
       row(i)=0
    5 continue
      DO 99 I=1,nset
C        PRINT*,'ENTER POSTCLOSURE TEMP DATA FILENAME FOR DATA SET #',i
C        READ(*,'(A80)') FNAME
        if(i .EQ. 1) then
         FNAME='bk1_poscls_tmp.xyp'
        elseif (i .EQ. 2) then
         FNAME='bk2_poscls_tmp.xyp'
        elseif(i .EQ. 3) then
         FNAME='bk3_poscls_tmp.xyp'
        elseif(i .EQ. 4) then
         FNAME='bk4_poscls_tmp.xyp'
        endif
        OPEN(UNIT=1,FILE=FNAME, STATUS='UNKNOWN',FORM='FORMATTED')
        nrow2_t=0
        DO 88 J=1,1000000
         READ(1,'(A)',END=77) LINE
         IF (LINE(1:1) .NE. '!') then
           nrow2_t=nrow2_t+1
           nrow_t=nrow2_t+nrow1
           READ(LINE,*) (VAR1(nrow_t,k),k=1,5)
           Time(nrow_t,i)=VAR1(nrow_t,1)+100
           Twp(nrow_t,i)=VAR1(nrow_t,2)
           Tw(nrow_t,i)=VAR1(nrow_t,4)
         ENDIF
   88   CONTINUE
   77   CONTINUE
        if (flag_t .LT. nrow_t) then
          flag_t=nrow_t
        endif
        row(i)=nrow_t
        print*, 'nrow_t=',nrow_t,' after nset# ',i
        print*, 'flag_t=',flag_t,' after nset# ',i
C        PRINT*,'ENTER POSTCLOSURE RH DATA FILENAME FOR DATA SET #',i
C        READ(*,'(A80)') FNAME
        if(i .EQ. 1) then
```

```
          FNAME='bk1_poscls_rh.xyp'
        elseif (i .EQ. 2) then
          FNAME='bk2_poscls_rh.xyp'
        elseif(i .EQ. 3) then
          FNAME='bk3_poscls_rh.xyp'
        elseif(i .EQ. 4) then
          FNAME='bk4_poscls_rh.xyp'
        endif
        OPEN(UNIT=1,FILE=FNAME,STATUS='UNKNOWN',FORM='FORMATTED')
        nrow2_r=0
        DO 1 J=1,1000000
         READ(1,'(A)',END=2) LINE
         IF (LINE(1:1) .NE. '!') THEN
           nrow2_r=nrow2_r+1
           nrow_r=nrow2_r+nrow1_r
           READ(LINE,*) (VAR2(nrow_r,k),k=1,5)
           RH(nrow_r,i)=VAR2(nrow_r,2)
         ENDIF
    1   CONTINUE
    2   CONTINUE
        if (flag_r .LT. nrow_r) then
           flag_r=nrow_r
        endif
        print*, 'nrow_r=',nrow_r,' after nset# ',i
        print*, 'flag_r=',flag_r,' after nset# ',i
   99   CONTINUE
C
C Write Out Data for EBSPAC
C
   98  Do 9 i=1,nset
       write(3,4000)
       if(i .NE. nset) then
        write(3,4400) i,i,i
       else
        write(3,4500) i,i,i
       endif
    9 continue
C
      Do 7 i=1,nset
       if(i .NE. nset) then
        write(3,5000) row(i), 99999.0, 99999.0, 99999.0
       else
        write(3,6000) row(i), 99999.0, 99999.0, 99999.0
       endif
    7 continue
C
      DO 3 I=1,flag_t
       do 4 j=1,nset
        if (j .ne. nset) then
         WRITE(3,2000) Time(i,j),Twp(i,j),Tw(i,j),RH(i,j)
        else
         WRITE(3,3000) Time(i,j),Twp(i,j),Tw(i,j),RH(i,j)
        endif
    4  CONTINUE
    3 CONTINUE
C
      print*, 'flag_t=',flag_t
```

```
      print*, 'flag_r=',flag_r
C
 2000 FORMAT(4E16.6, $)
 3000 FORMAT(4E16.6)
 4000 FORMAT(12x, 'Time', $)
 4400 FORMAT(5x,'Twp nset#',I2,6x,'Tw nset#',I2,6x,'RH nset#',I2, $)
 4500 FORMAT(5x,'Twp nset#',I2,6x,'Tw nset#',I2,6x,'RH nset#',I2)
 5000 FORMAT(I16,3E16.6,$)
 6000 FORMAT(I16,3E16.6)
      END
```

Appendix B

EBSPAC input file for analyzing the effect of backfill thermal conductivity

Filename: /export/home/rchen/TEFKTI/BK_cond/bk_cond_fail.inp

