LABORATORY NOTEBOOK

CNWRA/SwRI

NOTEBOOK NO. ______________

ISSUED TO ______________

ON ______________ **19** ____

DEPARTMENT ______________

RETURNED ______________ **19** ____

CNWRA
CONTROLLED
COPY 305

—SCIENTIFIC NOTEBOOK CO.—
2831 LAWRENCE AVE.
P.O. BOX 238
STEVENSVILLE, MI 49127
616-429-8285

INSTRUCTIONS

1. **The primary purpose of this notebook is to protect your and the Company's Patent-Rights by keeping records of all original work in a form acceptable as evidence if any legal conflict arises.**

2. • When starting a page, enter the title, project number, and book number.
   • Use <u>ink</u> for permanence -- avoid pencil.
   • Record your work as you progress, including any spur-of-the-moment ideas which may be developed later.
   • Avoid making notes on loose paper to be recopied.
   • Record your work in such a manner that a co-worker can continue from where you stop. You might be ill and to protect your priority it could be urgent that the work continue while you are absent.

3. • Give a complete account of your experiments and the results, both positive and negative, including your observations.
   • Record all diagrams, layouts, plans, procedures, new ideas, or anything pertinent to your work including the details of any discussions with suppliers, or other people outside the Company.
   • Do not try to erase any incorrect entries; draw lines deleting them, note the corrections, sign and date the changes. This extra care is worthwhile because of the necessity of original data to prove priority of new discoveries.

4. • After entering your data, sign and date the entries.
   • Explain your work to at least two witnesses who are not co-inventors, and have them sign and date the pages in the place provided.
   • Record the names of operators and witnesses present during any demonstration and have at least two witnesses sign the page. If no witnesses are present during an experiment of importance, repeat it in the presence of two witnesses.

5. Since computer programs can be patented these instructions apply to the development of computer software. In this case a description of the structure and operation of the program should be recorded in the notebook, together with a basic flow diagram which illustrates the essential features of the program. In the course of developing the code, the number of lines of code written each day should be recorded in the notebook, together with a statement of the portion of the flow diagram to which the section of code is directed.

6. This notebook and its contents are the exclusive property of the Company. It is confidential and the contents are not to be disclosed to anyone unless authorized by the Company. You must return it when completed, upon request, or upon termination of employment. It should be kept in a protected place. **If loss occurs, notify your supervisor immediately, and make a written report describing the circumstances of the loss.**

Form 590

Project No. 20-1402-561

TITLE ENFE Book No. 305 1

From Page No. ____

This Notebook is a continuation of the work recorded in Notebook 284

ECP 8/24/00 ECP 8/24/00 ECP 8/24/00

This work ~~has~~ ~~had~~ has evolved from thermal hydrological modeling of the drift scale – (top of mountain to water table) into coupled geochemical thermal hydrological modeling of mountain drift scale to drift scale heater test

Along the way, benchmark comparisons are being done by Lauren Browning and Bill Murphy using the equilibrium code EQ3/6

I'm using multiflo in the coupled METRA GEM and GEM standalone mode.

I refer to multiflo1.2β as either multiflo or mf and I refer to the version of multiflo which implements the operator splitting time integration ~~alg~~ algorithm as

ECP 8/24/00

Multiflo X

The executables are located at

~spainter/bin/multiflo and

~spainter/dhughson/multifloX

Putting my initials and today's DATE (Some 18 months after the fact) makes this better. ECP 8/24/2000

To Page No. ____

Witnessed & Understood by me,	Date	Invented by Debra Hughson	Date
		Recorded by DH	Feb 5 1999

Check on the effect of time integration in GEM, maximum difference between multiflo and EQ3/6 for the time dependent leaching box is about 8% for CO_3^{2-}. Refer to page 94 in notebook 284.

With multifloX at time 349.9yr, T= 87.42C P=7.4957e7 Pa

Component	s = 1 cm⁻¹ multifloX ①	s = 10 cm⁻¹ ②	s = 100 cm⁻¹ ③
Cl^-	1.8968e-3	1.8972e-3	1.8968e-3
Ca^{2+}	1.8785e-3	1.0141e-5	1.8814e-3
H^+	2.9208e-7	2.0951e-9	2.9251e-7
$CO_2(aq)$	1.0137e-3	9.1547e-6	1.0152e-3
$SiO_2(aq)$	5.6337e-3	5.6337e-3	5.6337e-3
OH^-	1.3446e-6	1.7866e-4	1.3427e-6
HCO_3^-	1.8578e-3	2.2304e-3	1.8578e-3
CO_3^{2-}	7.0798e-7	1.0740e-4	7.0708e-7
$CaCO_3(aq)$	6.9689e-6	6.9688e-6	6.9689e-6

EP 8/24/2000 Now the quality is improved. EP 8/24/00

① maximum timestep in masin.inp set to 100 years
Time step ~~at~~ ~~GEM~~ at 349 years is 0.1656 years in metra and 6.82e-2 to 9.743e-2 yr in GEM

→ Change max dt in masin.inp to 1.0 years
Time step at 349 years is 0.1656 years in metra and 3.219e-2 to 5.292e-2 years in Gem
concentrations at t= 349.9 yr are identical.

→ Change maxdt to 0.1 Gem time step 6.614e-3 years
exactly the same concentrations again

② change S from 1/cm to 10/cm } specific mineral surface area cm^2/cm^3
③ change S from 10/cm to 100/cm

component	④ s = 1000 cm⁻¹	⑤ s = 10⁴ cm⁻¹
Cl^-	1.8968e-3	1.8968e-3
Ca^{2+}	2.9331e-3	3.2866e-3
H^+	4.9108e-7	4.9375e-7
$CO_2(aq)$	1.8850e-3	1.7118e-3
$SiO_2(aq)$	5.6337e-3	5.6337e-3
OH^-	8.1851e-7	8.1864e-7
HCO_3^-	2.1024e-3	1.9093e-3
CO_3^{2-}	4.9989e-7	4.5678e-7
$CaCO_3(aq)$	~~6.98~~ 6.9688e-6 (EP 8/24/00)	6.9689e-6

MultifloX definetly Buggy
Does the same thing happen with multiflo 1.2β ?

Comp	s = 1 cm⁻¹	s = 10 cm⁻¹	s = 100 cm⁻¹	s = 10³ cm⁻¹
Cl^-	1.8968e-3	SAME	SAME	1.8968e-3
Ca^{2+}	1.8785e-3	SAME	SAME	1.8786e-3
H^+	2.9208e-7	SAME	"	2.9210e-7
$CO_2(aq)$	1.0137e-3	SAME	"	1.0138e-3
$SiO_2(aq)$	5.6337e-3	SAME	"	5.6337e-3
OH^-	1.3446e-6	SAME	"	1.3445e-6
HCO_3^-	1.8578e-3	SAME	"	same
CO_3^{2-}	7.0798e-7	SAME	"	7.0796e-7
$CaCO_3(aq)$	6.9689e-6	SAME	"	6.9688e-6

↳ metra dt = .1657 yr Gem dt = 7.787e-2 yr

Comp	
Cl^-	SAME
Ca^{2+}	SAME
H^+	SAME
$CO_2(aq)$	SAME
$SiO_2(aq)$	SAME
OH^-	SAME
HCO_3^-	SAME
CO_3^{2-}	SAME
$CaCO_3(aq)$	SAME

This with metra dt = 0.1656 years
gem dt = 6.6140e-4 years

Difference between multiflo and EQ3/6 does not appear to be a time intergation problem

Still need to look at activity coefficients and thermodynamic data base

From Page No.

With — Results

$S = 10\ cm^{-1}$ $DT(NSTPMAX+1) = 100$ — col (2) pg 2

$S = 10 cm^{-1}$ $DT(NSTPMAX+1) = 10$ — col (1) pg 2 ± 1 digit

$S = 10 cm^{-1}$ $DT(NSTPMAX+1) = 1$ — col (1) pg 2

Reaction Kinetics $n = \frac{W a^*}{\gamma} + \left(n_0 - \frac{W a^*}{\gamma}\right) \exp\left(\frac{-k s \gamma t}{W a^*}\right)$

S = mineral surface area cm^{-1}
K = rate const. $moles/cm^2/s$
$\gamma = 1$
W = mass of water Kg
$a^* = 10^{-2.72}$ moles/kg

$W = 110$ Kg $a^* = 10^{-2.72}$ moles/kg
$K = 10^{-11.34}$ $moles/cm^2/s$
$S = (10/cm)\ 10^6\ cm^3$

$$\frac{(110\ Kg)\ 10^{-2.72}\ moles/kg}{(10^{-11.34}\ moles/cm^2/s)(10/cm\ 10^6\ cm^3)} = 4600\ s$$

$= 1.45 \times 10^{-4}$ years

with $S = 10\ cm^{-1}$

TSTEP(1) = 1.5e-3 y DT(1) = 1.e-8 y
DT(2) = 10 y

Same results as col (1) pg 2

To Page No.

Witnessed & Understood by me,	Date	Invented by / Recorded by	Date
		DH	Feb 6 1999

From Page No.

Change tolc from 0.5 to 1e-10

Relative error % on Ca^{+2} H^+ $CO_2(aq)$ changed from about 0.039 ~~%~~ ECP 8/24/00 to 2.57e-2

but results are same as pg 2 col (1)

Change tolc from 1e-10 to 1e-15

Relative Error % Ca^{+2} H^+ $CO_2(aq)$ ~ 3e-10 but results are still the same as pg 2 col (1)

Begin a series of benchmark runs between MULTIFLO and EQ3/6 to track down the source of the 8% descrepancy from page 94 in notebook 284.

First Run Called Bill-25

Isothermal at 25° C

ECP 8/24/00

Component	$M(t=10^{-16} yr)$	$M(t=349.9y)$	~~EQ3~~
Cl^-	2.2493e-3	SAME	
Ca^{+2}	2.5e-3	SAME	
H^+	6.7097e-8	SAME	
$CO_2(aq)$	3.4064e-4	SAME	
$SiO_2(aq)$	1.0e-3	1.735e-3	
OH^-	1.8075e-7	SAME	
HCO_3^-	2.7451e-3	SAME	
CO_3^{2-}	2.7492e-6	SAME	
$CaCO_3(aq)$	7.0061e-6	SAME	

repeated following page

I am improving the quality of this work. ECP 8/24/00

To Page No.

Witnessed & Understood by me,	Date	Invented by / Recorded by	Date
		DH	Feb 10 1999

Project No. 20-1402-561
Book No. 305 TITLE ENFE

From Page No.

Comp	MX (t=10^-16 yr)	EQ3	% difference
Cl^-	2.2493e-3	2.2493e-3	0
Ca^{2+}	2.5e-3	2.5e-3	0
H^+	6.7097e-8	6.7097e-8	0
$CO_2(aq)$	3.4064e-4	3.4064e-4	0
$SiO_2(aq)$	1.0e-3	1.0e-3	0
OH^-	1.8075e-7	1.7929e-7	.814
HCO_3^-	2.7451e-3	2.7289e-3	.594
CO_3^{2-}	2.7492e-6	2.6959e-6	1.977
$CaCO_3(aq)$	7.0061e-6	7.0807e-6	-1.054

this is the same pattern of differences as on page 94 of NB # 284

Since Ca^{2+} and H^+ are the same, let's look at

$CaCO_3(calcite) + H^+ \rightleftharpoons HCO_3^- + Ca^{2+}$

For this reaction log K = 1.8487 @ 25 C in both EQ3 and mastertemp.V8.R5 data bases

MultifloX

	γ	a
HCO_3^-	.91315	$10^{-2.6009}$
Ca^{2+}	.70628	$10^{-2.753083}$
H^+	.92267	$10^{-7.20825}$

EQ3

log a	log γ	γ
-2.6021	-.0381	.9160
-2.7556	-.1535	.7023
-7.2095	-.0362	.9200

$$\frac{a_{HCO_3^-}\, a_{Ca^{2+}}}{a_{H^+}} = \frac{10^{-2.6009}\ 10^{-2.753083}}{10^{-7.20825}} = 10^{1.854267}$$

EQ3: = 1.8518

Neither multiflo nor EQ3 honor the K = 1.8487
But EQ3 is closer
0.17% vs. 0.3% in log K
0.72% vs. 1.37% in K

To Page No.

Witnessed & Understood by me, | Date | Invented by DH | Date Feb 10 1999
Recorded by

Project No. 20-1402-561
TITLE ENFE
Book No. 305

From Page No.

Concentrations for Ca^{2+} and H^+ are identical in MX and EQ3 yet a and γ are different.

BDOT $\dot{B}$ = bdot parameter
I = ionic strength
å = hard core diameter
A_γ = Debye-Hückel A
B_γ = Debye-Hückel B
z = charge

$$\log \gamma = \frac{A_\gamma z^2 \sqrt{I}}{1 + \mathring{a} B_\gamma \sqrt{I}} + \dot{B} I$$

Multiflo output Parameters @ 25 C: A = 0.5114, B = 0.3288, $\dot{B}$ = 4.1e-2

For Ca^{2+} from the database å = 6

~~then log γ =~~ Multiflo output I = 7.5028e-3

then log γ = 0.151636 γ = 0.705284

FOR HCO_3^- from database å = 4

then log γ = 0.04007 γ = 0.911855

For H^+ from database å = 9

then log γ = 0.035567 γ = 0.92137

EQ3 @ 25C A = 0.5114 B = 0.3288 $\dot{B}$ = 0.041

å is the same as above but I = 7.489962e-3

Comp	log γ	γ
H^+ ~~[illegible]~~	0.035542	0.92142
Ca^{2+}	0.151525	0.705465
HCO_3^- ~~[illegible]~~	0.040043	0.91192

ECP 8/24/00

My initials here must mean that I believe the line outs are correctly done. ECP 8/24/00

To Page No.

Witnessed & Understood by me, | Date | Invented by | Date Feb 10 1999
Recorded by DH

From Page No. ___

Concentration and Activity Coefficient Comparison MX and EQ3 — Summary

Parameters A = 0.5114 B = 0.3288 B̊ = 4.1e-2

Comp	å	z
Ca^{++}	6	2
H^+	9	1
HCO_3^-	4	1

Are identical in both codes

	MX			EQ3		
	I = 7.5028e-3			I = 7.489962e-3		
Comp	M	γ①	γ②	M	γ①	γ②
HCO_3^-	2.7451e-3	0.91315	0.911855	2.7289e-3	0.9160	0.91192
Ca^{2+}	2.5e-3	0.70628	0.705284	2.5e-3	0.7023	0.705465
H^+	6.7097e-8	0.92267	~~0.911~~ 0.92137	6.7097e-8	0.9200	0.92142

ECP 8/24/00 This is improved now! ECP 8/24/00

γ① reported by program in output file

γ② calculated using Bdot formula, parameters reported in output file (same for both), and Ionic strength reported in output file

I can not see one thing wrong but an accumulation of small errors and inconsistencies

To Page No. ___

Witnessed & Understood by me, | Date | Invented by | Date
Recorded by

From Page No. ___

Check BDOT Parameters MX and data0.com.R2

MX (mastertemp.V8.R5)				EQ3 (data0.com.R2)			
T	A	B	B̊	T	A	B	B̊
0	.4939	.3253	.0374	(0.01)	SAME	SAME	(.0394)
25	.5114	.3288	.041	SAME	SAME	SAME	SAME
60	.5465	.3346	.044	SAME	SAME	SAME	(.0438)
100	.5995	.3421	.046	SAME	SAME	SAME	SAME
150	.6855	.3525	.047	SAME	SAME	SAME	SAME
200	.7994	.3639	.047	SAME	SAME	SAME	SAME
250	.9593	.3766	.034	SAME	SAME	SAME	SAME
300	1.218	.3925	0	SAME	SAME	SAME	SAME

I found 3 differences in the temperature dependent bdot parameters between multiflox and EQ3 database data0.com.R2

After all this I was told I should have been using the EQ6 results

Comp	MX ($t = 10^{-16}$ yr)	EQ6	% diff	EQ6 log a
Cl^-	2.2493e-3	2.2493e-3	0	
Ca^{2+}	2.5e-3	2.4984e-3	.064	-2.7558
H^+	6.7097e-8	6.7463e-8	-.52	-7.2072
$CO_2(aq)$	3.4064e-4	3.4217e-4	-.45	
$SiO_2(aq)$	1.0e-3	—		
OH^-	1.8075e-7	1.7828e-7	1.39	
HCO_3^-	2.7451e-3	2.7259e-3	.70	-2.6026
CO_3^{2-}	2.7492e-6	2.6780e-6	2.66	
$CaCO_3(aq)$	7.0061e-6	7.0307e-6	-.35	

ECP 8/24/00

EQ6 $\frac{a_{HCO_3^-} a_{Ca^{2+}}}{a_{H^+}} = 1.8488$

To Page No. ___

Witnessed & Understood by me, | Date | Invented by | Date
Recorded by

From Page No.

With masin.inp file used previous pages & switch to master25.V8.R5 database gives runtime FP over flow error. S Painter rearrange primary & secondary species as follows:

Primary	itype	ctot		Secondary
Cl^-	-1	2.5e-10		OH^-
Ca^{2+}	7	2.5e-3		$CO_2(aq)$
H^+	3	2.5e-3	ec	CO_3^{2-}
HCO_3^-	4	-2.00	$CO_2(g)$	$CaCO_3(aq)$
$SiO_2(aq)$	7	1.e-3		

With these changes the following results are obtained

Comp	MX	EQ6	%diff
Cl^-	2.2809e-3	2.2493e-3	1.4
Ca^{2+}	2.50 e-3	2.4984e-3	.064
H^+	6.7183e-8	6.7463e-8	-.415
HCO_3^-	2.7136e-3	2.7259e-3	-.451
$SiO_2(aq)$	1.0e-3		
OH^-	1.7888e-7	1.78228e-7	.34
$CO_2(aq)$	3.3970e-4	3.4217e-4	-.72
CO_3^{2-}	2.6899e-6	2.6780e-6	.44
$CaCO_3(aq)$	7.0307e-6	7.0307e-6	0

	EQ3	File archive
Cl^-	2.2493e-3	
Ca^{2+}	2.5e-3	~dhughson/multiflo/
H^+	6.7097e-8	inputbak/
HCO_3^-	2.7289e-3	masin.inp.1
$SiO_2(aq)$	1.0e-3	
OH^-	1.7929e-7	EQ results for
$CO_2(aq)$	3.4064e-4	Bill25 taped
CO_3^{2-}	2.6959e-6	on page 12
$CaCO_3(aq)$	7.0807e-6	

To Page No.

Witnessed & Understood by me, | Date | Invented by | Recorded by DH | Date Mar 16 1999

From Page No.

Initial Simulation for Drift-Mountain Scale Reactive Transport Modeling – Yucca Mtn Site

~dhughson/multiflo/murphy/aqu

Simulation results for 1, 10, 100, 1000, & 10000 yrs

Model DCM – 20 hydrostratigraphic layers
Nevada-State Coordinates ~~170716 E~~ 170489 E
ECP 8/24/00 233748 N
INSTANT quality! ECP 8/24/2000

thermal-hydrologic properties same as Tables 3-18, 3-30, and 3-31 in TSPA-VA TBD

Thermal load equivalent to approx 85 MTU/acre

Primary Aqueous Species		Secondary Aqueous Sp.
Cl^-	charge balance	OH^-
Ca^{+2}	Initial conc.	HCO_3^-
H^+	Mineral Constraining	CO_3^{2-}
$CO_2(aq)$	Gas constraining	$CaCO_3(aq)$
$SiO_2(aq)$	Initial Conc.	

Minerals	Gas
	$CO_2(g)$
Calcite	
$SiO_2(am)$	

TO DO

1. Activity coefficient calculation check.
2. pH constraint on reaction rate
3. Representative mineralogy with appropriate speciation
4. Heterogeneous chemistry & parameters
5. Comparison with analysis for ambient conditions.
6. Thermal load

To Page No.

Witnessed & Understood by me, | Date | Invented by | Recorded by DH | Date Mar 9 1999

From Page No.

bill25aResults.txt

Date: Feb. 10, 1999

EQ3 RESULTS: Bill25a.3i

--- Distribution of Aqueous Species ---

(Species with concentrations .lt. 1.e-12 are not listed)

Species	Molality	Log molality	Log gamma	Log activity
HCO3-	2.7289E-03	-2.5640	-0.0381	-2.6021
Ca++	2.5000E-03	-2.6021	-0.1535	-2.7556
Cl-	2.2493E-03	-2.6480	-0.0392	-2.6871
SiO2(aq)	1.0000E-03	-3.0000	0.0000	-3.0000
CO2(aq)	3.4064E-04	-3.4677	0.0008	-3.4669
O2(aq)	2.5172E-04	-3.5991	0.0008	-3.5983
CaCO3(aq)	7.0807E-06	-5.1499	0.0000	-5.1499
CO3--	2.6959E-06	-5.5693	-0.1521	-5.7214
OH-	1.7929E-07	-6.7465	-0.0392	-6.7856
H+	6.7097E-08	-7.1733	-0.0362	-7.2095

EQ3

LLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLL

EQ6 RESULTS: Bill25a.6i

Time = 1.127E+10 sec
= 1.304E+05 days
= 3.570E+02 years

EQ6

Log sec = 10.052
Log days = 5.115
Log years = 2.553

Temperature = 25.000 degrees C
total pressure = 1.013 bars

DH 3/16/99

Species	Molality	Log molality	Log gamma	Log activity
O2(aq)	6.3228E-03	-2.1991	0.0008	-2.1983
HCO3-	2.7259E-03	-2.5645	-0.0381	-2.6026
Ca++	2.4984E-03	-2.6023	-0.1535	-2.7558
Cl-	2.2493E-03	-2.6480	-0.0392	-2.6871
SiO2(aq)	1.8631E-03	-2.7298	0.0000	-2.7298
CO2(aq)	3.4217E-04	-3.4658	0.0008	-3.4650
CaCO3(aq)	7.0307E-06	-5.1530	0.0000	-5.1530
CO3--	2.6780E-06	-5.5722	-0.1521	-5.7243
OH-	1.7828E-07	-6.7489	-0.0392	-6.7881
H+	6.7463E-08	-7.1709	-0.0362	-7.2072

Witnessed & Understood by me, | Date | Invented by | Date mar 16 1999
Recorded by DH

From Page No.

Bill25U Redox Benchmark

Same input as Bill25 except add

Primary	itype	cbst
UO_2^{2+}	7	1e-20
$O_2(aq)$	7	2.75182e-4

ECP 8/24/00

To Page No.

Witnessed & Understood by me, | Date | Invented by | Date
Recorded by

From Page No.

May 7 1999 Hydrology for Lauren's geochem model

volf of top block = 6.94e-5

say 20 mm/yr = 6.33e-7 kg/m²/s

So apply 20 mm/yr / volf = 9.1e-3 kg/m²/s to top

Ptn24 and Ch3zc fractures are still dry
ECP 8/24/00

Try 40 mm/yr = 1.824e-2 kg/m²/s

Part of Ptn and CH fractures still dry

Try 60 mm/yr = 2.736e-2 kg/m²/s

Still dry, try 80 mm/yr = 3.65e-2
still dry

All fractures are wet at 8.5e-2 kg/m²/s = 186.4 mm/yr

Mass balance

In fracture = 4.13e-5 kg/s Out fracture = -1.351e-8 kg/s
matrix = 1.503e-8 kg/s matrix = -4.13e-5 kg/s
4.1315e-5 kg/s 4.1314e-5 kg/s

Flux in = 186.5 mm/yr OK

This work in support of
Browning L, W M Murphy, D L Hughson - Benchmarking & Calibration of a Model for Predicting Reactive Transport at Yucca Mountain, Nevada, EOS Transactions, AGU 1999 Spring meeting Vol 80 No 17 April 27, 1999 H51E-08 p S155
Has been completed

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	June 25 1999

From Page No. This is the beginning of a new Project

An archeological site at Akrotiri, Greece, as a natural analog for radionuclide transport: Implications for validity of performance assessments.

To be presented at Fall 1999 Meeting of the Materials Research Society Nov 29 - Dec 3, 1999

Computer files will be stored in two places

PC D:\documents\akrotiri and
SUN /home/dhughson/multiflo/murphy/akrotiri

Reference: Murphy, W.M., E C Pearcy, R T Green, J D Prikryl, S Mohanty, B W Leslie, A Nedungadi, A test of long-term predictive, geochemical transport modeling at the Akrotiri archaeological site, J. of Cont. Hyd 29 (1998) 245-279

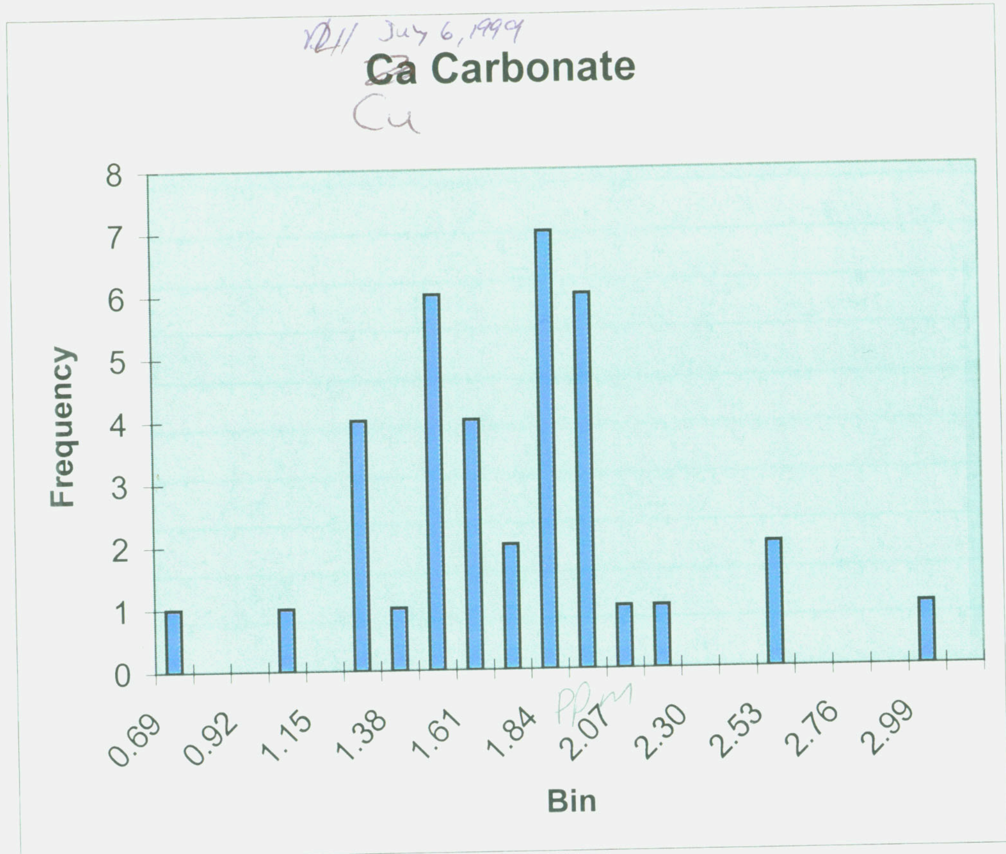
- Reconstruct field data from notebooks & old files
- data visualization & hypothesis formulation
- Construction of alternative conceptual models
- hypothesis testing using alternative conceptual models
- Insights into PA abstraction of Unsaturated zone flow & transport

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	June 25 1999

Project No. 20-1402-561
Book No. 305 TITLE ENFE

From Page No.



37 data $CuCO_3$

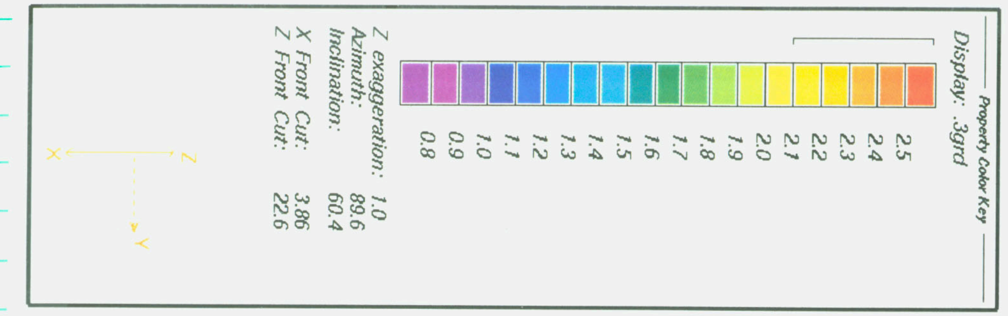
$\mu = 1.67$
$\sigma^2 = 0.183$
$\sigma = .428$
min = .69
max = 2.99

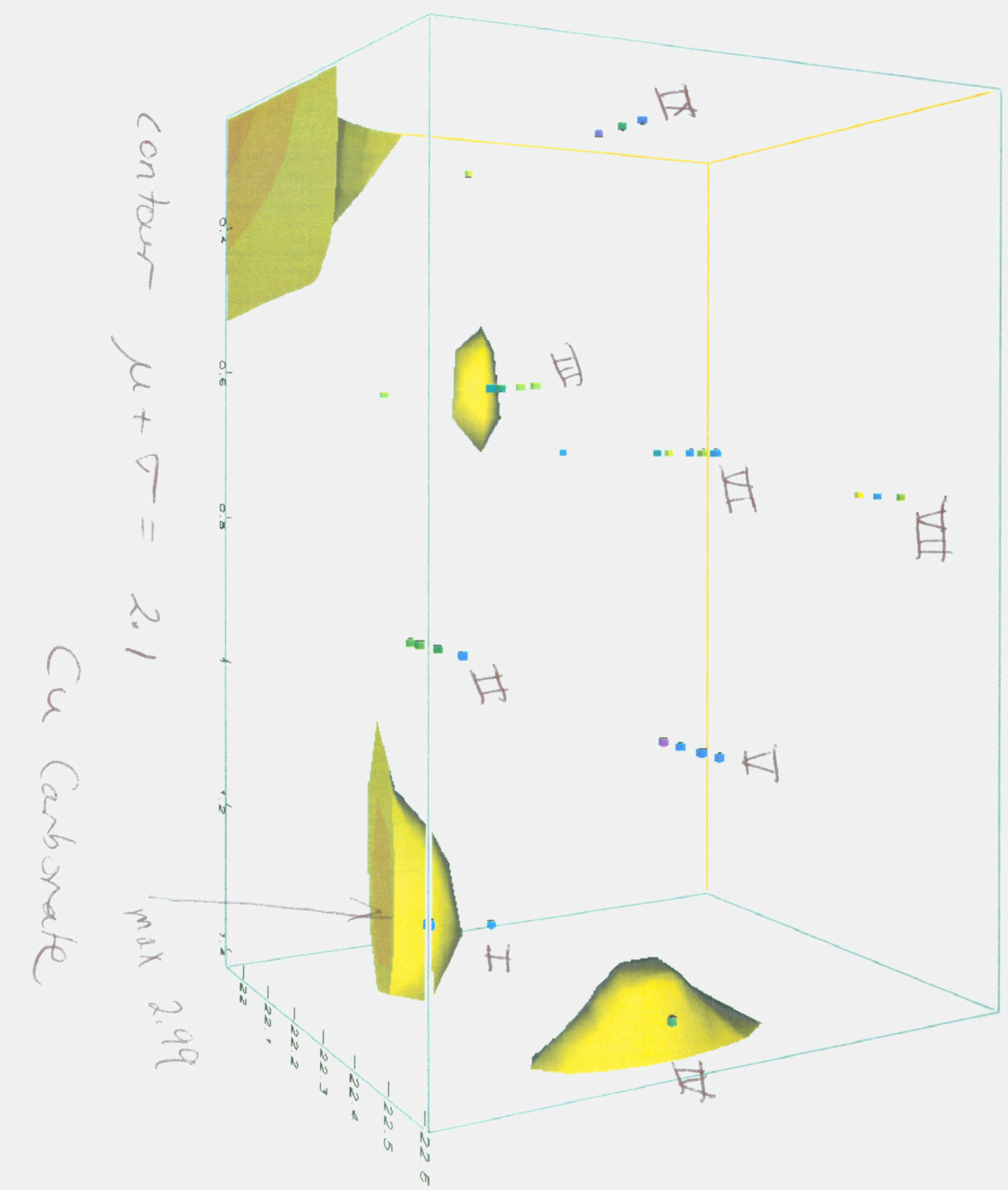
To Page No.

Witnessed & Understood by me, | Date | Invented by | Date
Recorded by RDH | July 26 1999

Project No. 20-1402-561
Book No. 305
TITLE ENFE Akrotiri

From Page No.



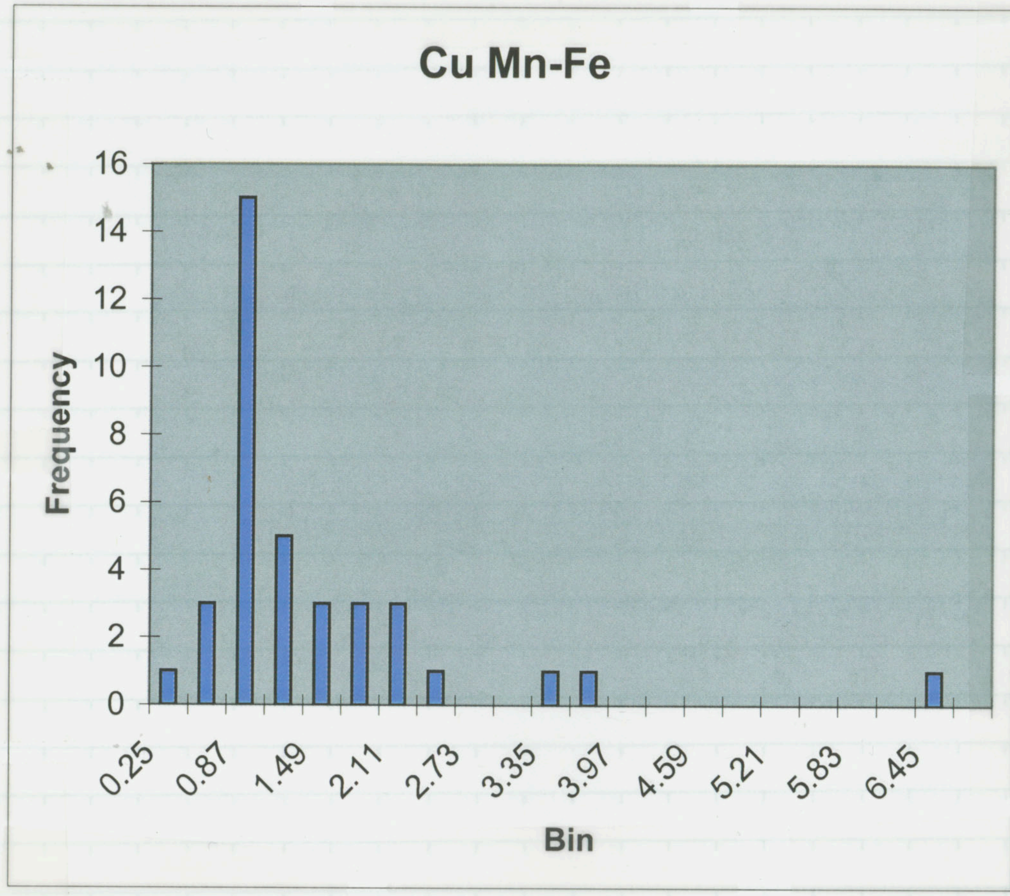


To Page No.

Witnessed & Understood by me, | Date | Invented by | Date
Recorded by RDH | July 26 1999

From Page No.

Akrotiri



37 data Cu (ppm, Fe-Mn oxide)

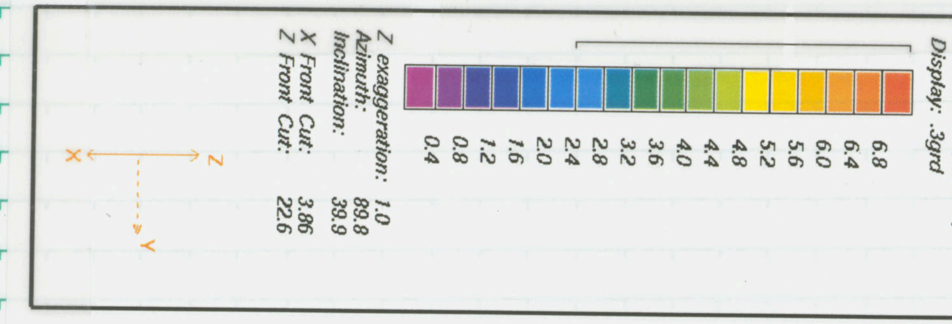
$\mu = 1.25$
$\sigma^2 = 1.27$
$\sigma = 1.128$
min = 0.25
max = 6.45

To Page No.

Witnessed & Understood by me,	Date	Invented by / Recorded by	Date
		DH	July 26 1999

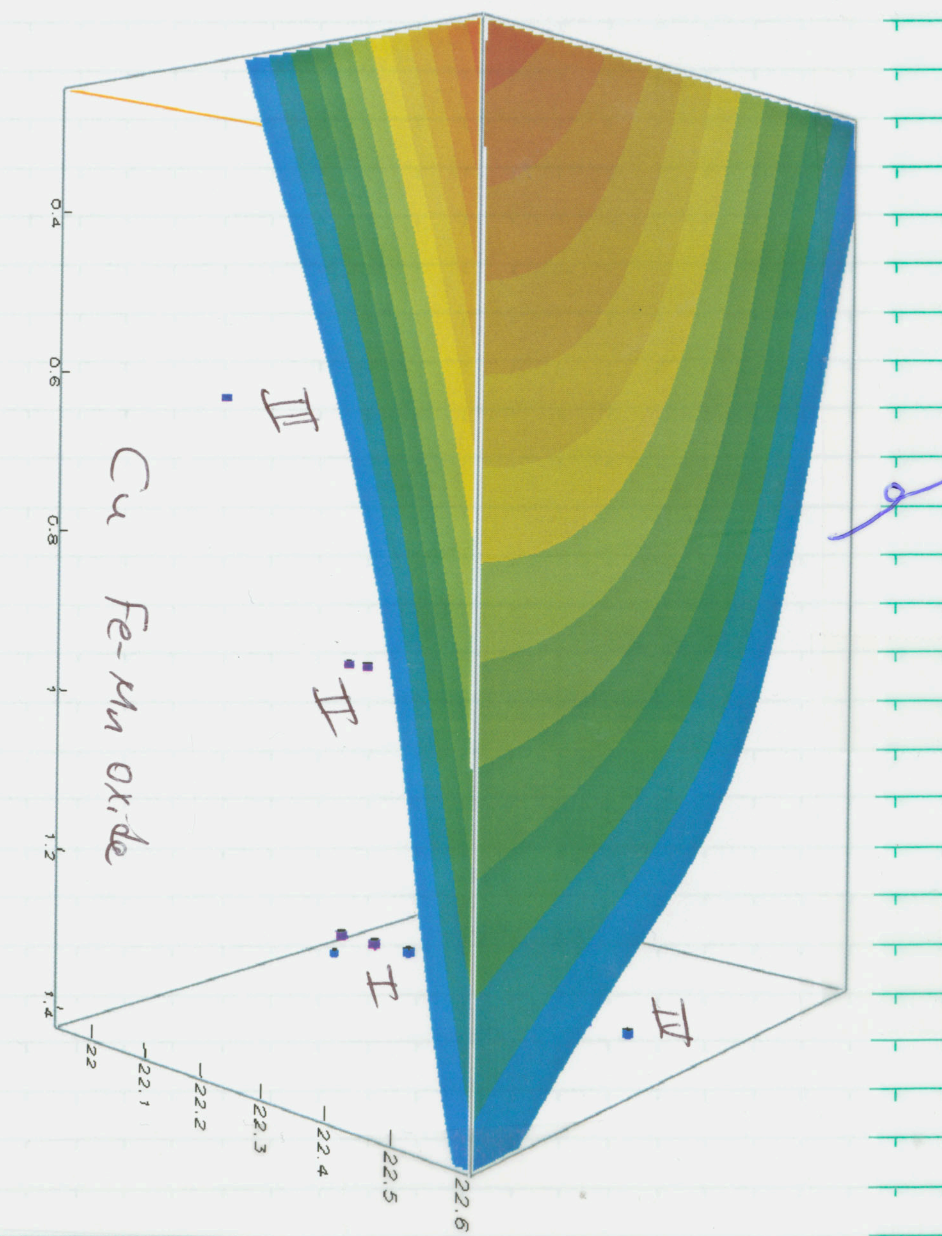
From Page No.

Akrotiri



$\mu + \sigma \approx 2.4$ contour

Cu Fe-Mn Oxide

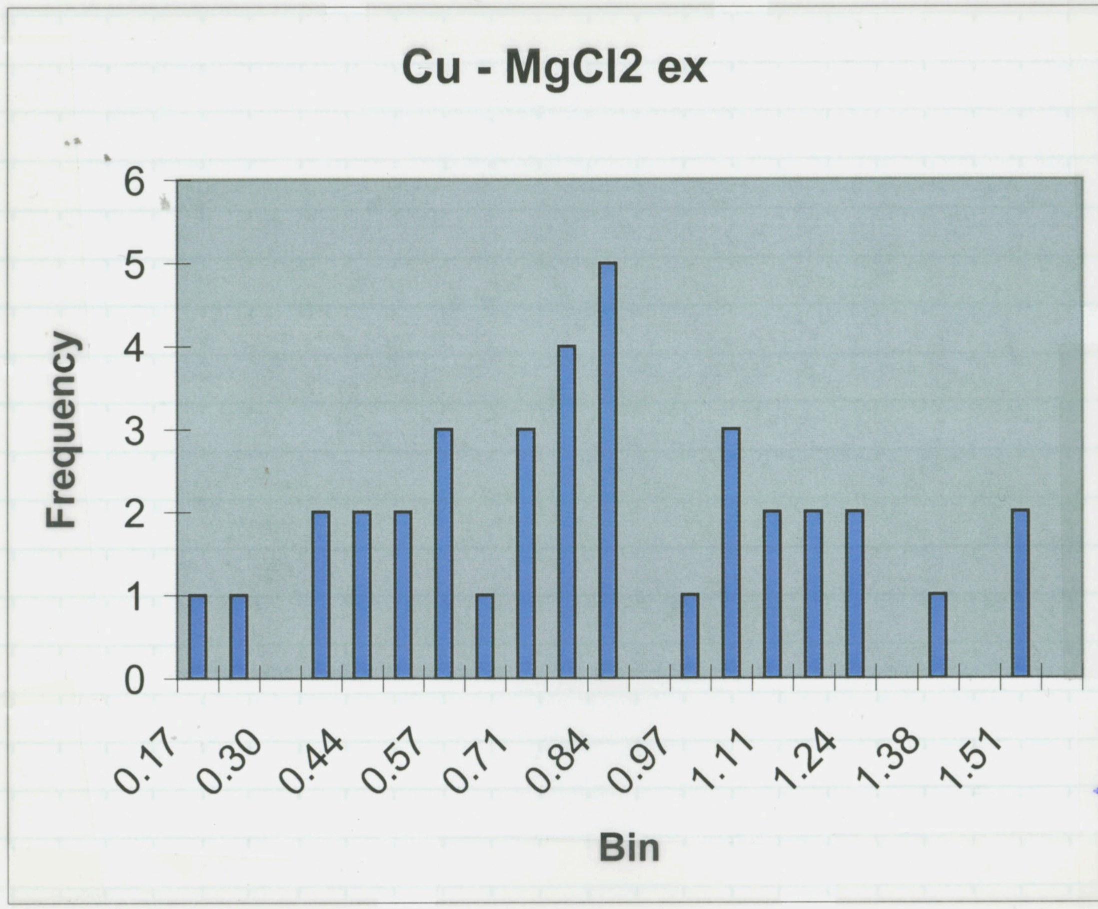


To Page No.

Witnessed & Understood by me,	Date	Invented by / Recorded by	Date
		DH	July 26 1999

From Page No.

Akrotiri

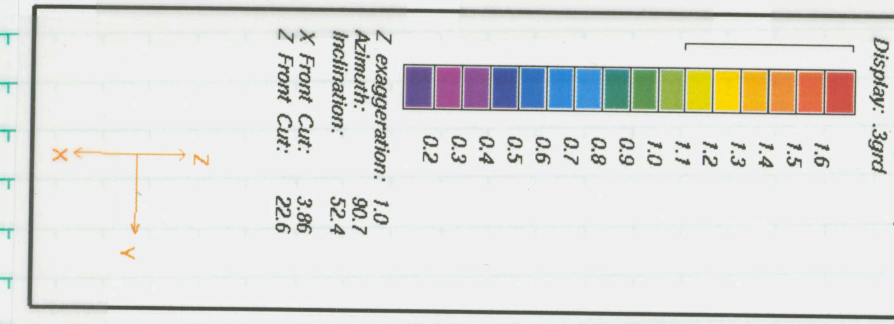


$\mu = 0.79$
$\sigma^2 = .1176$
$\sigma = .343$
min = 0.17
max = 1.51

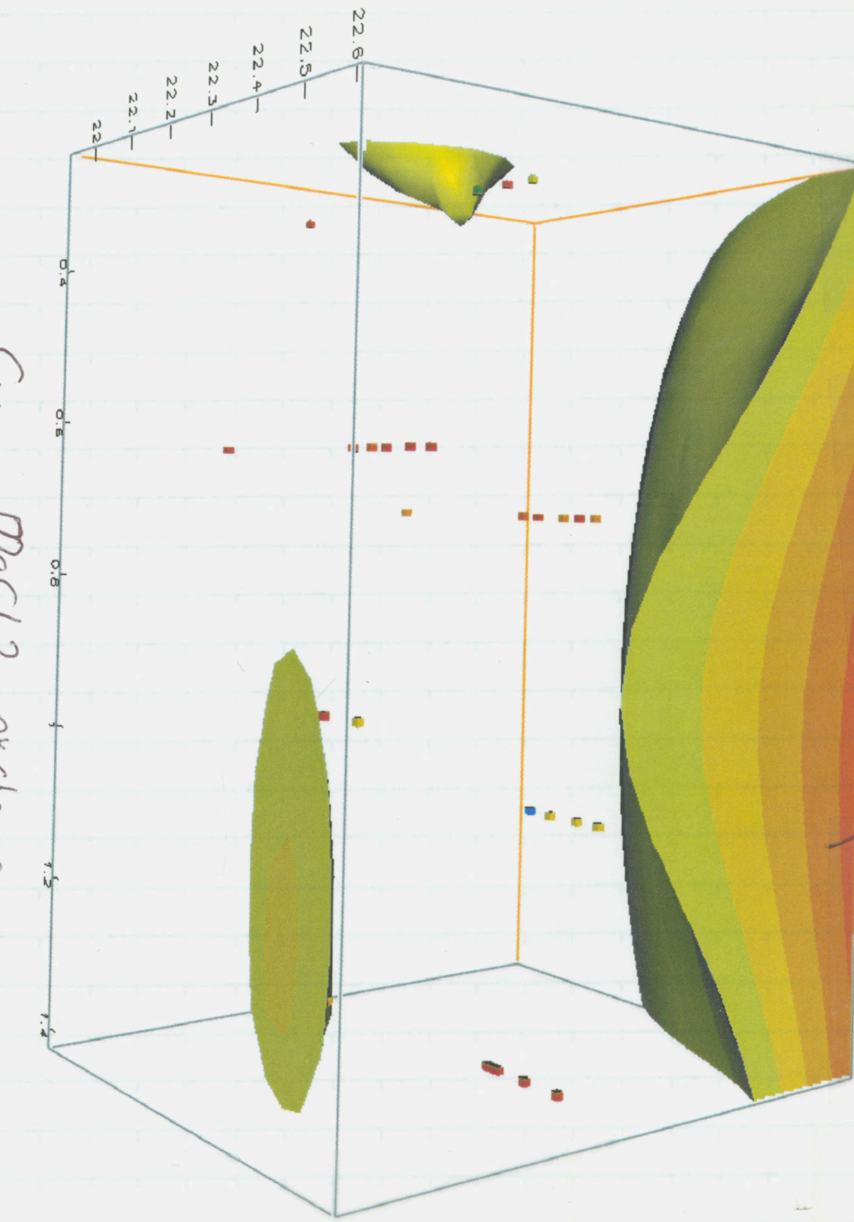
Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DJ	July 26 1999

From Page No.

Akrotiri



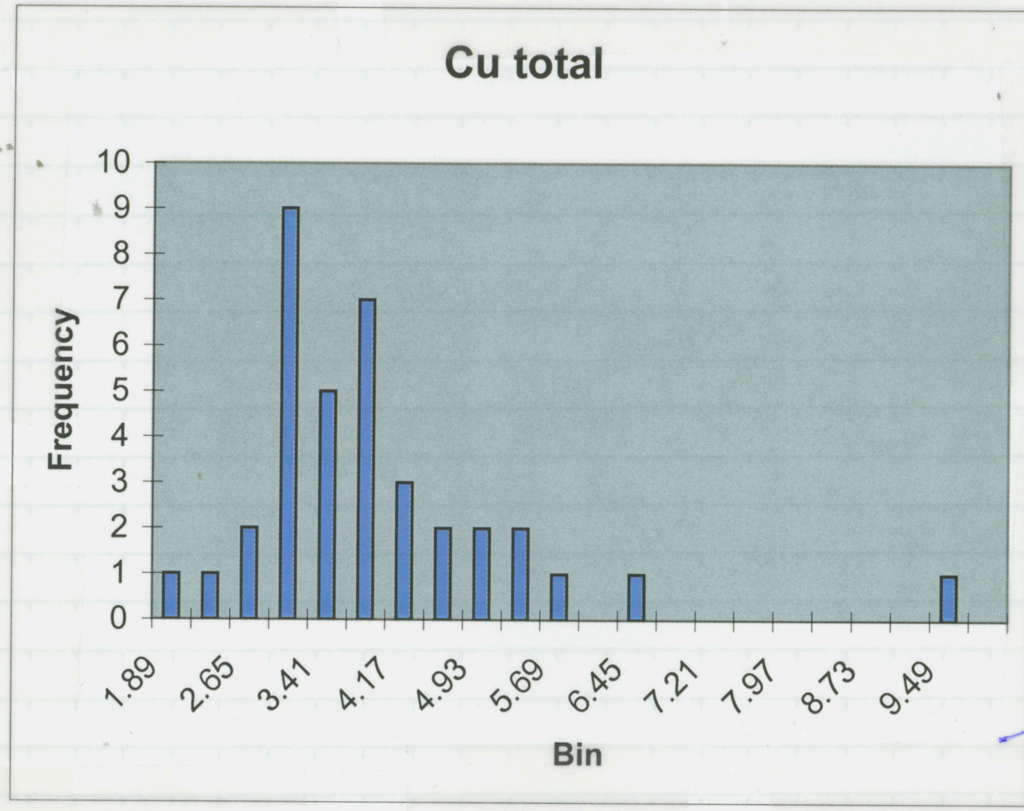
Cu MgCl2 exchange
contour $\mu + \sigma \approx 1.1$



Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DJ	July 26 1999

From Page No.