```
\example input file for ebspac_fail
!
\simulation time
10000.                  ! tend: simulation time length [yr]
\               ! when iflag=1 (defined later)
\
5.682, 1.802            ! wplen,wpdia: wp length and diameter [m]
0.1, 0.02               ! cthick1,cthick2: wp layers 1&2 thicknesses [m]
!
\choose source of temperature data
2               ! iflag 1: emp. equation, 2: tab.data
1               ! nset (temp.-rel hum. relationship to use
49.9999999              ! timintv (used when iflag=2)
!
\other temperature parameters
0.              ! age of fuel (not used in this version)
!
\Dry oxidation of wp outer overpack
5.              ! grainr: metal grain radius [micrometer]
25              ! nseries (terms in the infinite series)
0.7e-3                  ! gbthick [micrometer]
1.e-2                   ! constant: used in the dry oxidation equn.
!
\evaporation-condensation
0.65                    ! humdc: critical relative humidity
2.e-3                   ! filmthk: thickness of water film [m]
97.             ! ctemp: boiling point of water [C]
!
\Corrosion Parameters(Ep: pitting potential [mV]; Erp: repassivation potential [mV])
-584.8                  ! xipto: outer overpack Ep intercept
3.92                    ! pttemo: temp. coef. of outer overpack Ep intercept
-24.5                   ! slpto: outer overpack Ep slope
-1.1                    ! slpttemo: temp. coef. of outer overpack Ep slope
-620.3                  ! xirpo: outer overpack Erp intercept
0.47                    ! rptemo: temp. coef. of outer overpack Erp intercept
-95.2                   ! slrpo: outer overpack Erp slope
0.88                    ! slrptemo: temp. coef. of outer overpack Erp slope
200.                    ! xipti: inner overpack Ep intercept
0.              ! pttemi: temp. coef. of inner overpack Ep intercept
-240.                   ! slpti: inner overpack Ep slope
0.              ! slpttemi: temp. coef. of inner overpack Ep slope
422.8                   ! xirpi: inner overpack Erp intercept
-4.1                    ! rptemi: temp. coef. of inner overpack Erp intercept
-64.                    ! slrpi: inner overpack Erp slope
-0.80                   ! slrptemi: temp. coef. of inner overpack Erp slope
0.75, 0.5       ! betaox1, betahy1: beta kinetics parameters
\                 for oxygen and water for WP outer overpack
0.75, 0.5       ! betaox2, betahy2: beta kinetics parameters for
\                 oxygen and water for WP inner overpack
3.80e12, 1.6e-1                 ! rkox1 [c*m/y/mol], rkhy1 [c/m2/yr]
37300., 25000.                  ! gox1 [J/mol], ghy1 [J/mol]
3.0e10, 3.2             ! rkox2 [c*m/y/m], rkhy2 [c/m2/yr]
40000., 25000.                  ! gox2 [J/mol], ghy2 [J/mol]
3.15e5, 0.0, 0.0        ! aa(1,1) [C/m2/yr], aa(1,2), aa(1,3)
6.30e4, 0.0, 0.0        ! aa(2,1) [C/m2/yr], aa(2,2), aa(2,3)
```

```
-0.46                   ! eexpt: in Vshe
8.66e-3                 ! rcoef:
0.45                    ! rexpont:
2.05e-4                 ! crate2: m/yr corrosion rate
0.0                ! xcouple, a fractional coupling strength
0.0                ! xread
3.e-1                   ! clconc: chloride concentration [mol/L]
3.e-4                   ! clcrit1: crit. chloride conc. for 1st layer [mol/L]
2.e-3                   ! clcrit2: crit. chloride conc. for 2nd layer [mol/L]
100.                    ! cfactor: chloride dilution factor
9.0                     ! refph: reference pH
1.0, 1.0           ! taus:deposit tortuosity,spor:deposit porosity
!
\Runge-kutta control parameters
1.e-3, 1.e0             ! dtini, dtmax
1.e-2, 1.e-30           ! errrel (same as eps), errabs (same as tiny)
!
\end
////2000                ! nhista (used when iflag=1)
```