Akrotiri



$\mu = 3.71$
$\sigma^2 = 1.76$
$\sigma = 1.326$
min = 1.89
max = 9.49

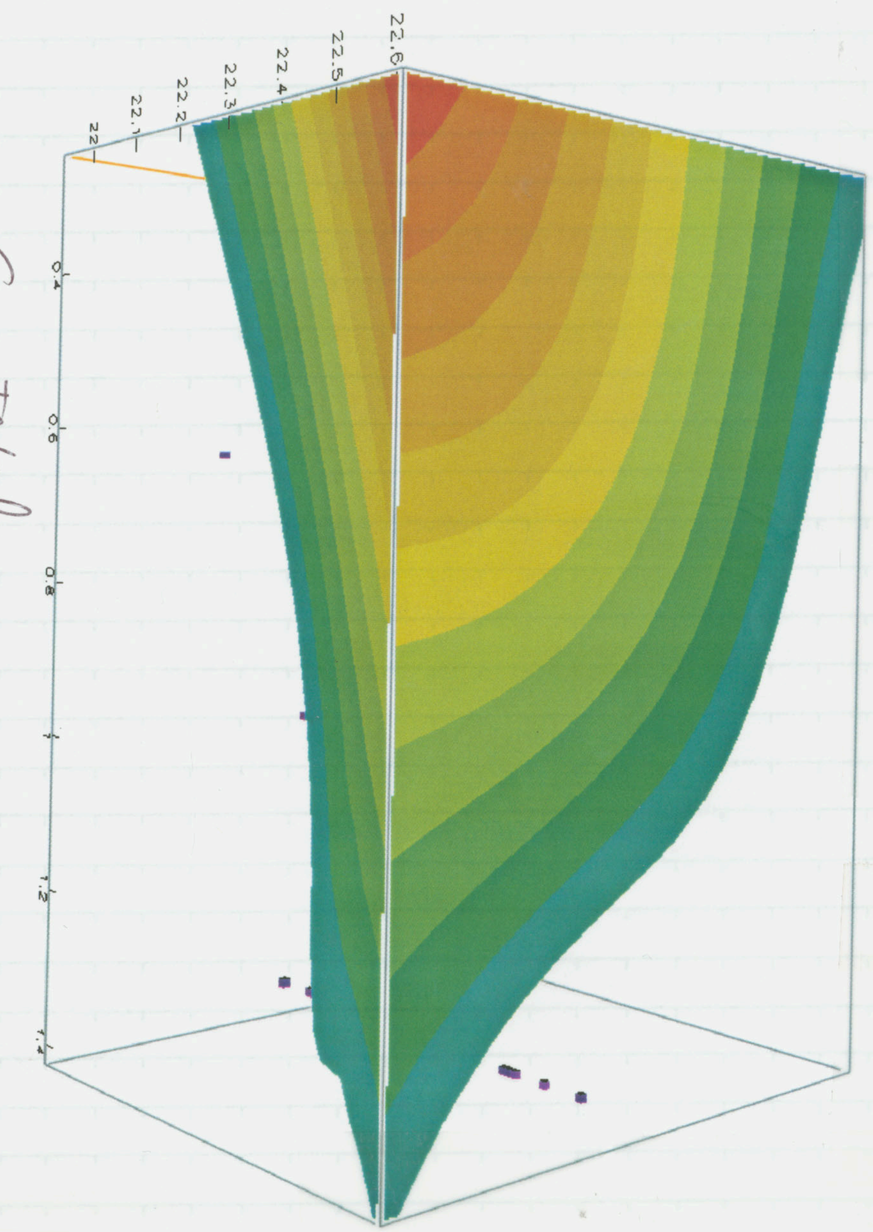
throw out 9.49 datum

$\mu = 3.55$
$\sigma^2 = .83$
$\sigma = .91$
min = 1.89
max = 6.09

From Page No.

Akrotiri

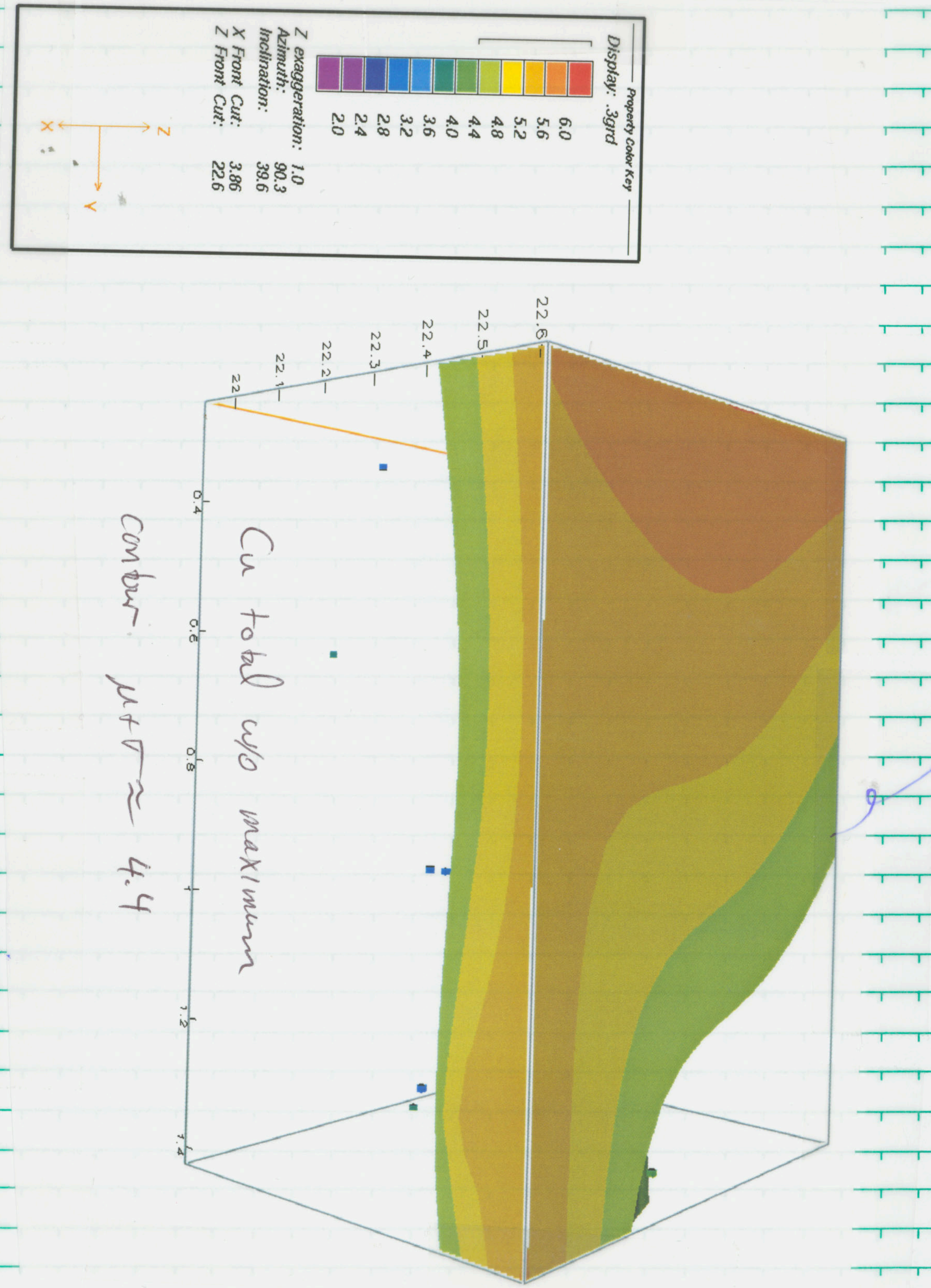
Cu Total
$\mu + \sigma \approx 5.0$ (5.2) contour



Project No. 20-1402-561
Book No. 305 TITLE ENFE

From Page No.

Akrotiri



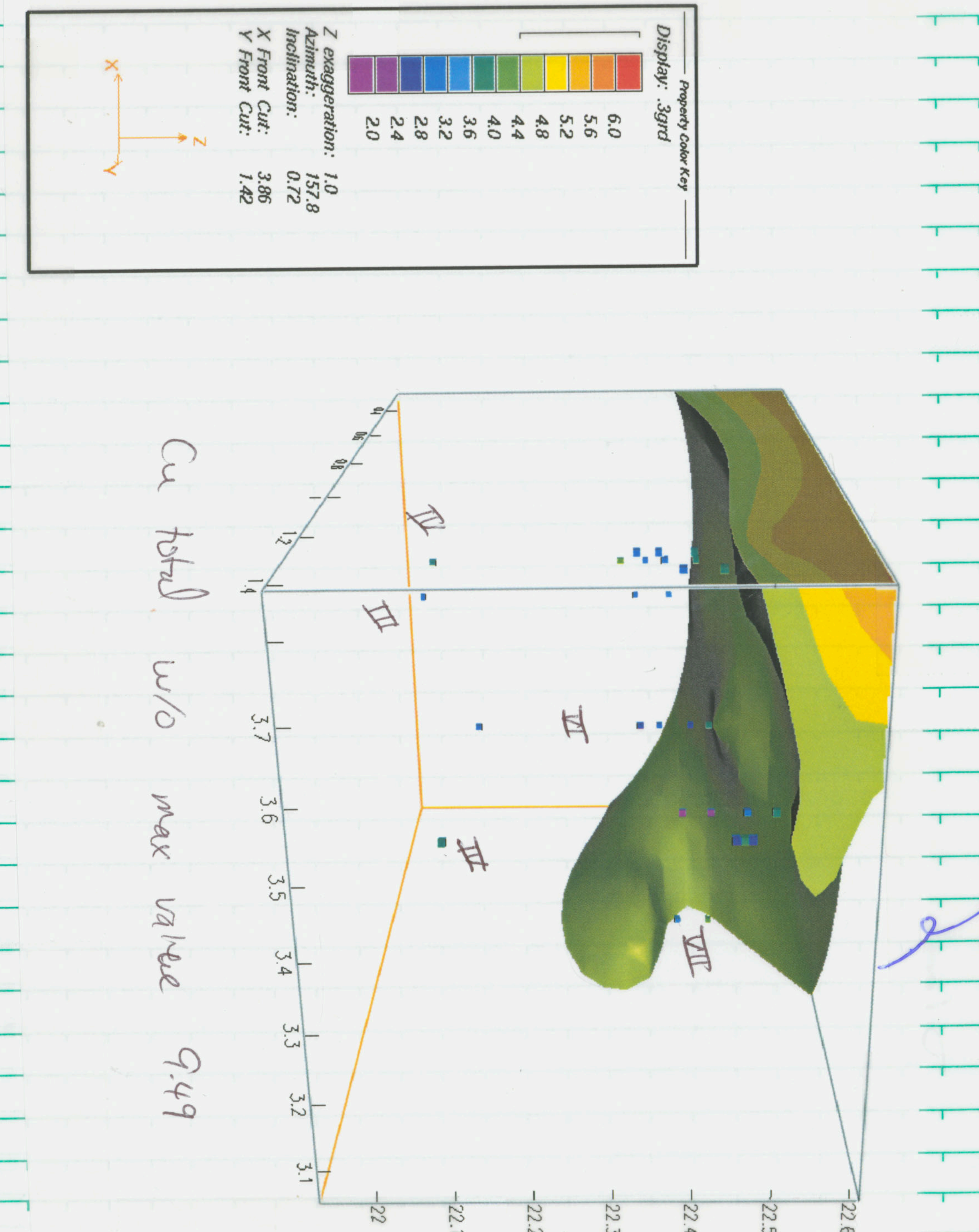
To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by [signature]	July 26 1999

Project No. 20-1402-561
Book No. 305
TITLE ENFE

From Page No.

Akrotiri



To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by [signature]	July 26 1999

Project No. 20-1402-561
Book No. 305 TITLE ENFE – Akrotiri

From Page No.____

Information potentially subject to copyright protection was redacted from this section.
The redacted material is from the following reference:

Hughson, D.L., L. Browning, W.M. Murphy, and R. Green. "An Archeological Site at Akrotiri, Greece, as a Natural Analog for Radionuclide Transport: Implications for Validity of Performance Assessments." Proceedings of the Scientific Basis for Nuclear Waste Management XXIII. D. Shoesmith and R. Smith, eds. Materials Research Society. 1999.

Paper due circa Oct 1, 1999 according to Bill Murphy.

1D & 3D models w/ parameter & BC variations

To Page No.____

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Aug 2 1999

TITLE ENFE – Akrotiri
Project No. 20-1402-561
Book No. 305

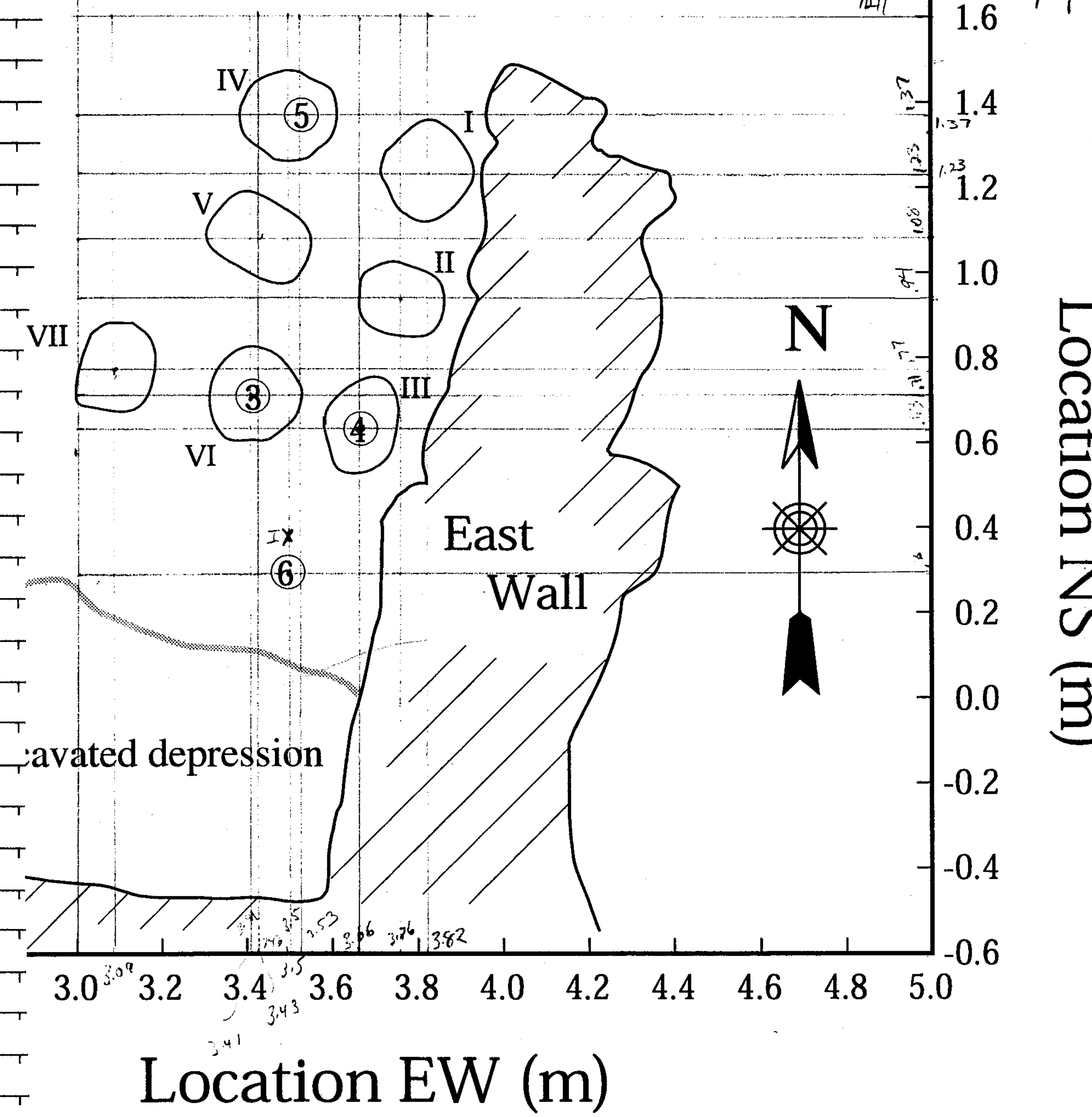
From P

HOLE	X	Y	m Zelev top0	cm Δ packed earth		ref
I	3.82	1.23	22.55	4.5	22.51	18.05
II	3.76	0.94	22.52	6.0	22.46	16.52
III	3.66	0.63	22.49	2.0	22.47	20.49
IV	3.53	1.37	22.59	3.5	22.56	19.09
V	3.43	1.08	22.54	2.0	22.52	20.54
VI	3.41	0.71	22.50	0	22.5	22.50
VII	3.09	0.77	22.50	0	22.5	22.50
IX	3.5	0.3	22.47	3.0	22.44	19.47

DH

ECP 8/24/00

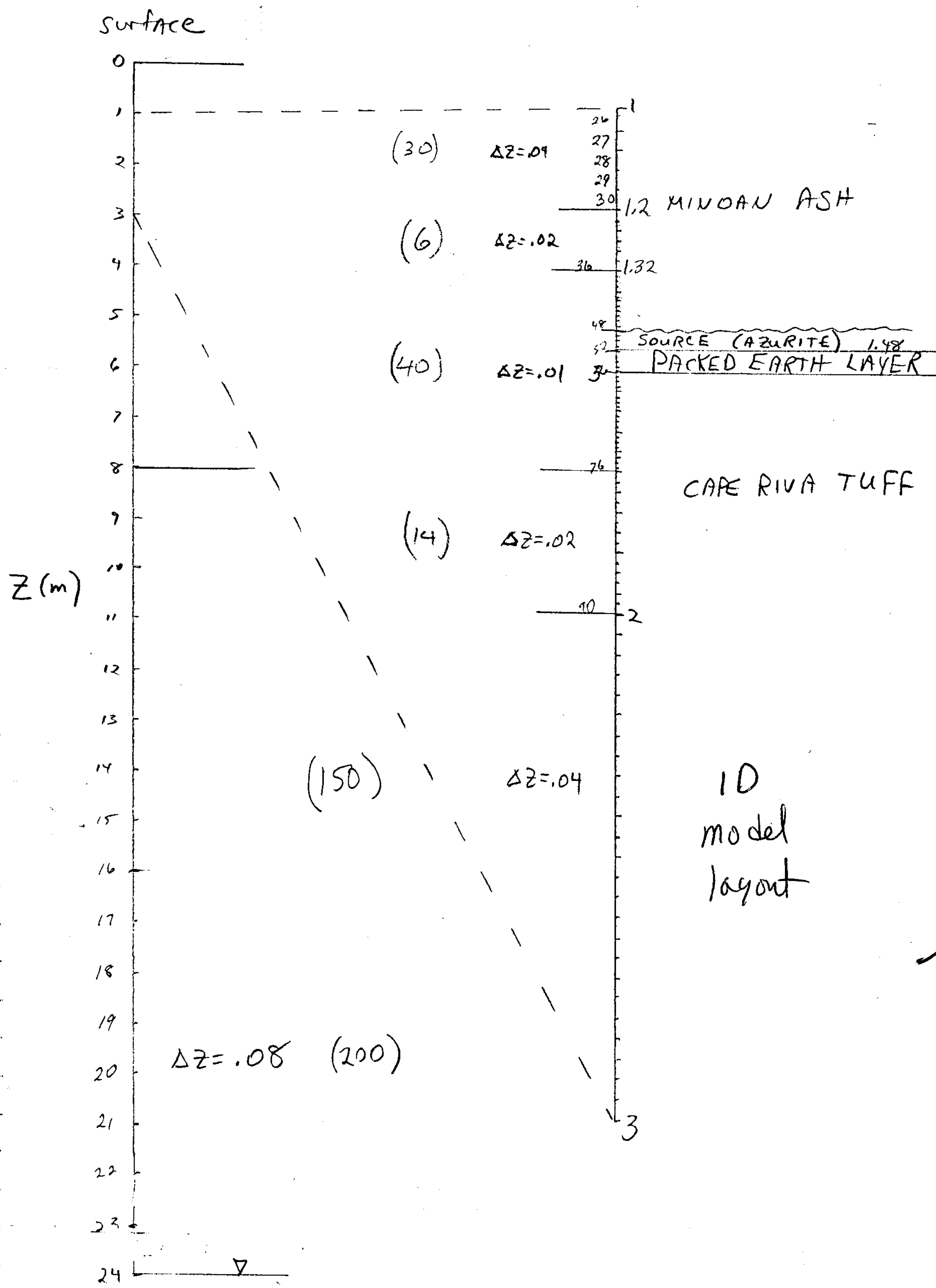
Wow! ECP 8/24/00



Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Aug 2 1999

Project No. 20-1402-561
Book No. 305 TITLE EWFE- Akrotiri

From Page No.____



To Page No.____

Witnessed & Understood by me,	Date	Invented by / Recorded by	Date
			Aug 2 1999

TITLE ENFE - Akrotiri

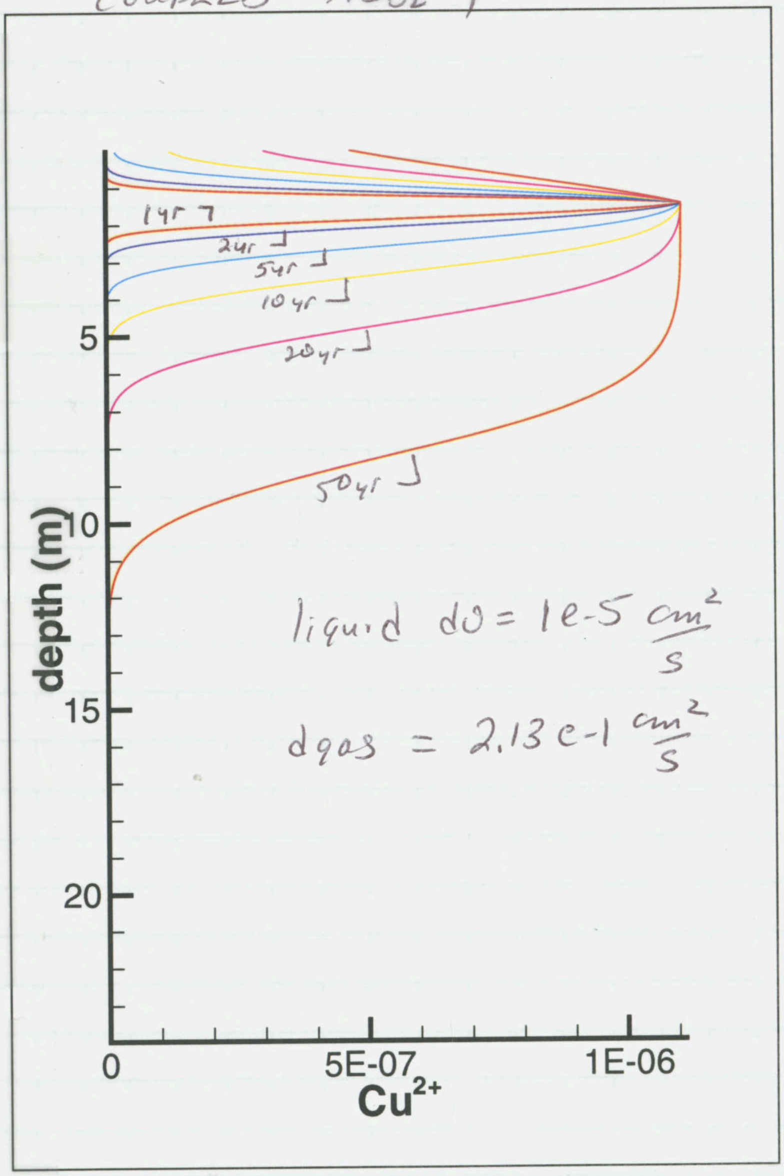
Project No. 20-1402-561

Book No. 305

From Page No.

COUPLED MODE 4

ITYPEBC = 1



Problems found with itypebc = 5 & reported to S Painter Aug 2, 1999. S_g at bc adjusted by trial & error to give ~ 10.5 mm/yr infiltration

To Page No.

Witnessed & Understood by me,

Date

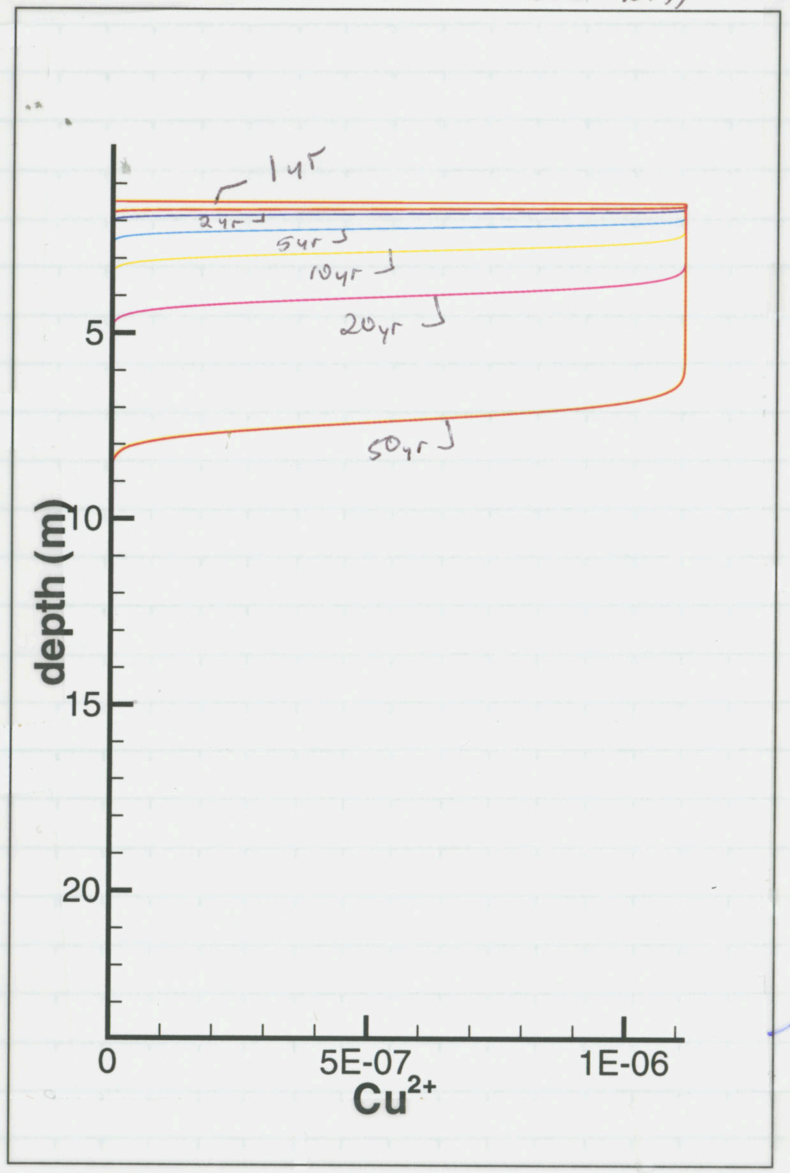
Invented by Aug 2, 1999

Recorded by

Date

From Page No.

COUPLED MODE 4 NO DIFFUSION



θ aqueous & gaseous diffusion

$q_z \approx 10.5 \frac{mm}{yr}$

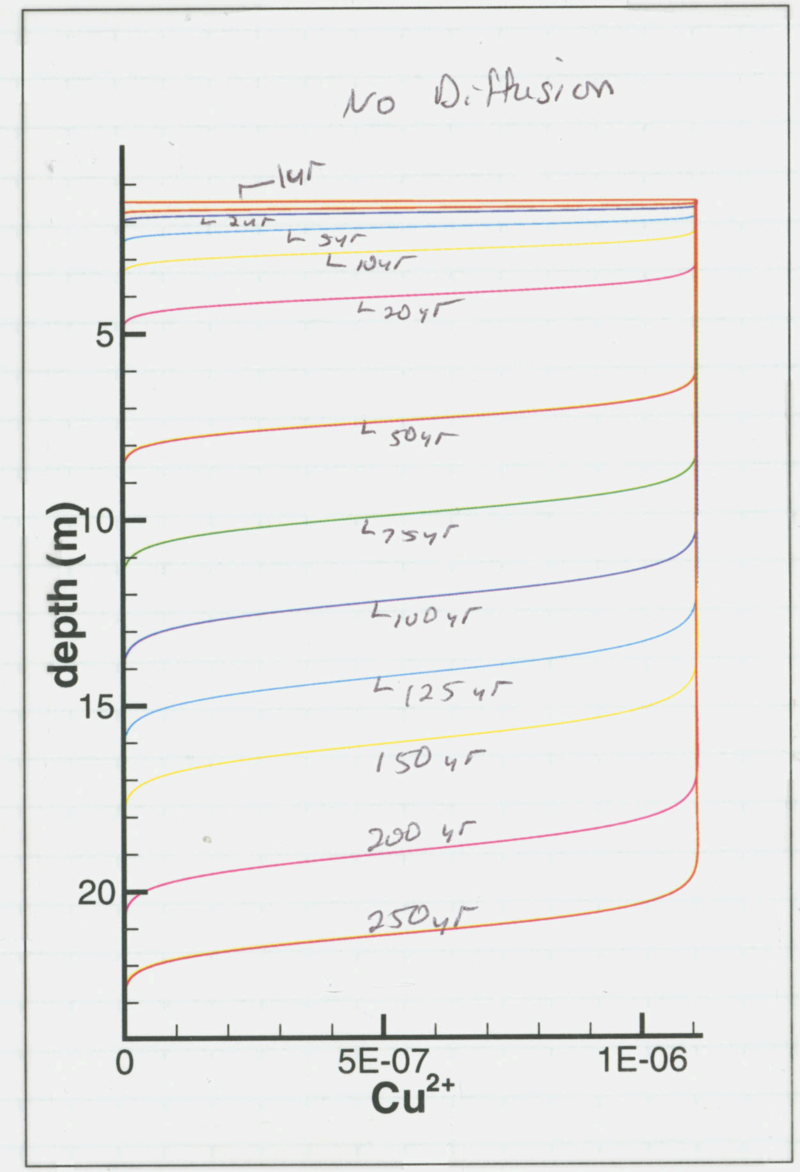
$\phi = .52 \quad S_e = .18 = \frac{\theta}{\phi} \quad \theta = 9.36e{-2}$

$v = \frac{q}{\theta} = \frac{10.5 \frac{mm}{yr}}{9.36e{-2}} = 112 \frac{mm}{yr}$ @ 50yr = 5.6 m

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	DH Aug 2, 1999

From Page No.



10.5 $\frac{mm}{yr}$ infiltration

with advective transport alone & 10.5 mm/yr flux, plume will arrive at the water table in about 300 years

using base case properties

~dhughson/multiflo/murphy/akrotiri/1D/inputfiles/

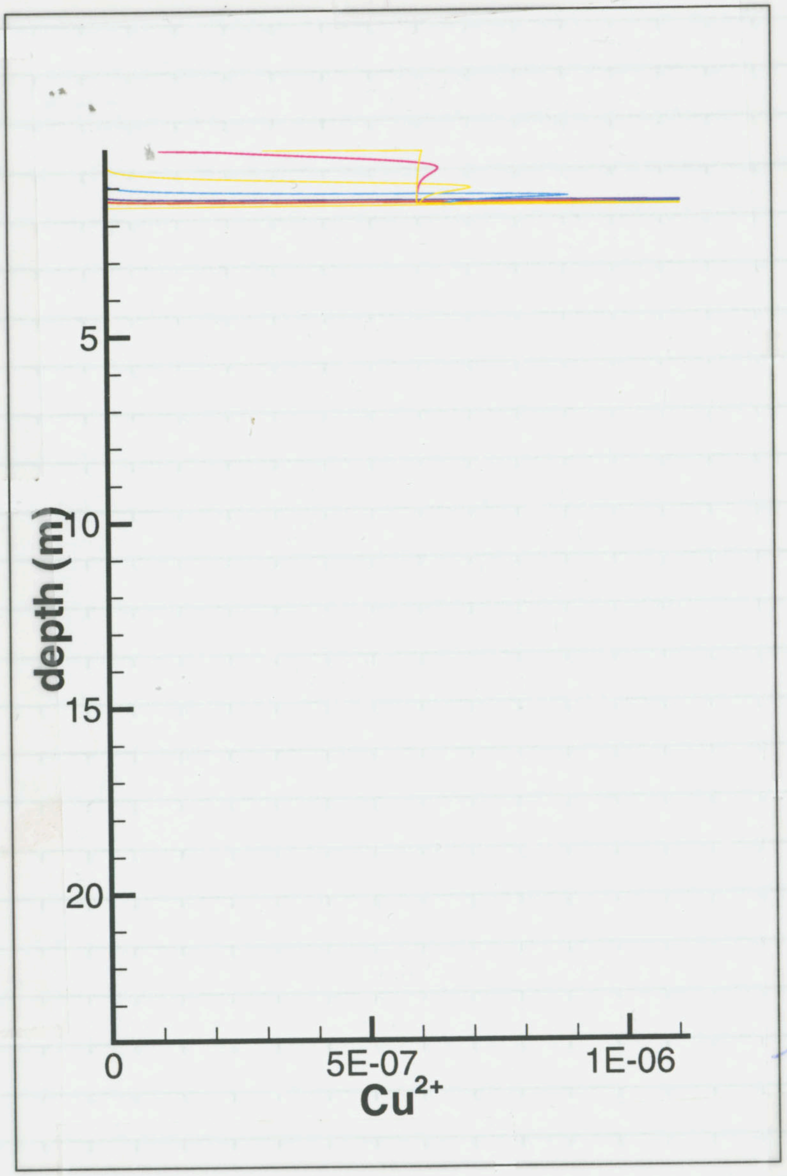
multi.1 masin.1

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Aug 2 1999

Project No. 20-1402-561
Book No. 305 TITLE EWFE- Akrotiri

From Page No. ____



S_g at top BC = 0.9

S_l = 0.10

Results in upward liquid flux of ~ −4.75 mm/yr

Aqueous diffusion

D_d = 0

Simulation to ~~20~~ 250 years

ECP 8/24/00

THE quality of this page is now improved. ECP 8/24/00

Note
Murphy et al (1998) represent infil taken @ 15 cm/yr = 150 mm/yr

To Page No. ____

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by [initials]	Aug 3 1999

From Page No.

Sq Top BC	Flux in top layer
0.43	10.6 mm/yr
0.40	15.0 mm/yr
0.30	47.0 mm/yr
0.20	205.0 mm/yr
0.10	48110 mm/yr

@ 25C

mean annual precip = 32cm/yr = 320 mm/yr

Est mean annual infiltration = 150 mm/yr ?
~~Est~~ mean annual temp = 17 C
ECP 8/24/2000

Sq at Top BC	Flux in top layer
0.4	12.4 mm/yr
0.3	38.8 mm/yr
0.2	169.6 mm/yr
0.1	34632 mm/yr
.19	209 mm/yr
.18	263 mm/yr
.17	342.1 mm/yr
.16	466 mm/yr
.15	680.8 mm/yr
.14	1129.5 mm/yr
.13	2808.4 mm/yr
.10	33790 mm/yr
0.9	-3.75 mm/yr
0.95	-4 mm/yr @ 17C
0.95	-5 mm/yr approx 25C @ TOP 17C @ bottom
0.12	16429 mm/yr ≅ 4.5 mm/day

@ 17C

Use as initial condition (→ 12.4 mm/yr)

To Page No.

Witnessed & Understood by me, | Date | Invented by | Recorded by [signature] | Date Aug 11 1999

From Page No.

Hellenic National Meteorological Service
Climatological Data Base
Lat N 36.25 Long E 25.26 1974-1991

Mon	Total mm	Max 24 hr	Avg Monthly Total
Jan	59.4	47.6	13.2
Feb	60.2	58.5	13.38
Mar	53.2	114.5	11.8
Apr	15.0	41.0	3.3
May	3.6	21.6	0.8
Jun	.9	4.0	0.2
Jul	.0	0.8	0
Aug	.1	2.0	.022
Sep	5.6	64.4	1.24
Oct	19.9	40.2	4.42
Nov	50.1	46.3	11.1
Dec	52.7	33.0	11.7
	320.7		

← Number of rainy days per month if ~~infiltration~~ ~~is 4~~ precip is 4.5 mm/day ~

S_l at surface = 0.12 which gives 16.429 mm/yr

ECP 8/24/00

Unlikely to be < 10 mm/yr infiltration

Simulated precipitation model did not work ~ floating pt errors, terrible mass balance, etc.

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Aug 10 1999

From Page No.

3D model setup

Bottom BC from 1D model
for S_q = 0.41 at TOP BC q_{in} = 11.03 mm/yr

1D model at depth 4.5 m

ρ = 101170 Pa T = 17°C S_l = 0.1836
= 0.186 @ 4.98 m

Grid size 12 x 9 x 30 = 3240

Run for 2 days trying to get initial condition steady state. Reached 0.8 years

3D model has impossibly long run times.
Try 2D model of slice through 3D. ECP
ECP 8/24/00 These were not marked, but I realize now that this helps. 8/24/00
↳ ~~Fre~~ P. File multi.11mm initialized to ~ 10.6 mm/yr infiltration on type 5 bc

Results with 20 mm/y & 130 mm/yr show lots of Cu^{2+} below packed earth ~ to 4.5 m z at 10 yrs.

Retry using initialization flux of ~ 1.4 mm/yr

Step to ~ 15 mm/yr for transport.

– Results in Cu^{2+} at 4.5m z in ~ 50 years

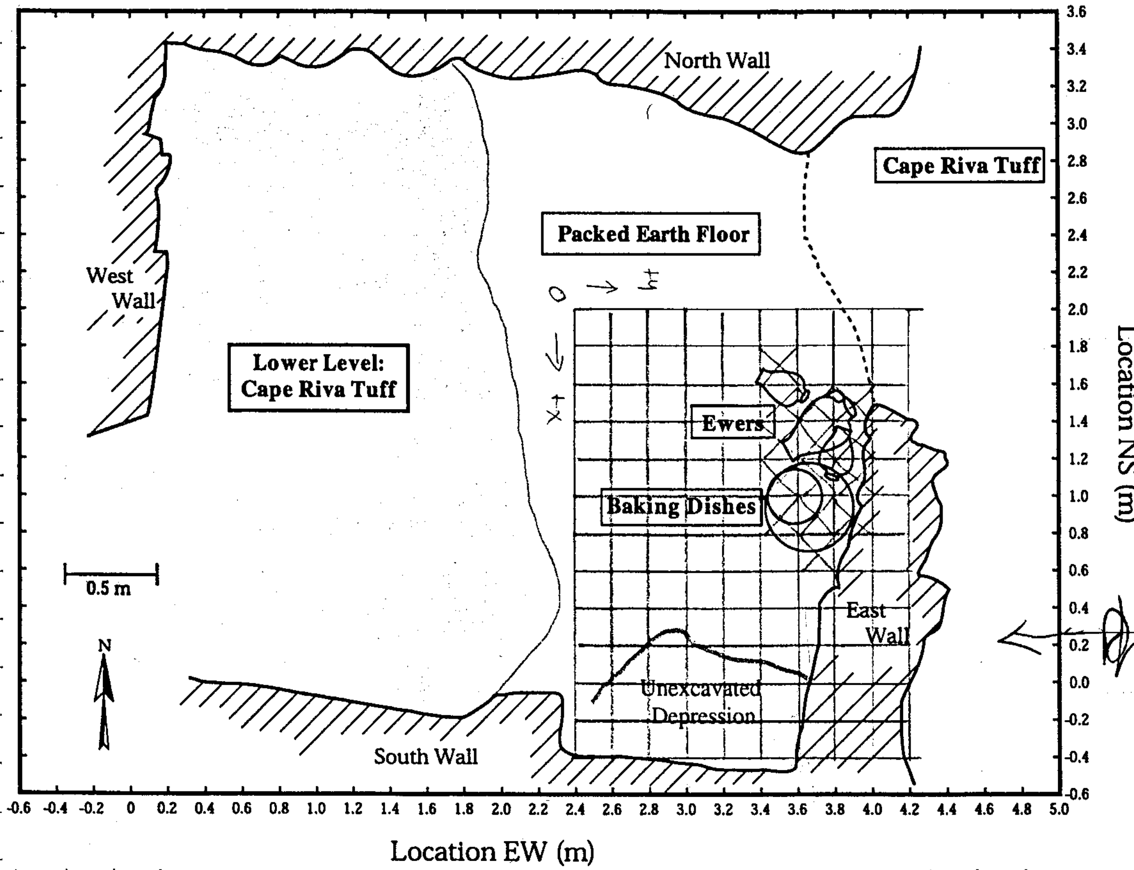
Retry initializing to hydrostatic

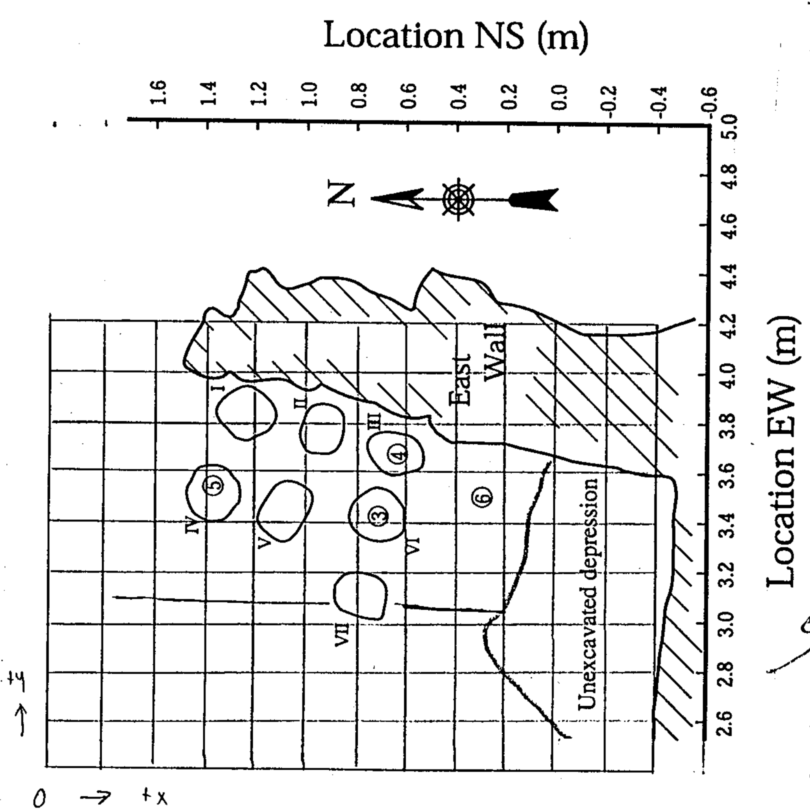
To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Aug 10 1999

Project No. 20-1402-561
Book No. 305 TITLE ENFE Akrotiri

From Page





Source term in Blocks marked X

Relation of sampling holes to grid & coordinates

X = 2m N
y = 2.4m W
is origin

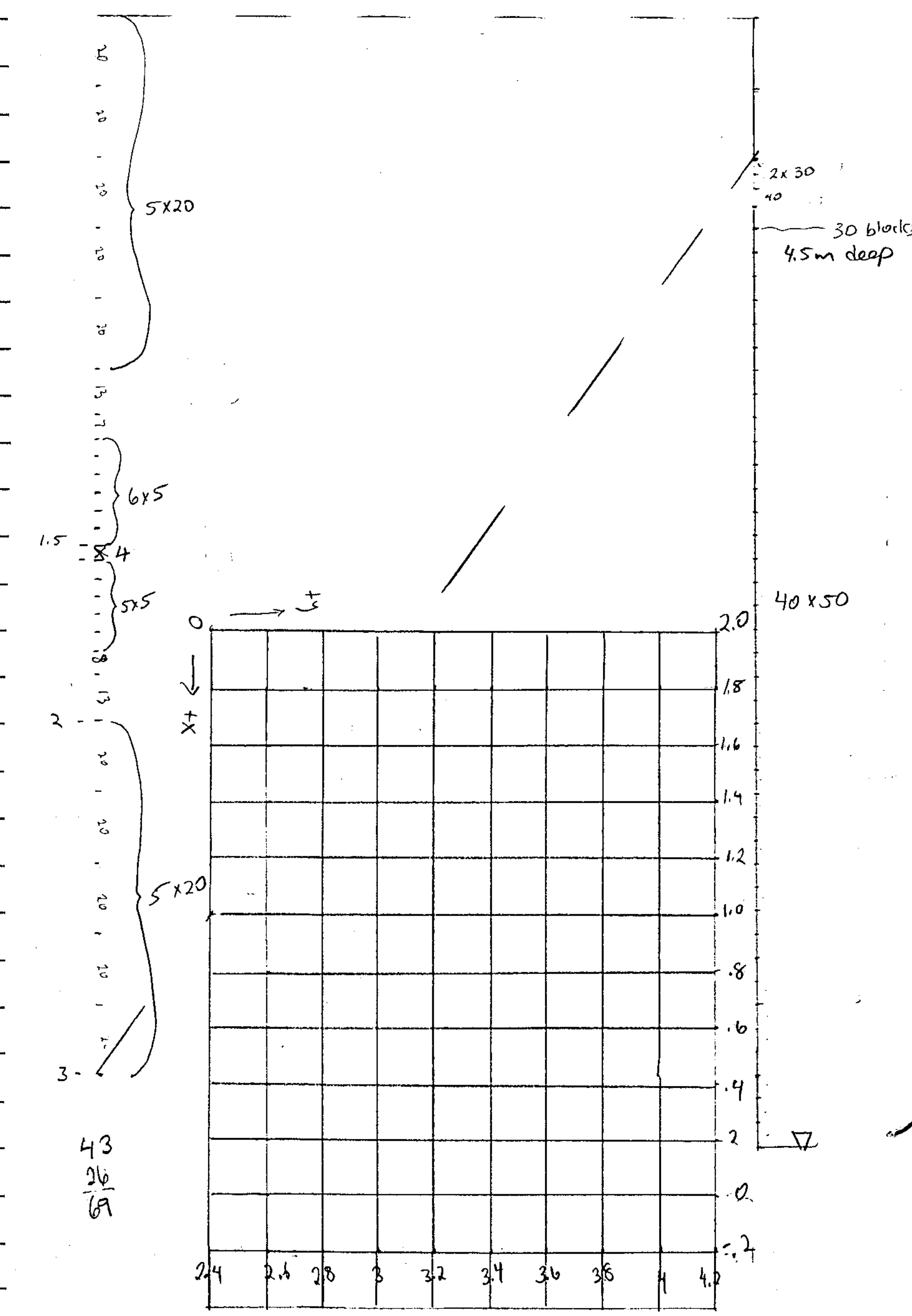
To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Aug 10 1999

TITLE 20-1402-561
Project No.
Book No. 305

From Page No.

3D model discretization



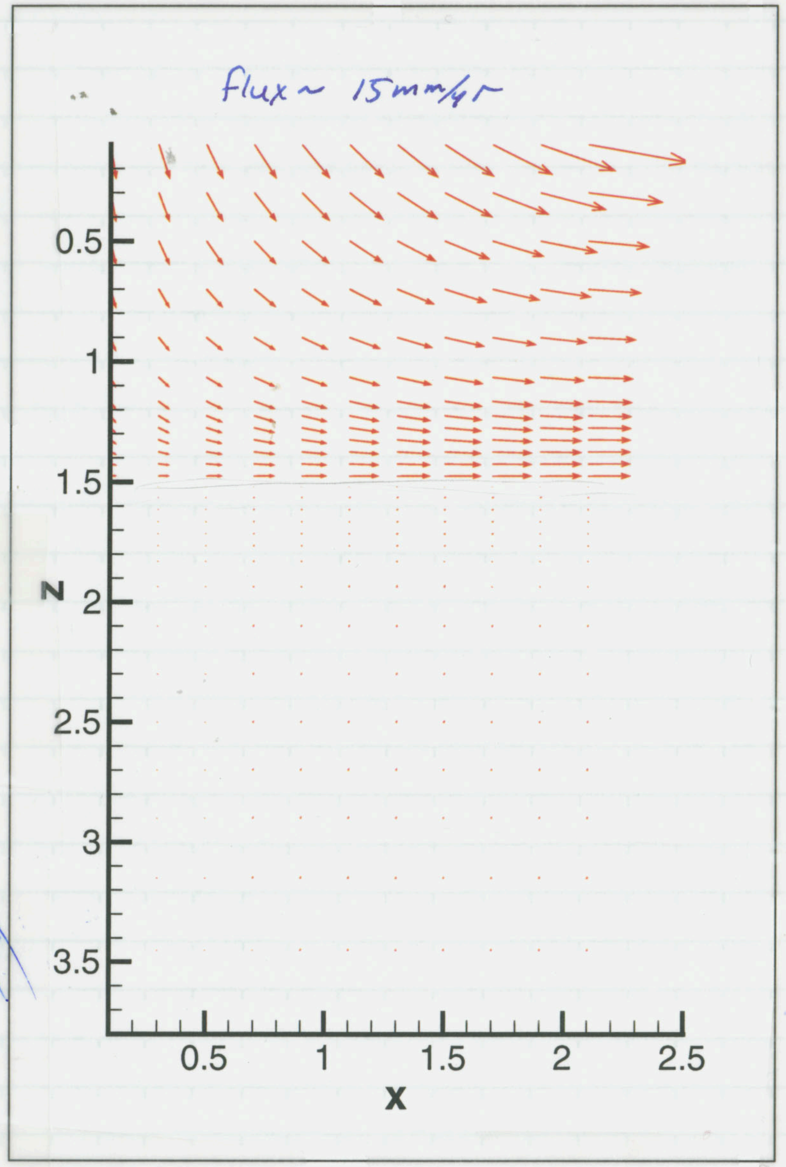
truncated at Z = 4.5m

bottom BC set to Sg from 1D model

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Aug 10 1999

From Page No.



No-flow on left side

Large block reservoir on right side (prescribed sate)

Initial cond close to hydrostatic

Flux on top set to 15mm/yr

Z vel slightly less ~13. mm/yr

shows the diversion capacity of the packed earth layer

Slope ∠ set to 10° sloping south

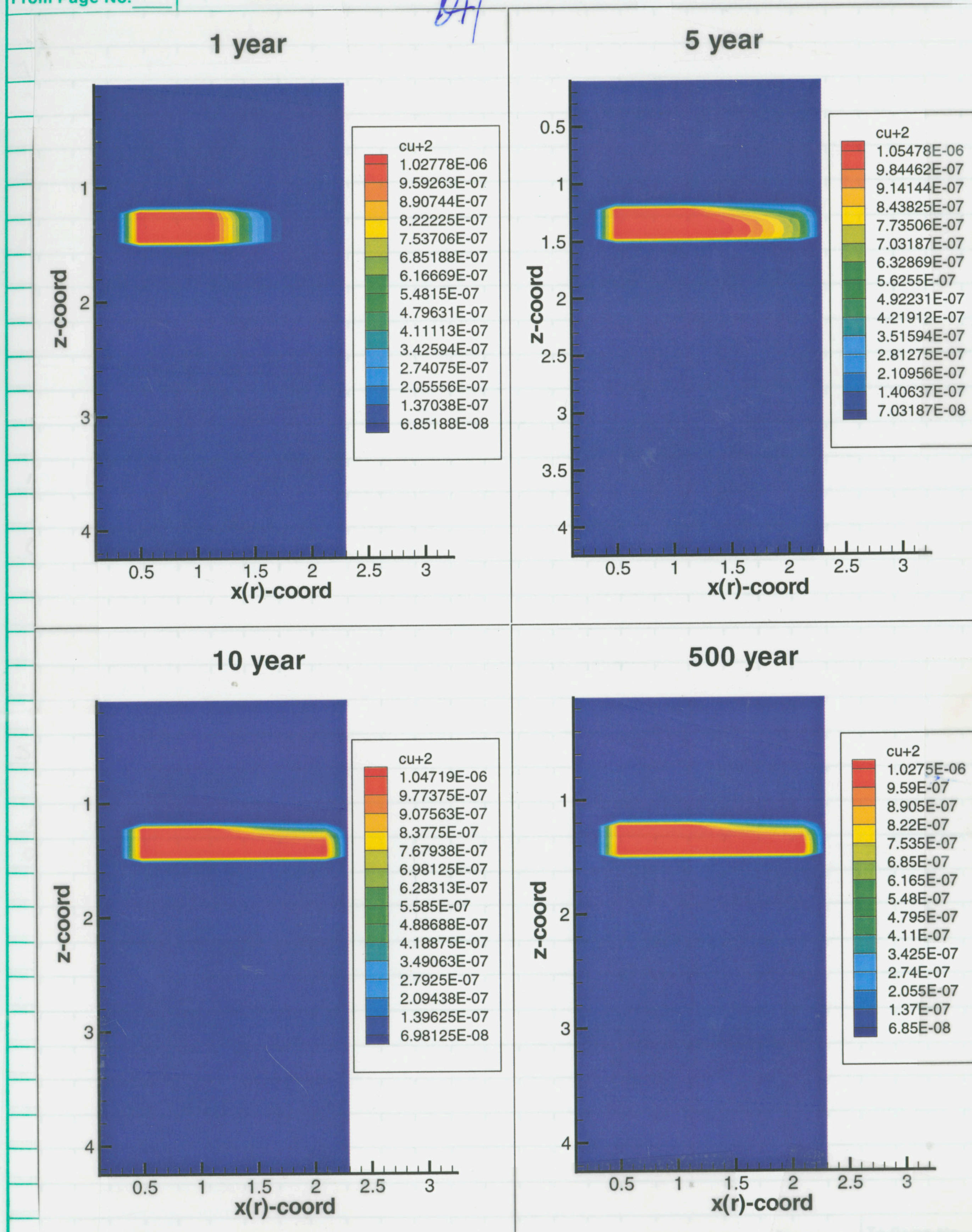
DH

Graphs on following page show Cu^{+2} transport due to advection only. Aqueous Diffusion set to zero. No Cu^{+2} below packed earth in 500 yrs.

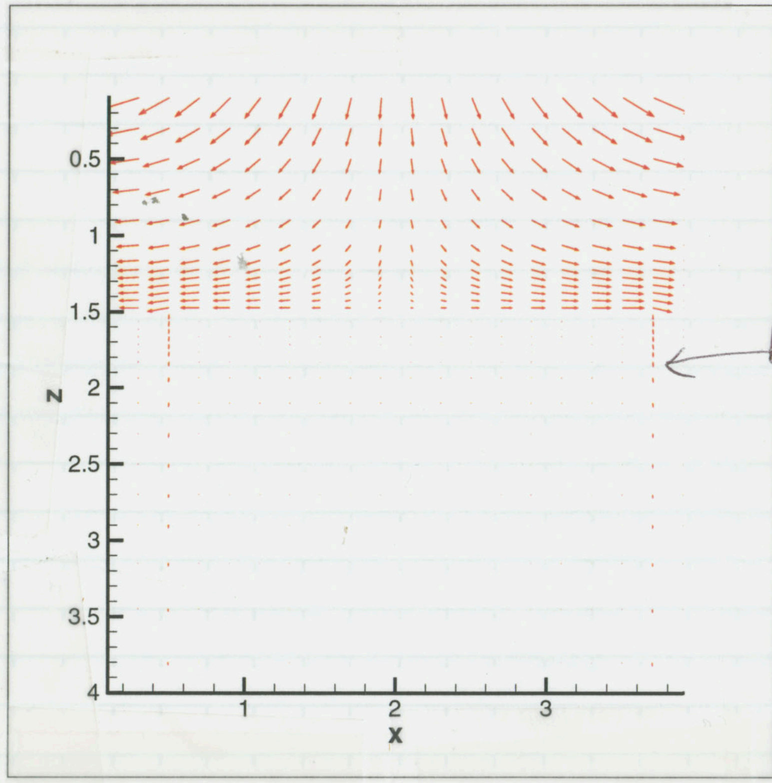
To Page No.

From Page No.

DH



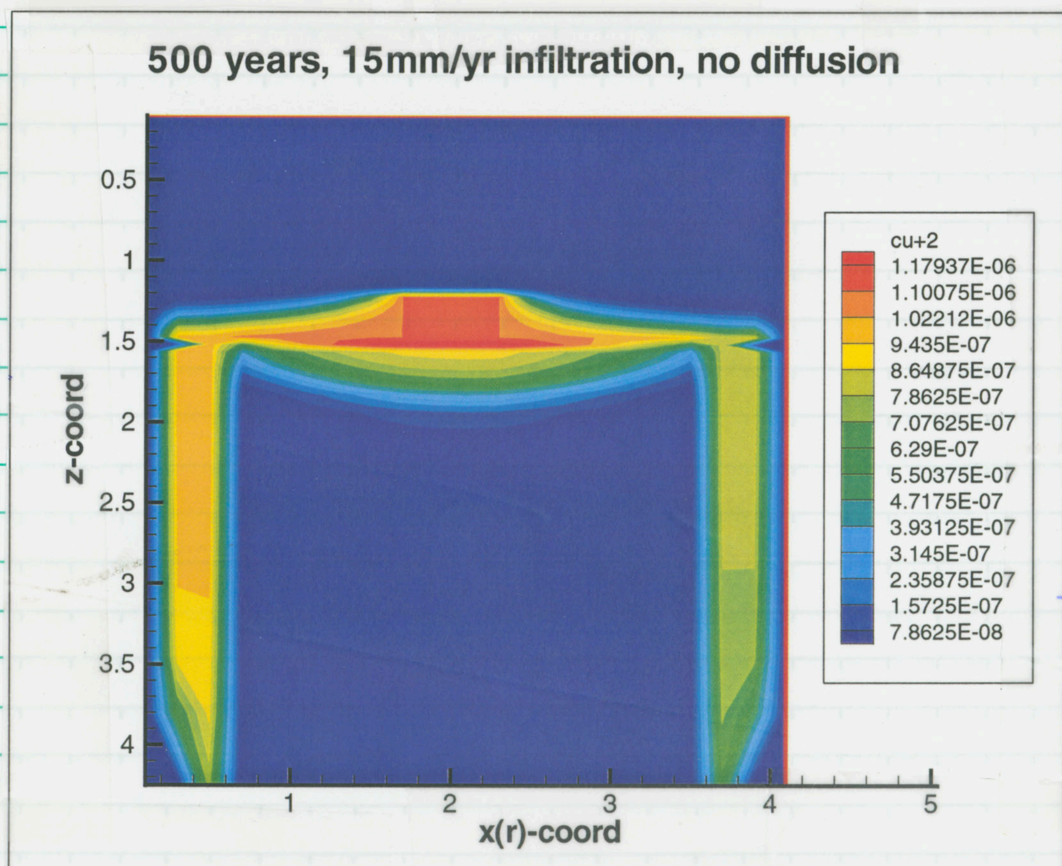
From Page No. ___



Initialized to nearly hydrostatic the 15 mm/yr infiltration to steady state ~ prescribed state BC right and left with high K zones for fracture conduits. BC dominate this model & give rise to diversion above the contact.

← DH

Numerical diffusion results from residual velocities



.1 to .01 mm/yr in the supposed hydrostatic initial condition prior to flux at the top.

To Page No. ___

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Aug 12 1999

From Page No. ___

Previous page input file saved as

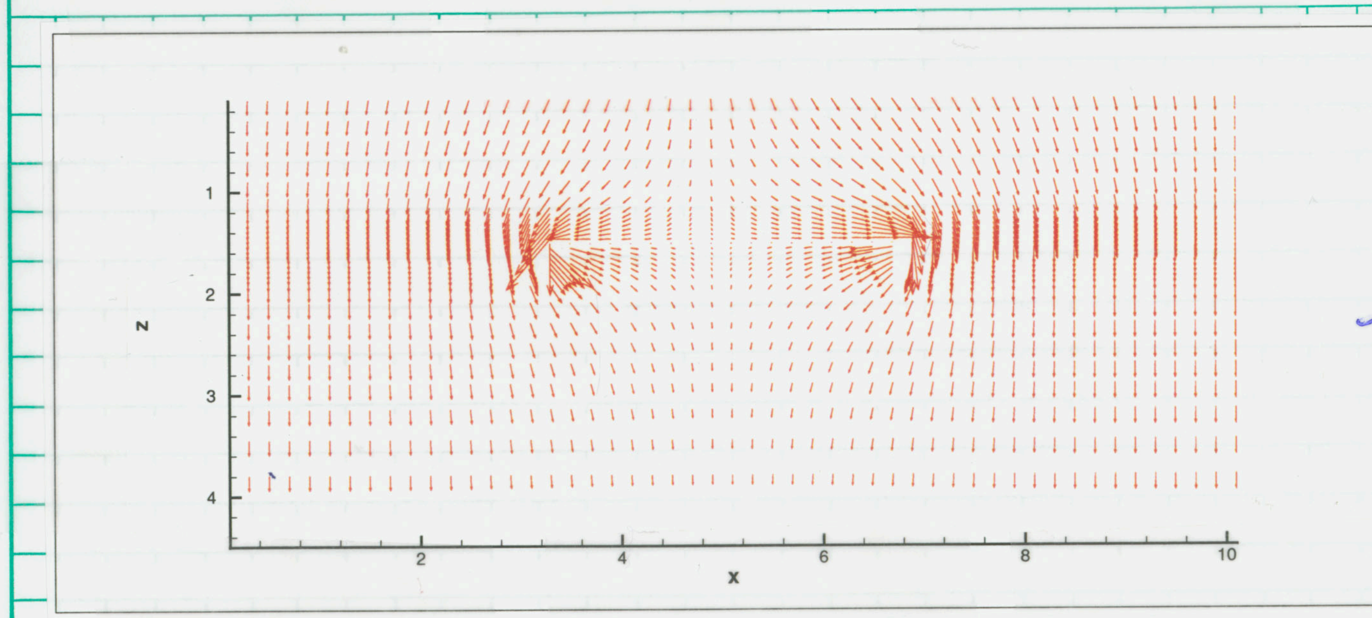
~dhughson/multiflo/murphy/akrotiri/2D/inputfiles
multi.1 and masin.1

Need to widen model domain to move BC farther away.

52 columns at 0.2 m wide - same depth 4.5m

Packed earth in middle 17 cols
Ash on Cape Riva otherwise

No flow bc left and right
~15 mm/yr infiltration

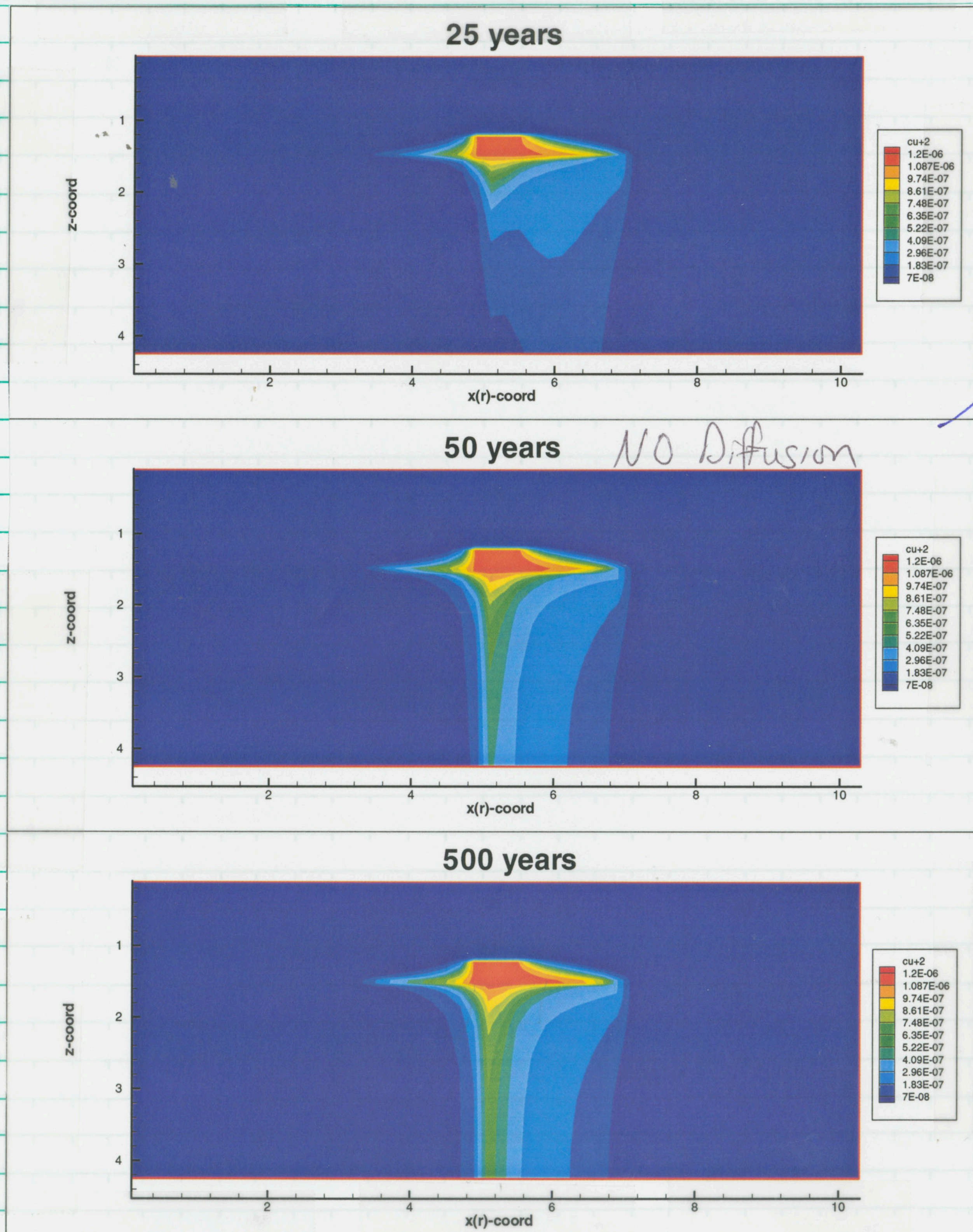


To Page No. ___

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Aug 12 1999

Project No. 20-1402-561
Book No. 305
TITLE ENFE Akrotiri

From Page No.

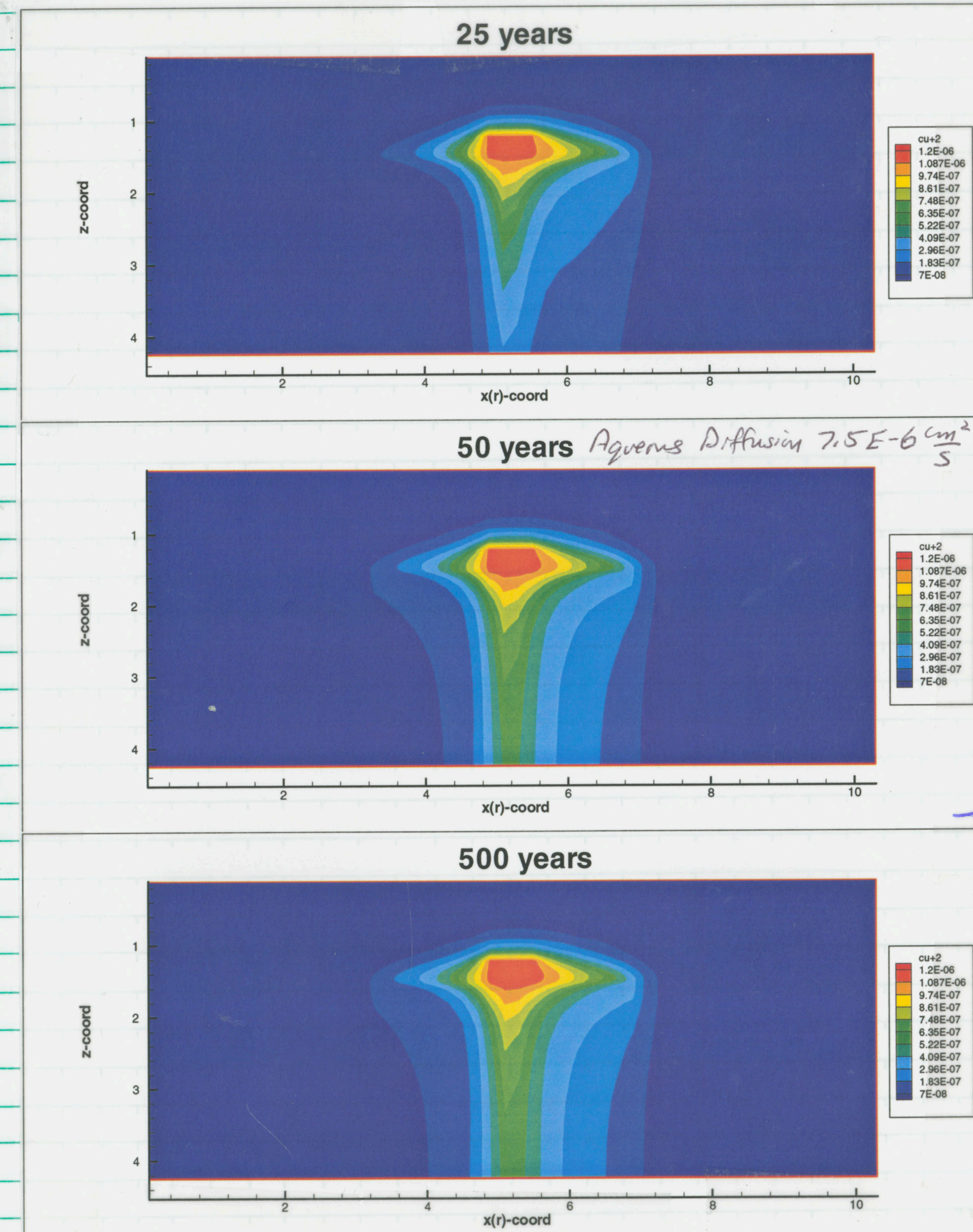


To Page No.

Witnessed & Understood by me,	Date	Invented by / Recorded by	Date
		DH	Aug 12 1999

TITLE ENFE - Akrotiri
Project No. 20-1402-561
Book No. 305

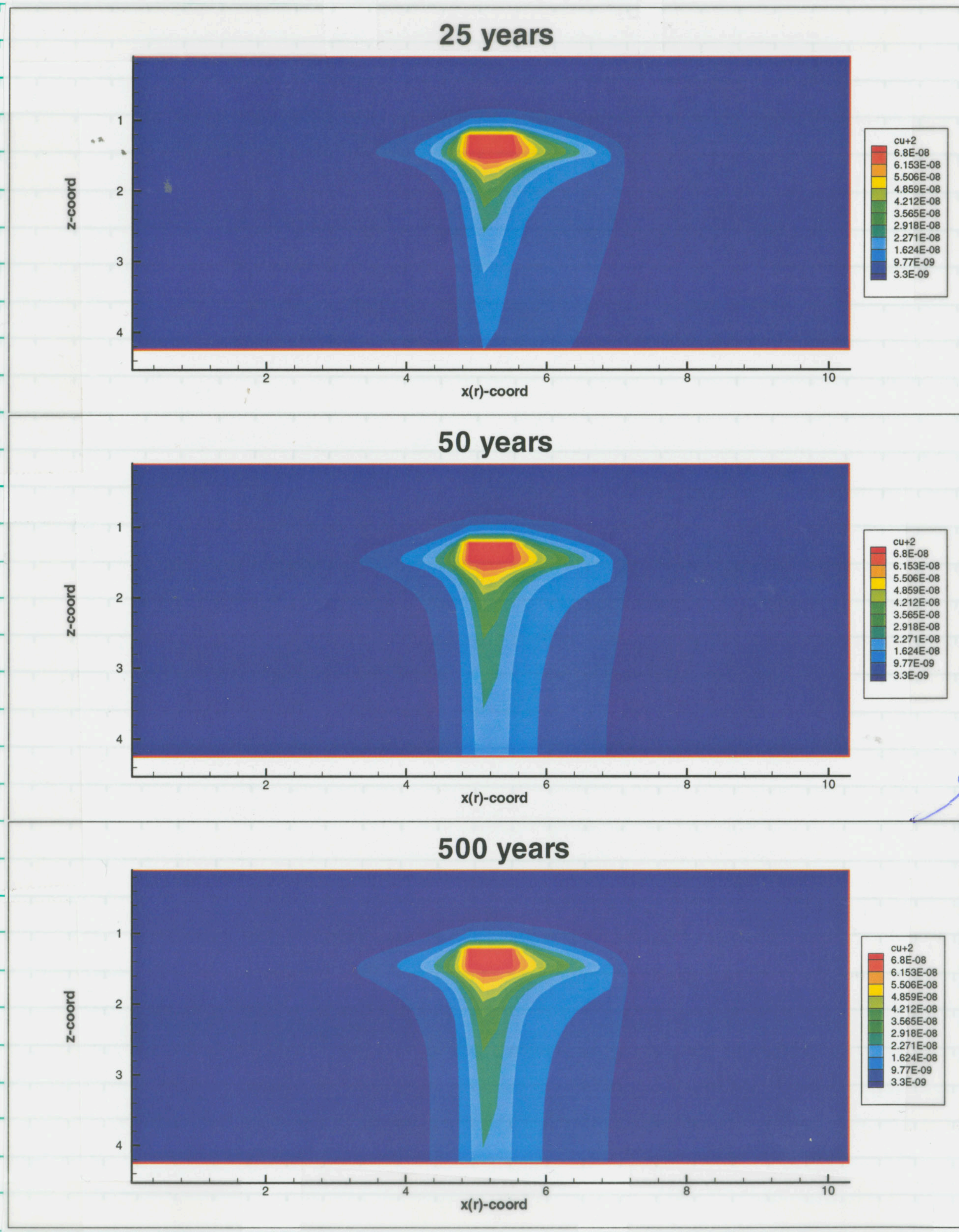
From Page No.



To Page No.

Witnessed & Understood by me,	Date	Invented by / Recorded by	Date
		DH	Aug 13 1999

From Page No. ___



To Page No. ___

From Page No. ___

Using mineral atacamite as the source instead of azurite results in Cu^{2+} concentration reduction but same general shape. ← But undersaturated

~dhughson/multiflo/murphy/akrotiri/2D/inputfiles/
multi.2 masin.2

Potential Evaporation Hamon [1963] from Federer et al. WRR 32(7) p 2319 1996

$$PE = \frac{715.5\,\Lambda\,e^*}{T_m + 273.2}$$

Λ Day length days

T_m = mean air Temp for day °C

$e^*(T)$ saturated vapor press at T kPa

↑ from CRC 72nd ed

Lauren reworked the constraints & aqueous species ~~to~~ so that atacamite is ~~not~~ closer to equilibrium with the water around the source.

This results ~~the~~ in ~~peak~~ concentrations going up about 3 orders of magnitude but plume is about the same shape.

ECP 8/24/2000 This page is now 4X better. ECP 8/24/00

Plot on page 49 input file saved as

~dhughson/multiflo/murphy/akrotiri/2D/inputfiles/masin.3
multi.3

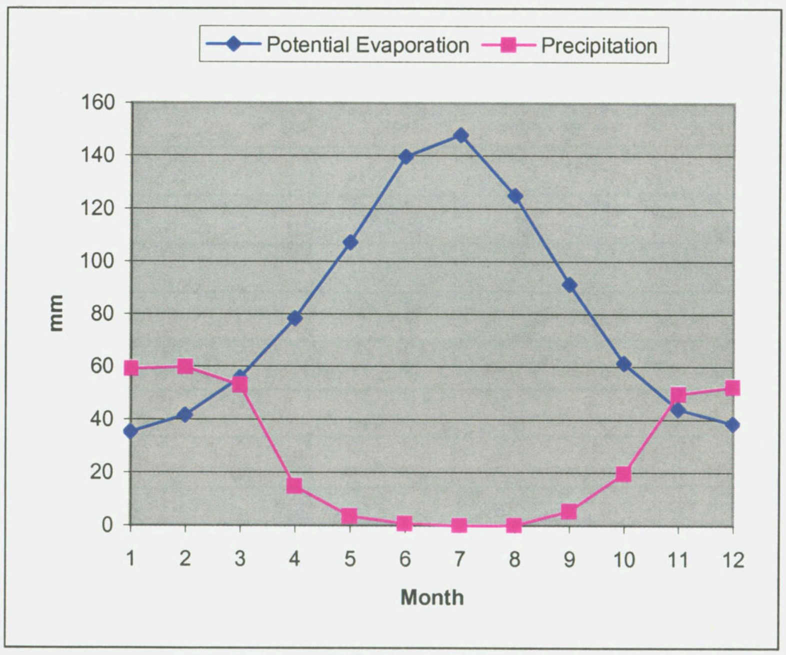
To Page No. ___

Project No. 20-1402-561
Book No. 305 TITLE ENFE Akrotiri

From Page No.

Method of Haman (1963)

Month	Mean T	vap press	day length	PE	Total Prec
Jan	11.2	1.3309	0.348395	35.48204	59.4
Feb	11.2	1.3309	0.409893	41.74532	60.2
Mar	12.7	1.4693	0.5	55.92263	53.2
Apr	15.5	1.76205	0.590107	78.38326	15
May	19.1	2.2119	0.651605	107.3106	3.6
Jun	23.3	2.8628	0.66497	139.73	0.9
Jul	25.4	3.2466	0.625958	148.1172	0
Aug	24.8	3.1322	0.546955	125.1141	0.1
Sep	22.6	2.7441	0.453045	91.4669	5.6
Oct	19.1	2.2119	0.374042	61.59961	19.9
Nov	15.4	1.7508	0.33503	44.23284	50.1
Dec	12.6	1.4598	0.348395	38.72789	52.7



To Page No.

Witnessed & Understood by me, | Date | Invented by | Date Aug 16 1999
Recorded by DH

HELLENIC NATIONAL METEOROGICAL SERVICE
DIVISIONS II-III/STAT. CLIMAT. SECTION
CLIMATOLOGICAL DATA BASE

DATCLIM MET. PAR.69

STATION ΘHPA 744
LATITUDE N 36.25 DEGR LONGITUDE E 25.26 DEGR ALTITUDE OF BAROM. 36.50 METERS

PERIOD 1974-1991

MONTH	PRESS(M.S.L.)	T E M P E R A T U R E MEAN	AV.MAX	AV.MIN	ABS MAX	ABS MIN	REL HUM.	AV.CLOUD.	PRECIPITATION(IN MM) TOTAL	MAX 24H
JANUARY	1018.0	11.2	13.2	9.1	21.8	1.0	71.4	4.6	59.4	47.6
FEBRUARY	1015.9	11.2	13.5	9.2	22.0	-2.0	70.7	4.7	60.2	58.5
MARCH	1014.6	12.7	15.1	10.2	25.6	1.6	72.4	4.1	53.2	114.5
APRIL	1012.9	15.5	16.2	12.5	28.4	6.6	69.8	3.5	15.0	41.0
MAY	1013.0	19.1	22.1	15.7	32.6	9.0	67.7	2.7	3.6	21.6
JUNE	1011.6	23.3	26.6	19.6	39.0	12.0	62.5	1.1	.9	4.0
JULY	1010.1	25.4	28.3	21.8	39.4	13.6	59.9	.3	.0	.8
AUGUST	1010.2	24.8	27.9	21.6	36.6	16.0	61.8	.4	.1	2.0
SEPTEMBER	1013.7	22.6	25.6	19.4	35.0	10.4	65.5	1.0	5.6	64.4
OCTOBER	1016.6	19.1	21.8	16.4	33.8	10.0	70.1	2.6	19.9	40.2
NOVEMBER	1016.8	15.4	18.0	13.1	27.4	.8	72.1	3.8	50.1	46.3
DECEMBER	1016.6	12.6	14.8	10.0	22.2	.0	71.6	4.4	52.7	33.0

N U M B E R O F D A Y S W I T H

MONTH	CLOUDINES (0 - 8/8) 0-1.5	1.6-6.4	6.5-8.0	PREC.	RAIN	SNOW	THUND	HAIL	ST GND	FOG	DEW	H.FROST	TEMPERATURE MIN LE 0.0	MAX LE 0.0	WI GE 6B
JANUARY	2.3	23.8	4.8	9.4	9.1	.0	1.2	.1	.1	.0	.4	.0	.0	.0	8.2
FEBRUARY	1.9	21.4	4.8	9.4	8.9	.4	1.3	.0	.1	.1	1.1	.0	.2	.0	8.3
MARCH	5.5	20.5	5.0	7.2	6.9	.2	1.7	.1	.0	.2	1.1	.0	.0	.0	6.8
APRIL	7.8	19.4	2.8	4.6	4.5	.0	.5	.0	.0	.1	.5	.0	.0	.0	5.0
MAY	12.2	17.3	1.5	1.8	1.6	.0	.2	.0	.0	.0	.3	.0	.0	.0	2.7
JUNE	22.1	7.8	.1	.6	.6	.0	.1	.0	.0	.0	.0	.0	.0	.0	2.6
JULY	28.9	2.0	.1	.4	.4	.0	.1	.0	.0	.0	.1	.0	.0	.0	3.8
AUGUST	28.3	2.7	.1	.1	.1	.0	.0	.0	.0	.0	.2	.0	.0	.0	2.6
SEPTEMBER	23.2	6.4	.3	.9	.9	.0	.1	.0	.0	.1	.2	.0	.0	.0	3.1
OCTOBER	13.0	16.2	1.8	3.9	3.7	.0	.6	.0	.0	.1	.9	.0	.0	.0	4.3
NOVEMBER	5.3	21.6	3.2	7.2	7.2	.0	1.4	.0	.0	.2	1.5	.0	.0	.0	5.5
DECEMBER	3.2	22.9	4.8	10.2	9.4	.0	1.5	.1	.0	.1	.9	.0	.1	.0	8.3

To Page No.
From Page No.

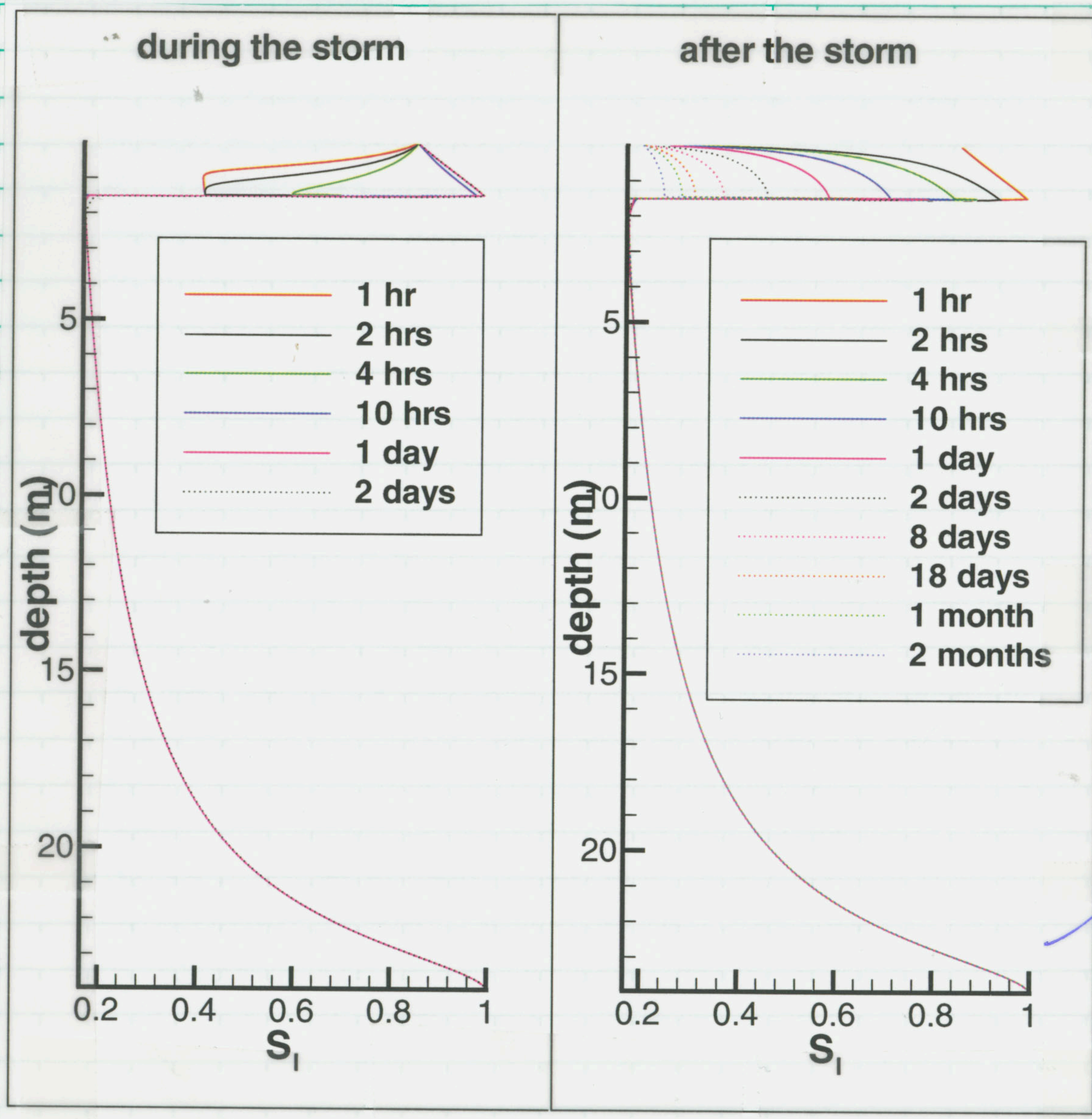
TITLE ENFE-Akrotiri

Project No. 20-1402-501
Book No. 305

Date Aug 16 1999
Invented by
Recorded by
Date
Witnessed & Understood by me,

From Page No.

Suppose Initial hydrostatic ~ S_l at surface ~ 0.4. 2 day rain causes surface S_l = 0.85. After rain, sun comes out & dries soil to S_l = 0.2

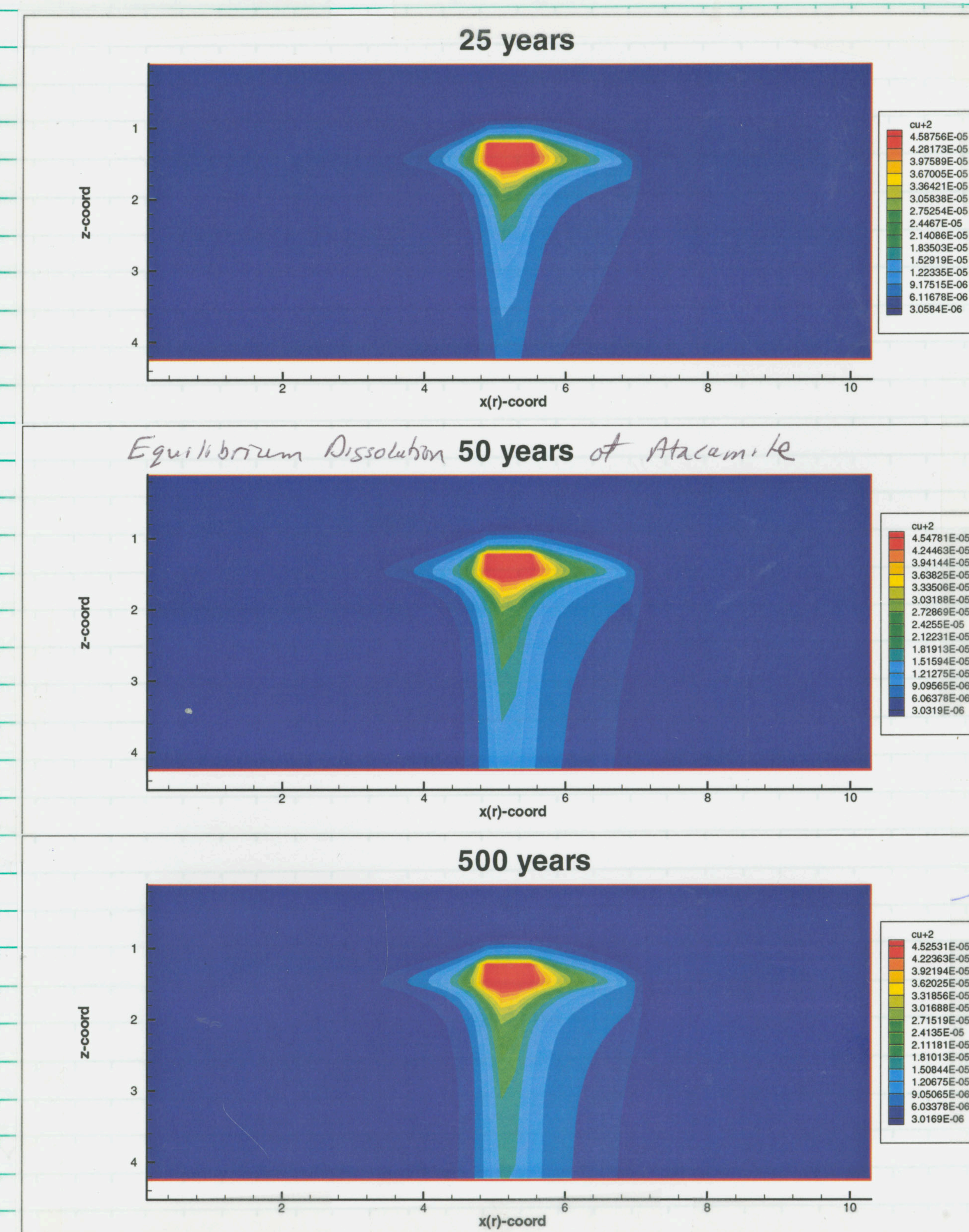


Water goes below packed earth after 1 day of rain but dries out to hydrostatic S_l = 0.4 between 2 and 8 days

To Page No.

Witnessed & Understood by me, | Date | Invented by | Recorded by DH | Date Aug 16 1999

From Page No.



~dhughson/multiflo/murphy/akrotiri/2D/inputfiles/masin.4 & part.4

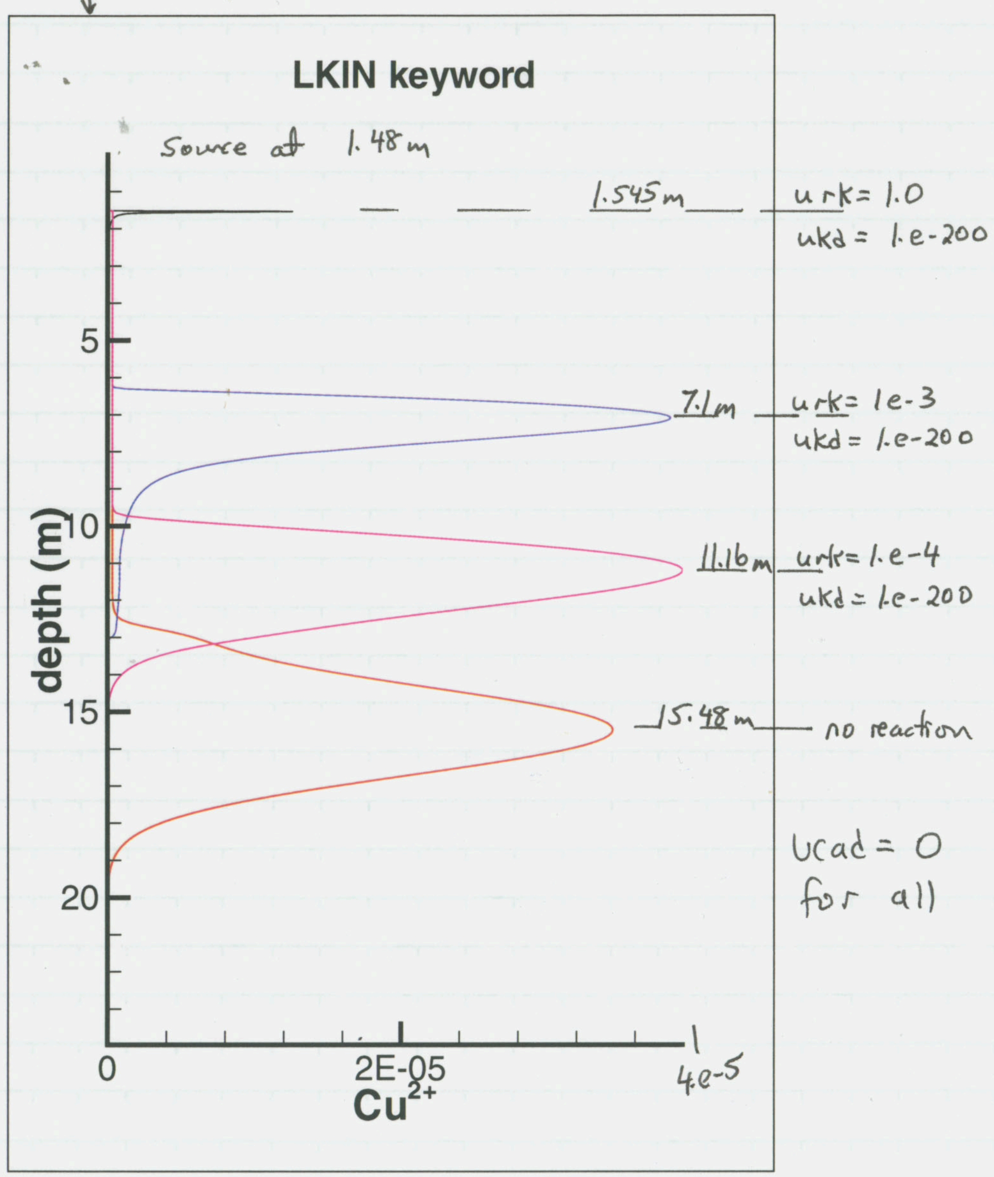
To Page No.

Witnessed & Understood by me, | Date | Invented by | Recorded by DH | Date Aug 20 1999

Project No. 20-1402-561
Book No. 305 TITLE ENFE Akrotiri

From Page No.

↓ V_L = 1 m/yr S = .2 ϕ = .5



Gem only test runs using LKIN keyword for sorption

~dhughson/multiflo/murphy/akrotiri/1D/inputfiles/masin.2

To Page No.

Witnessed & Understood by me,	Date	Invented by / Recorded by	Date
		[signature]	Sep 1 1999

TITLE ENFE-Ambient GeochemYM Project No. 20-1402-561
Book No. 305

From Page No.

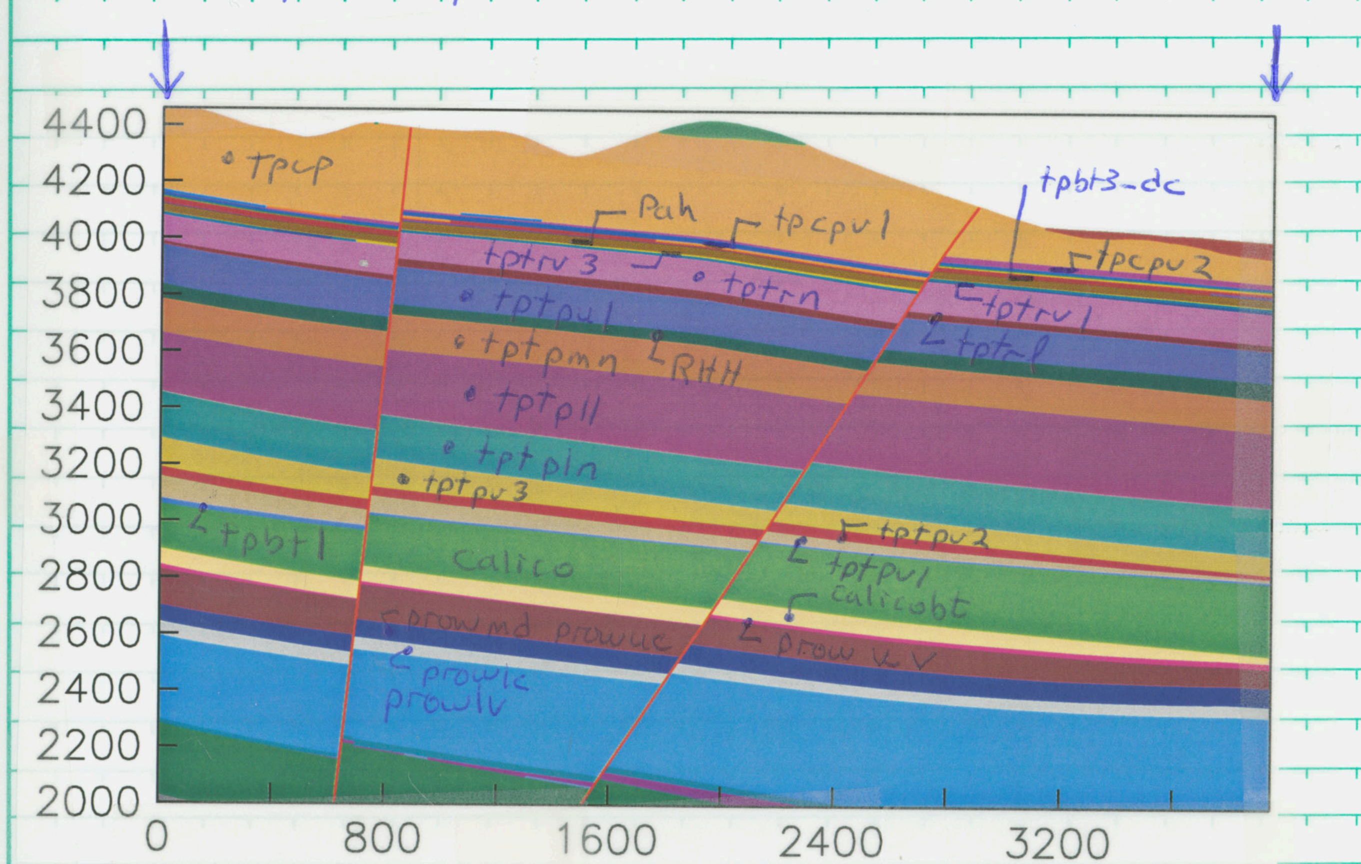
2-D Flow model for Fall 1999 AGU
Ambient Geochem at YM

Cross-section from GEM3_1_HiRes, unsliced, faces in earth vision from SD-7 to UZ-16

SD-7 231328 m N 171066 m E elev 1359 m TD 632m
758949 ft N 561239 ft E
perched water at 480 m depth 880 masl

UZ-16
760535.2 ft N 564857.5 ft E elev 4000.6 ft TD 1521.5 ft

tpbt3 = ptn23 tpcpu = tcw13
tpcpvl = ptn21



tpbt1 = chlvc tptpln = tsw36 tptpmn = tsw34 tptrn = tsw32
tptpv = tsw37 tptpll = tsw35 tptpul = tsw33 tptrv = tsw31

To Page No.

Witnessed & Understood by me,	Date	Invented by / Recorded by	Date
		[signature]	Sept 1 1999

From Page No. ____

Table 3: Stratigraphic Unit Upper Contacts and Unit Thicknesses for the USW SD-7 Drill Hole
[--: not present in this hole, or otherwise not identified]

Lithostratigraphic Unit	Abbreviation	Depth to Upper contact (ft)	Apparent thickness (ft)	Tops from Stratigraphic Compendium (ft)
Tiva Canyon Tuff (Tpc) — 277.9 ft thick†				
Crystal-poor middle nonlithophysal zone	Tpcpmn	50.1†	24.7†	50.2
lower nonlithophysal subzone	Tpcpmn1	50.1†	24.7†	50.2
Crystal-poor lower lithophysal zone	Tpcpll	74.8	120.2	140.0
Crystal-poor lower nonlithophysal zone	Tpcpln	195.0	100.4	195.2
hackly subzone	Tpcplnh	195.0	60.8	--
columnar subzone	Tpcplnc	255.8	39.6	--
Crystal-poor vitric zone ("shardy base")	Tpcpv	295.4	32.6	295.0
moderately welded subzone	Tpcpv2	295.4	21.0	--

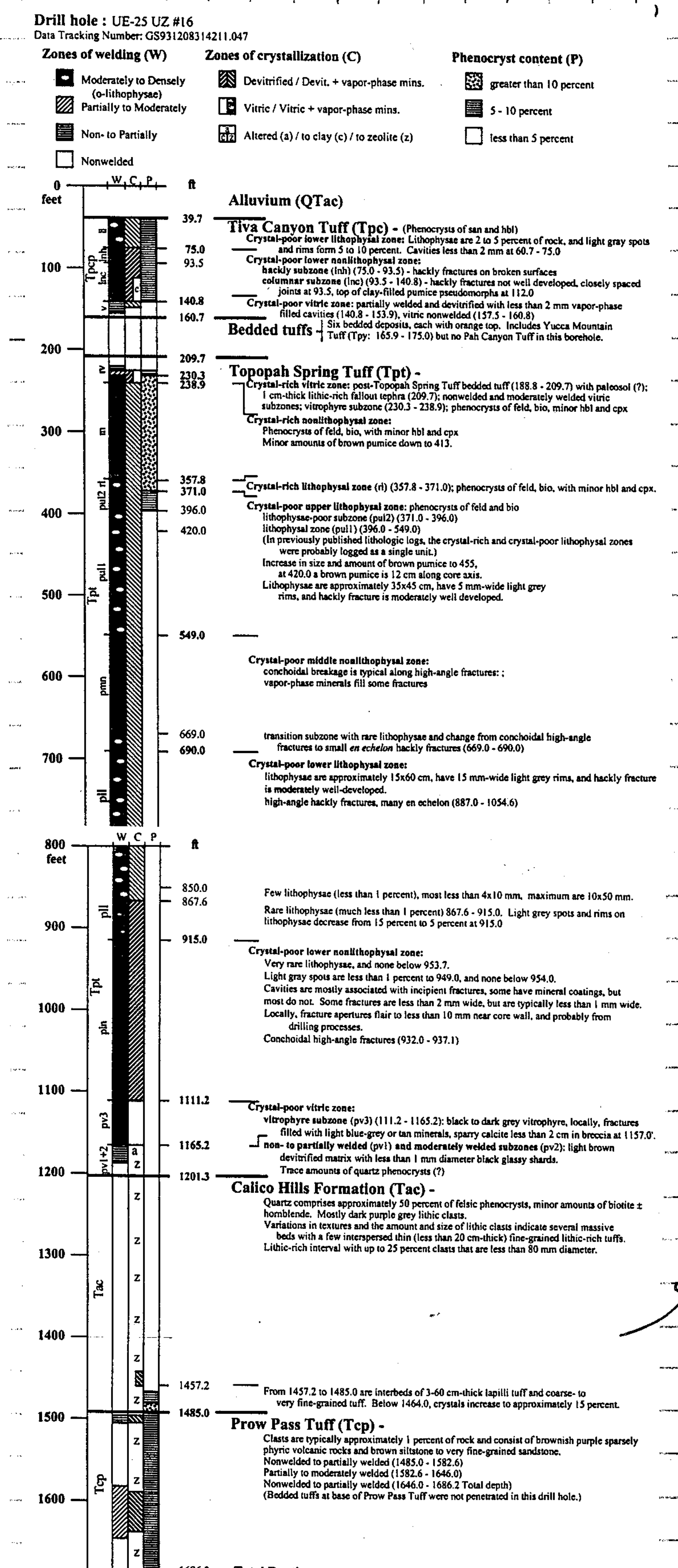
Table 3: Stratigraphic Unit Upper Contacts and Unit Thicknesses for the USW SD-7 Drill Hole (Continued)

Lithostratigraphic Unit	Abbreviation	Depth to Upper contact (ft)	Apparent thickness (ft)	Tops from Stratigraphic Compendium (ft)
nonwelded subzone	Tpcpv1	316.4	11.6	--
Pre-Tiva Canyon Tuff bedded tuff	Tpcbt4	328	2.5	326.0
Yucca Mountain Tuff (Tpy) — not present		--	0.0	
Pre-Yucca Mountain Tuff bedded tuff	Tpbt3	330.5‡	0.0‡	
Pah Canyon Tuff (Tpp) — 14.5 ft thick		345‡	14.5‡	
Pre-Pah Canyon Tuff bedded tuff	Tpbt2	357‡	1.5‡	
Topopah Spring Tuff (Tpt) — 1005.5 ft thick				
Crystal-rich vitric zone	Tptrv	358.5‡	29.8	366.0
nonwelded subzone	Tptrv1	358.5‡	22.5	366.0
moderately welded subzone	Tptrv2	381	6.2	--
densely welded subzone	Tptrv3	387.2	1.1	387.0
Crystal-rich nonlithophysal zone	Tptrn	388.3	99.5	393.0
Crystal-rich lithophysal zone	Tptrl	--	0.0	--
Crystal transition interval	--	473?-487.8	14.8	--
Compositional transition	--	472.2-532.0	59.8	--
Crystal-poor upper lithophysal zone	Tptpul	487.8	194.7	490.0
Crystal-poor middle nonlithophysal zone	Tptpmn	682.5	120.8	640.0
Crystal-poor lower lithophysal zone	Tptpll	803.3	216.7	829.0
Crystal-poor lower nonlithophysal zone	Tptpln	1020.0	171.4	1020.0
Crystal-poor vitric zone	Tptpv	1191.4	172.6	1182.1
densely welded subzone	Tptpv3	1191.4	83.1	1182.1
moderately welded subzone	Tptpv2	1274.5	20.5	1274.6
nonwelded subzone	Tptpv1	1295.0	69.0	--
Pre-Topopah Spring Tuff bedded tuff	Tpbt1	1364‡	41‡	1357.0
Calico Hills Formation (Tac) — 221.2 ft thick				
unit 3	Tac3	1405‡	88.3‡	1381.0
unit 2	Tac2	1493.3	30.5	
unit 1	Tac1	1523.8	43.4	
bedded tuff unit	Tacbt	1567.2	43.1	
basal sandstone unit	Tacbs	1610.3	15.9	
Prow Pass tuff (Tcp) — 554.0 ft				
unit 4	Tcp4	1626.2	28.8	
unit 3	Tcp3	1655.0	182.8	
unit 2	Tcp2	1837.8	40.2	
unit 1	Tcp1	1878.5	289.0	
bedded tuff unit	Tcpbt	2167.5	12.7	
Bullfrog Tuff (Tcb) — 417.8 ft				
unit 4	Tcb4	2180.2	37.8	
unit 3	Tcb3	2218.0††	260.0††	

Table 3: Stratigraphic Unit Upper Contacts and Unit Thicknesses for the USW SD-7 Drill Hole (Continued)

Lithostratigraphic Unit	Abbreviation	Depth to Upper contact (ft)	Apparent thickness (ft)	Tops from Stratigraphic Compendium (ft)
unit 2	Tcb2	2478.0††	3.5††	
unit1	Tcb1	2481.5	97.9	
tuffaceous sandstone unit	Tcbts	2579.4	18.6	
Tram Tuff (Tct) — 77.1 ft†				
upper ash-flow unit		2598.0	77.1†	

† Entire unit not penetrated; partial thickness only.
‡ Extremely poor core recovery in this general interval makes it impossible to determine exact contacts, or in some cases, the presence/absence of units; contacts have been inferred through interpretation of petrophysical logs. See geologic log sheets in Appendix B for interpretation and detailed descriptions of available evidence.
†† Fault contact; partial thickness only.



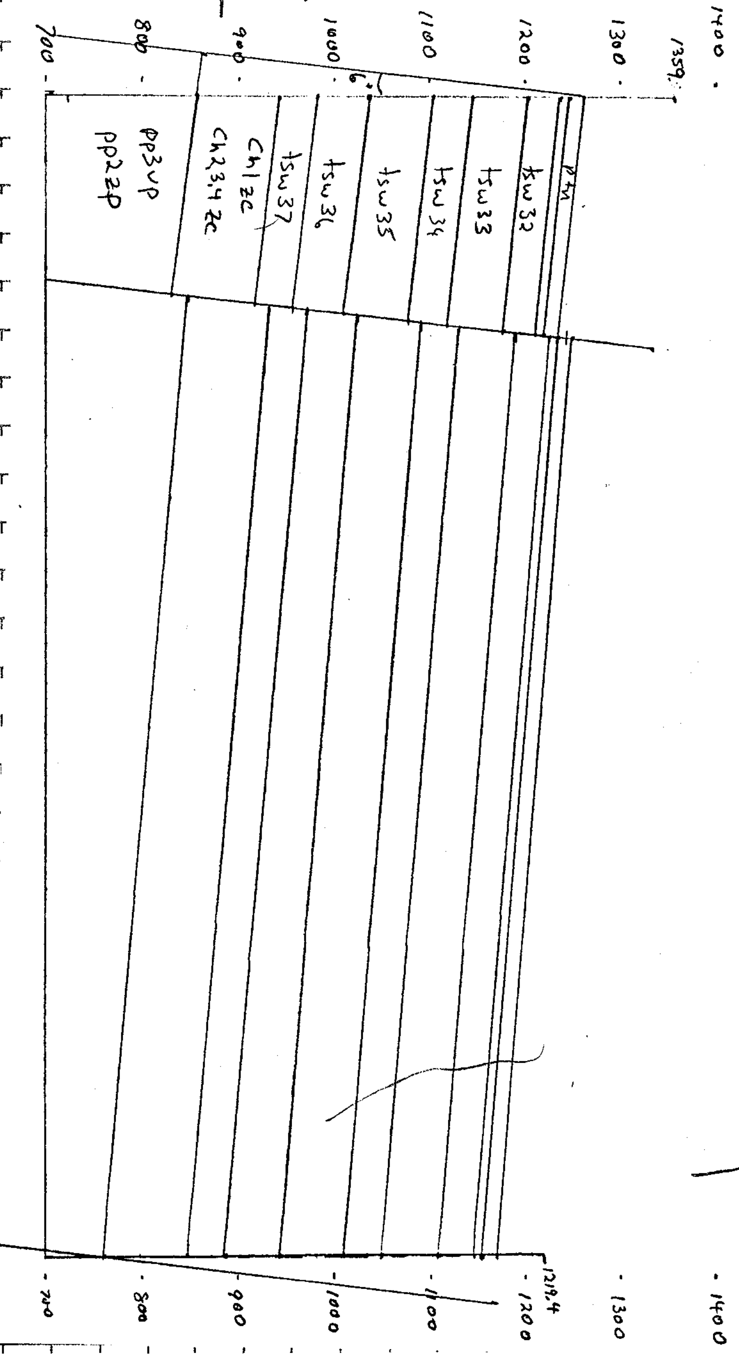
Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by [signature]	Sept 1 1999

From Page No. ____

Rautman, Christopher A. & Dale A. Engstrom, Geology of the USW SD-7 Drill Hole, Yucca Mountain, Nevada, Sandia Report SAND96-1474 UC-814, Sept. 1996 Sandia National Labs, Albuquerque NM

Geslin, Jeffrey K., Thomas C. Moyer & David C. Buesch, Summary of Lithologic Logging of New and Existing Boreholes at Yucca Mountain, Nevada, Aug 1993 to Feb 1994, US Geological Survey Open-File Report 94-342, Denver, CO 1995

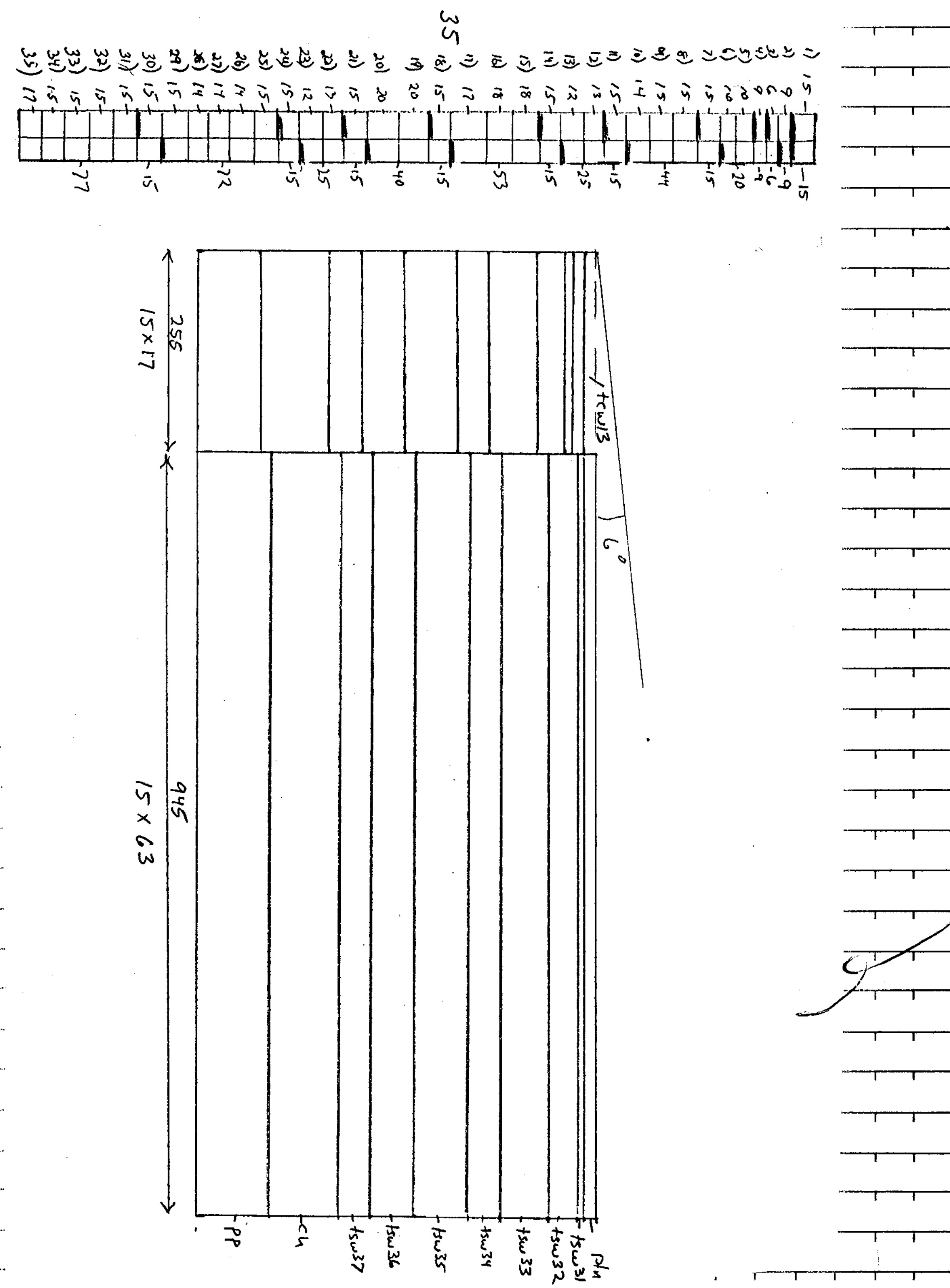
	thickness (m)	
Ptn	15	15
Tsw31	9	24
tsw32	35	59
tsw33	59	118
tsw34	40	158
tsw35	68	226
tsw36	55	281
tsw37	40	321
Ch	87	408
pp3vp, pp2p	172	580



To Page No. ____

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by [signature]	Sept 1 1999

From Page No. ___



To Page No. ___

From Page No. ___

Check on MULTIFLO 1-D simulations using SWMS-3D

Minoan Ash

$K_s = 1.7e\text{-}4 \ \frac{m}{s} = 14.688 \ m/day$ $\qquad K_s = \frac{k\rho g}{\mu}$

$k = \frac{K_s \mu}{\rho g} = \frac{1.7e\text{-}4 \frac{m}{s} \ .01119 \frac{g}{cm\,s} \ \frac{100cm}{m}}{998.3 \frac{kg}{m^3} \ \frac{1000g}{kg} \ 9.8 \frac{m}{s^2}} = 1.944e\text{-}11 \ m^2$

$\alpha = .4904 \ m^{-1} \ \frac{m^3}{998.3 kg} \ \frac{s^2}{9.8 m} = 5.01e\text{-}5 \ Pa^{-1}$ (initials) 8/24/00

$n = 1.4$ ~~$m = 1 - 1/m$~~ ~~$m = \frac{1}{1-n}$~~ $m = 1 - 1/n = .2857$

$S_r = .02$ $\quad \phi = .6$ $\quad \theta_r = S_r \phi = .012$

$K_d = .0027 \ m^3/kg \ \frac{kg}{1000g} = 2.7e\text{-}6 \ \frac{m^3}{g}$

Packed Earth

$K_s = 1.0e\text{-}7 \ m/s = 8.64e\text{-}3 \ m/d$

$k = 1.144e\text{-}14 \ m^2$ $\quad n = 1.13$ $\quad m = 0.115$

$\alpha = 2.7 \ m^{-1} = 2.76e\text{-}4 \ Pa^{-1}$ $\quad S_r = 0.1$ $\quad \phi = .3$ $\quad \theta_r = .03$

$K_d = 0.45 \ m^3/kg = 4.5e\text{-}4 \ m^3/g$

Cape Riva $\quad K_s = 1.5e\text{-}4 \ m/s = 12.96 \ m/d$

$k = 1.716e\text{-}11 \ m^2$ $\quad n = 1.7$ $\quad m = .4118$

$\alpha = .6865 \ m^{-1} = 7.02e\text{-}5 \ Pa^{-1}$ $\quad S_r = .02$ $\quad \phi = .52$ $\quad \theta_r = .0104$

$K_d = .0027 \ m^3/kg = 2.7e\text{-}6 \ m^3/g$

To Page No. ___

Project No. 20-1402-561
Book No. 305 TITLE ENFE Akrotiri

From Page No.

EQ 3/6 Run Cu^{2+} in Equilibrium with Atacamite = 4.67e-5 moles/kg

1-D MULTIFLO RUN TO 30 years 15 cm/yr recharge
no sorption

In the source term blocks Cu^{2+} = 4.829e-5 moles/Kg

$\frac{C}{C_0} = 0.5$ Front at z = 17.1 m
Transport distance 17.1 - 1.48 = 15.62 m

Here's error in Sl causing bad results DH Sept 21 '99

1-D SWMS-3D Run to 30 years 15 cm/yr recharge
no sorption

Source term B.C. 4.67e-5 mole/Kg ~~Kg/1000g~~ ~~998.3kg/m^3~~ ~~1000g/Kg~~ ~~63.546g/mole~~

= 2.96 g/m^3

ECP 8/24/00 I HAVE NOW increased the quality of this record. ECP 8/24/00

$Cu_2Cl(OH)_3$ Atacamite

2(63.546)
35.453
3(15.9994)
3(1.0079)
213.55 g/mole

Murphy $\left(\frac{15cm}{yr}\right)(m^2)\left(\frac{100cm}{m}\right)^2 \frac{1e\text{-}5\ mole}{L} \frac{L}{1000cm^3}$ 3600y

= 5.4 mole Cu = 576.6g Atacamite per sq meter

$\left(\frac{15cm}{yr}\right)(1m^2)\left(\frac{100cm}{m}\right)^2 \left(\frac{.9983g}{cm^3}\right)\left(\frac{Kg}{1000g}\right)\left(\frac{4.67e\text{-}5\ mole}{Kg}\right)$ 3570 yr

= 25 mole Cu = 2669 g Atacamite per sq meter

Source Footprint 4(.2m)(.2m) = .16 m^2 = 427g Atacamite

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Sept 22 1999

Project No. 20-1402-561
TITLE ENFE Akrotiri Book No. 305

From Page No.

Final Vol. Fraction from multiflo at 3600 y

0.002 block vol m^3 — 56.8 cm^3/mole — 213.545 g/mole

Initial Volume fraction of atacamite / Initial mass in place

0.1	0.1	0.1	0.1	751.919	751.919	751.919	751.919
0.1	0.1	0.1	0.1	751.919	751.919	751.919	751.919
0.1	0.1	0.1	0.1	751.919	751.919	751.919	751.919
0.1	0.1	0.1	0.1	751.919	751.919	751.919	751.919
0.1	0.1	0.1	0.1	751.919	751.919	751.919	751.919
0.1	0.1	0.1	0.1	751.919	751.919	751.919	751.919

Final volume fraction 1.5 cm/yr infiltration / final mass in place

0.09888	0.09956	0.099561	0.099518	743.4975	748.6106	748.6181	748.2948
0.099374	0.1	0.1	0.099996	747.212	751.919	751.919	751.8889
0.099375	0.1	0.1	0.099998	747.2195	751.919	751.919	751.904
0.099375	0.1	0.1	0.099999	747.2195	751.919	751.919	751.9115
0.099377	0.1	0.1	0.1	747.2346	751.919	751.919	751.919
0.099334	0.099982	0.09989	0.099993	746.9112	751.7837	751.0919	751.8664

Final volume fraction 15 cm/yr infiltration / final mass in place

0.091857	0.096945	0.096631	0.096049	690.6902	728.9479	726.5869	722.2107
0.094748	0.1	0.1	0.099994	712.4282	751.919	751.919	751.8739
0.094721	0.1	0.1	0.099998	712.2252	751.919	751.919	751.904
0.094693	0.1	0.1	0.099999	712.0147	751.919	751.919	751.9115
0.094666	0.1	0.1	0.1	711.8117	751.919	751.919	751.919
0.094529	0.099925	0.099949	0.099964	710.7815	751.3551	751.5355	751.6483

mass loss 43.52107

8.421493	3.308444	3.300924	3.62425
4.707013	0	0	0.030077
4.699494	0	0	0.015038
4.699494	0	0	0.007519
4.684455	0	0	0
5.007781	0.135345	0.827111	0.052634

mass loss 340.8599

61.22877	22.97113	25.33215	29.70832
39.49079	0	0	0.045115
39.6938	0	0	0.015038
39.90434	0	0	0.007519
40.10736	0	0	0
41.13749	0.563939	0.383479	0.270691

7.832066

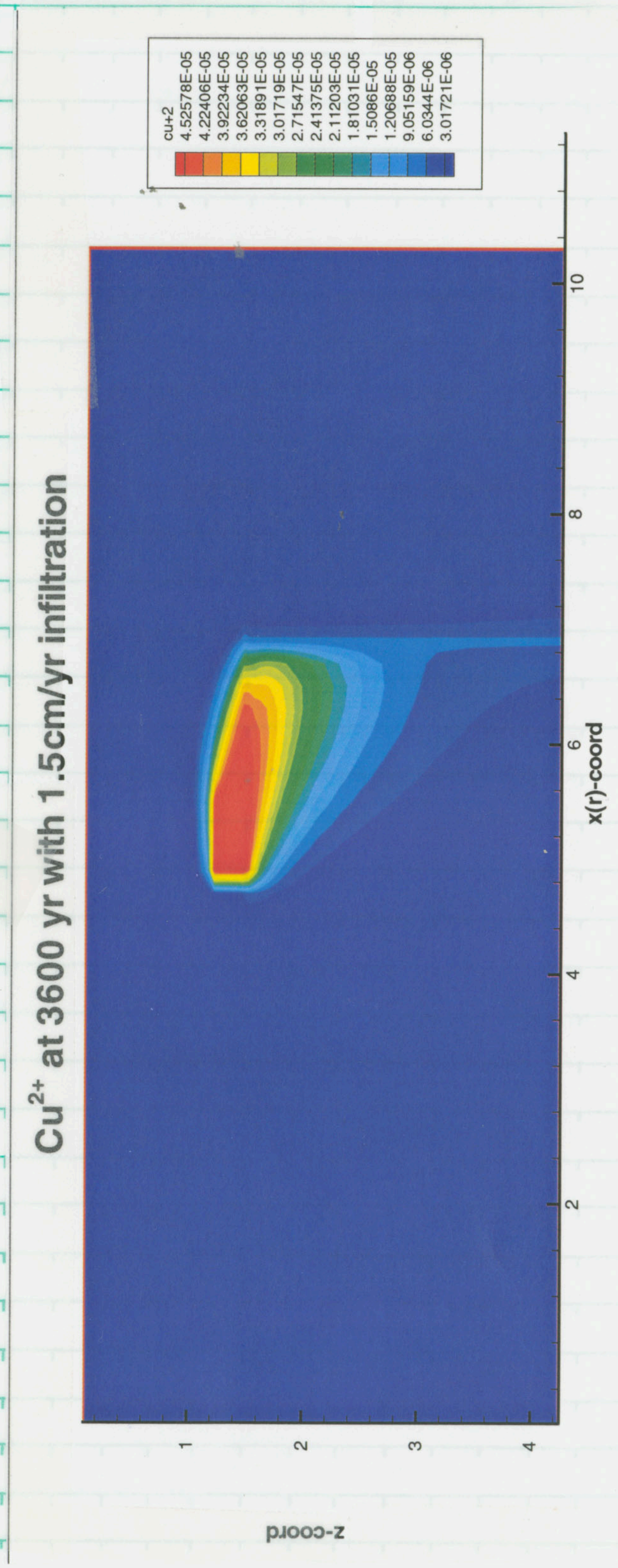
DH

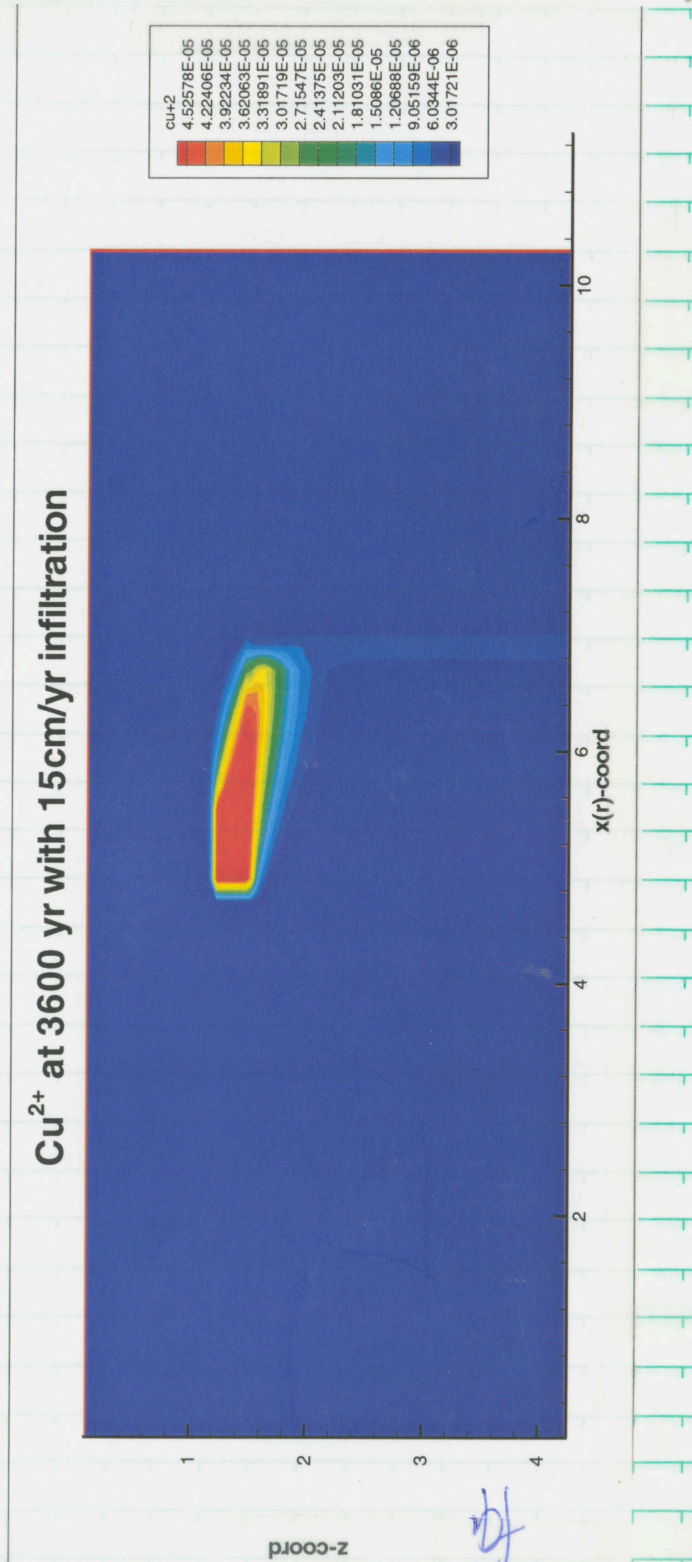
To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Sept 23 1999

Project No. 20-1402-561
Book No. 305 TITLE ENF E Akrotiri

From Page No.



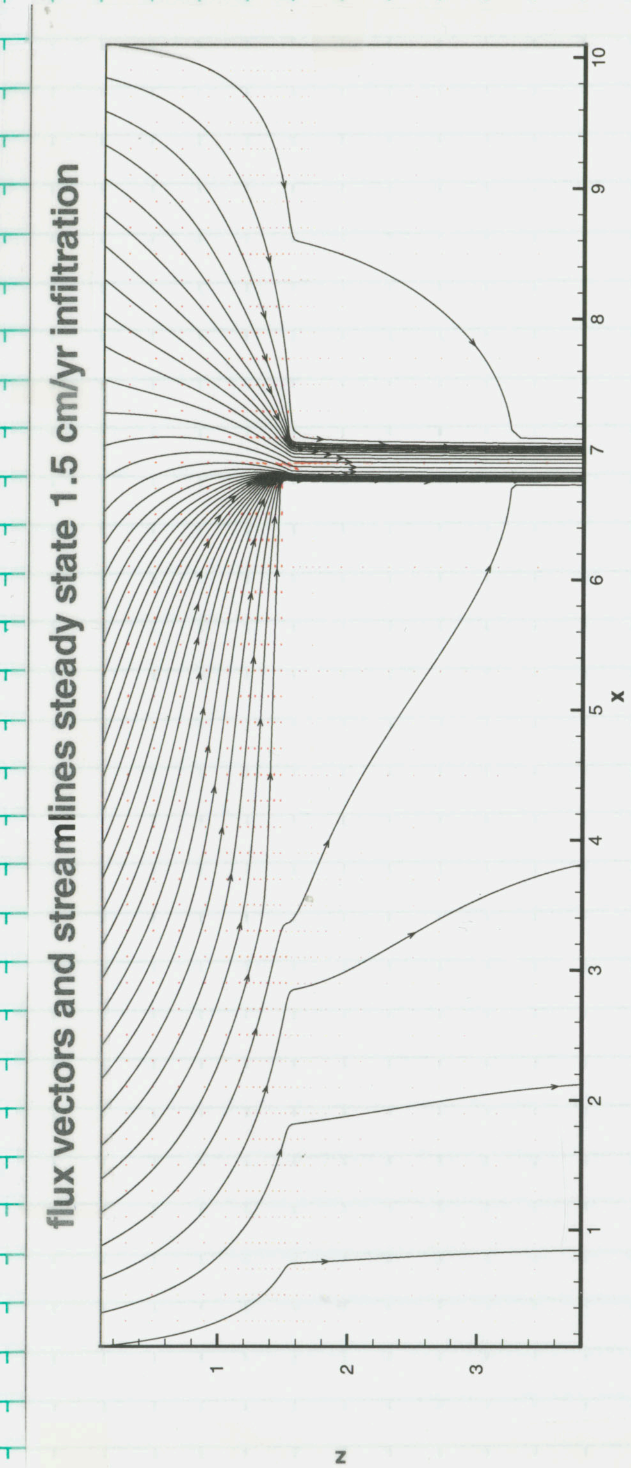


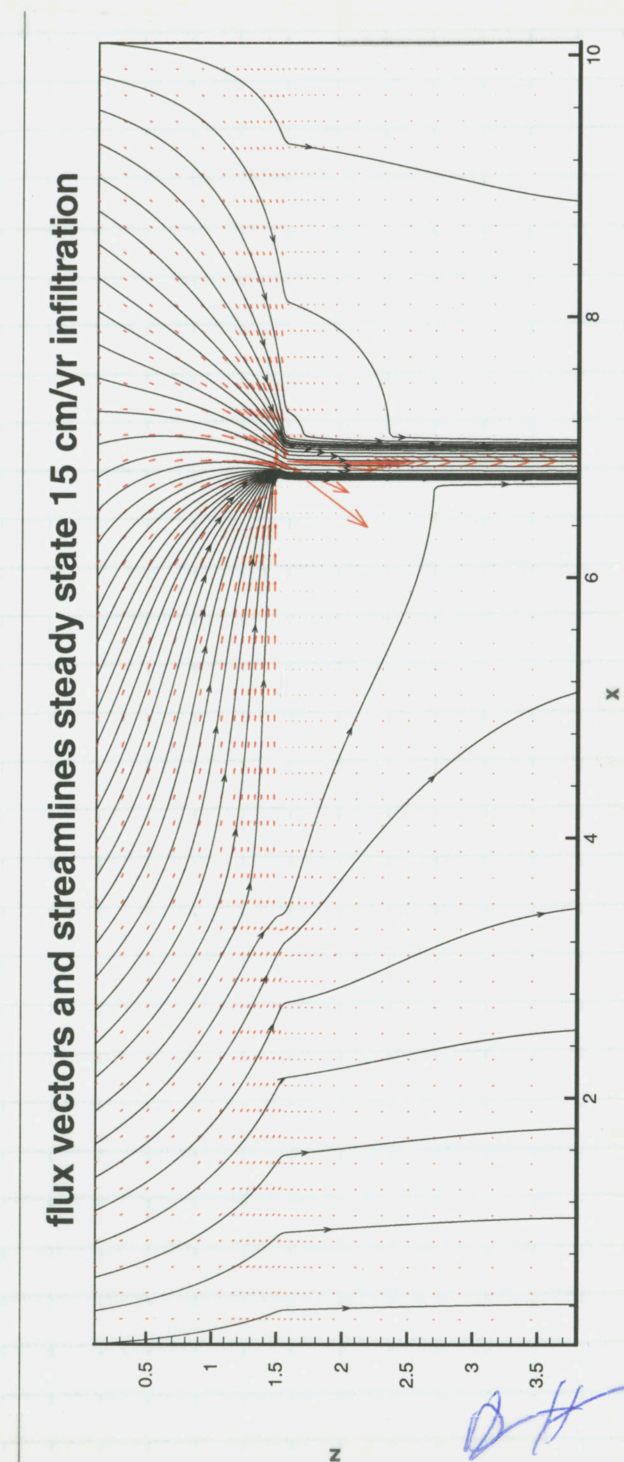
To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Sept 22 1999

TITLE ENFE Akrotiri
Project No. 20-1402-561
Book No. 305

From Page No.





To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Sept 23 1999

Information potentially subject to copyright protection was redacted from this section. The redacted material, pages 60 through 74 of this scientific notebook is from the following reference:

Hughson, D.L., L. Browning, W.M. Murphy, and R. Green. "An Archeological Site at Akrotiri, Greece, as a Natural Analog for Radionuclide Transport: Implications for Validity of Performance Assessments." Proceedings of the Scientific Basis for Nuclear Waste Management XXIII. D. Shoesmith and R. Smith, eds. Materials Research Society. 1999.

Project No. 20-1402-871
Book No. 305 TITLE RT

From Page No. ___

To Page No. ___

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Jan 6 2000

TITLE RT
Project No. 20-1402-871
Book No. 305

From Page No. ___

Following pages are some odds & ends of graphs & diagrams that I used but did not paste into this notebook in sequence

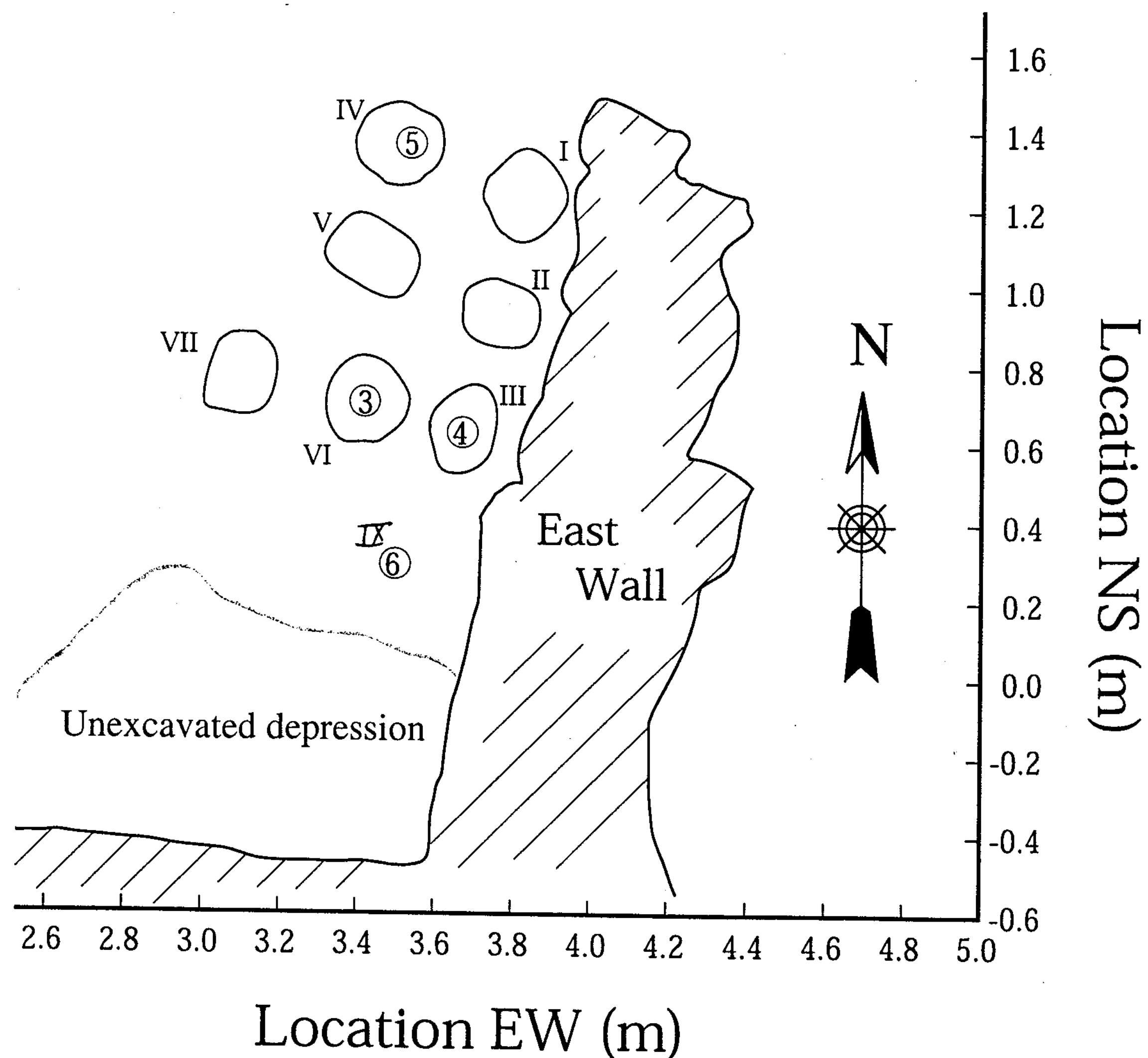
To Page No. ___

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Jan 6 2000

Project No. 20-1402-871

Book No. 305 TITLE RT

From Page No.



Jun 6 2000

Sample Hole Locations

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	Jun 6 2000

Project No. 1402-871

TITLE RT Book No. 308

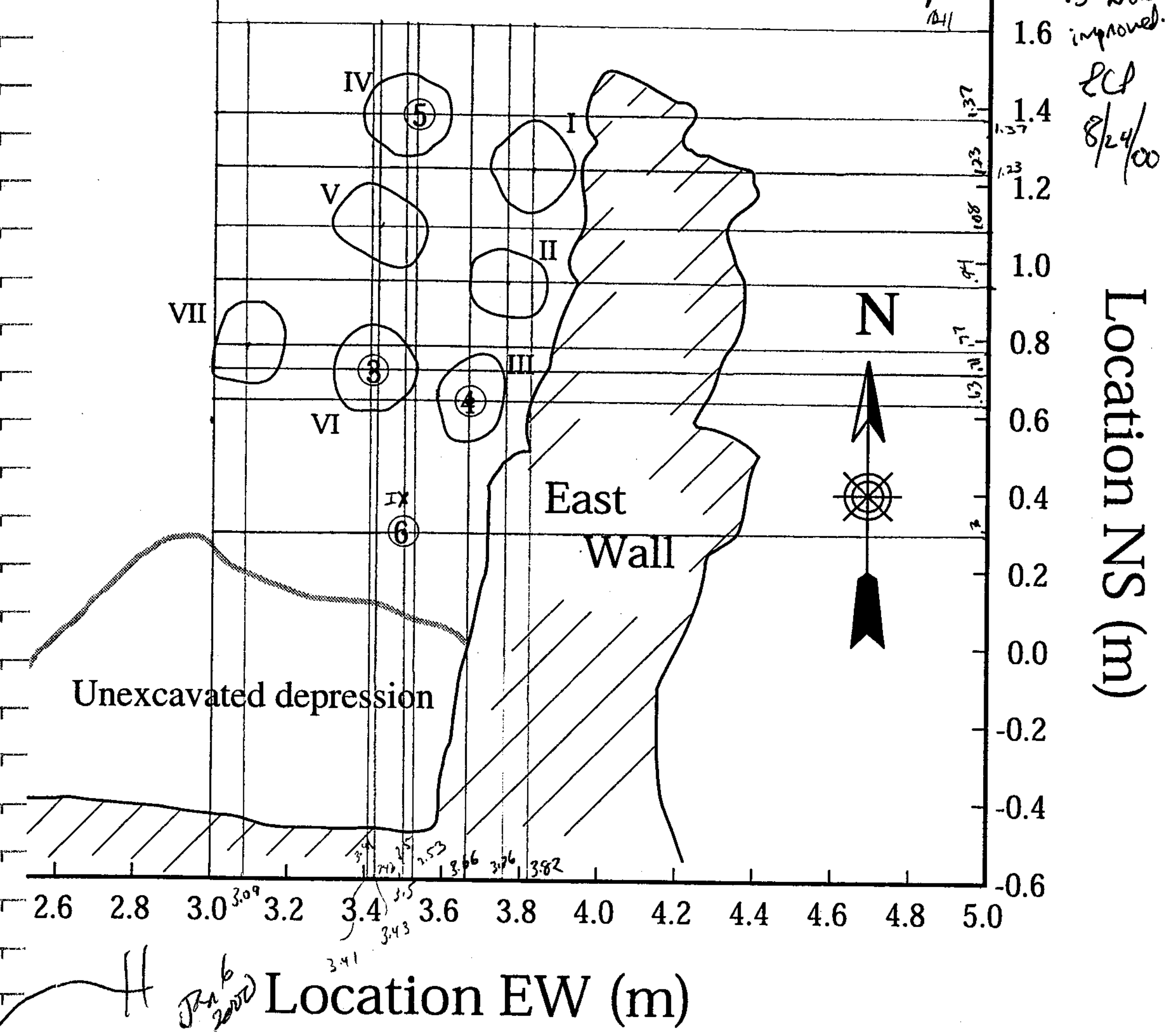
From Page No.

HOLE	X	Y	m Zelev topo	cm Δ packed earth		ref
I	3.82	1.23	22.55	4.5	22.51	18.65
II	3.76	0.94	22.52	6.0	22.46	16.52
III	3.66	0.63	22.49	2.0	22.47	20.49
IV	3.53	1.37	22.59	3.5	22.56	19.09
V	3.43	1.08	22.54	2.0	22.52	20.54
VI	3.41	0.71	22.50	0	22.5	22.50
VII	3.09	0.77	22.50	0	22.5	22.50
IX	3.5	0.3	22.47	3.0	22.44	19.47

ECP 8/24/00

The quality of this page is now improved.

ECP 8/24/00



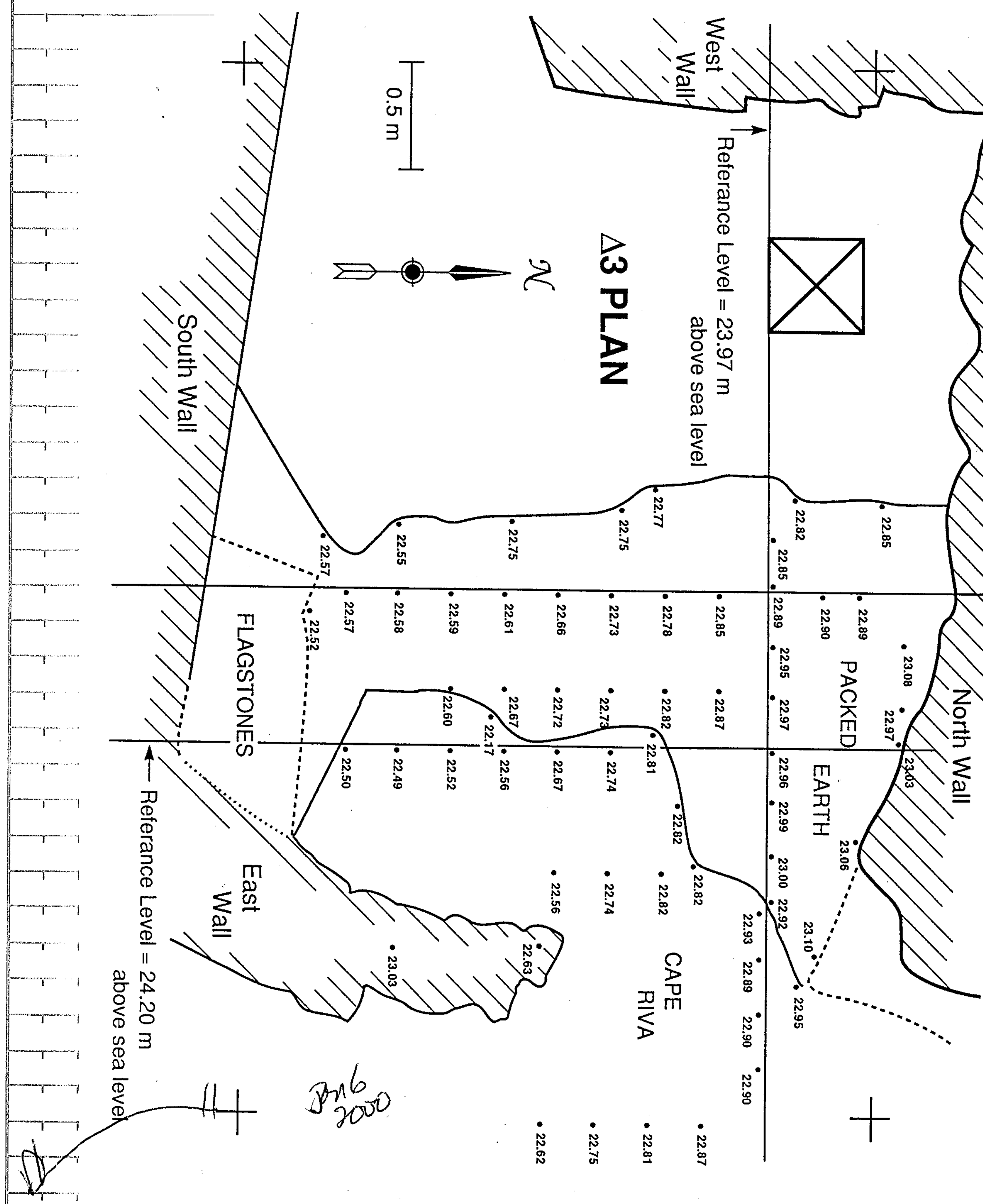
Jun 6 2000

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by Jun 6 2000	

Project No. 1402-871
Book No. 305 TITLE RT

From Page No.



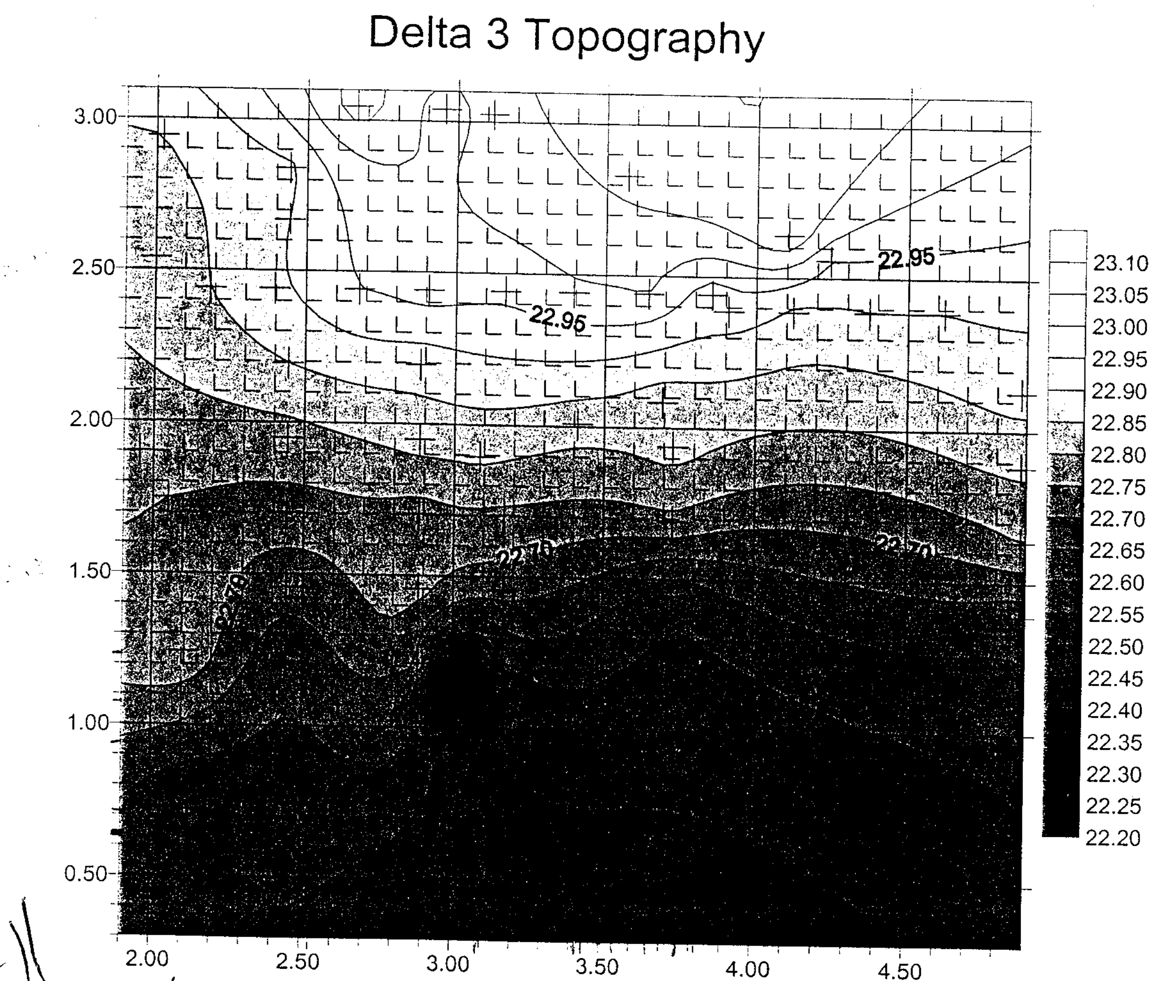
Jan 6 2000

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Jan 6 2000

TITLE RT Project No. 1402-871
Book No. 305

From Page No.



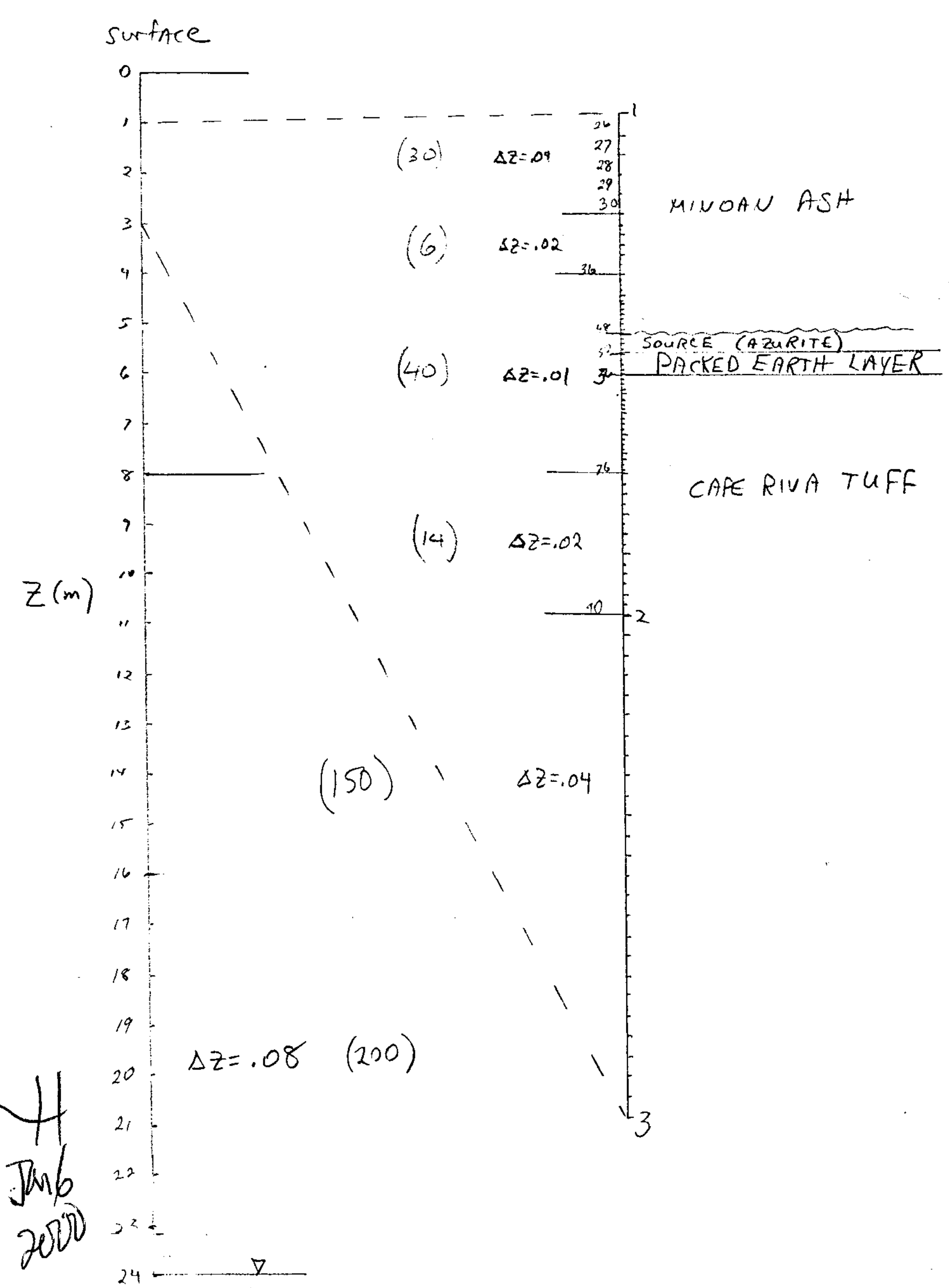
Jan 6 2000

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH Jan 6 2000	

Project No. 1402-871
Book No. 305 TITLE RT

From Page No.



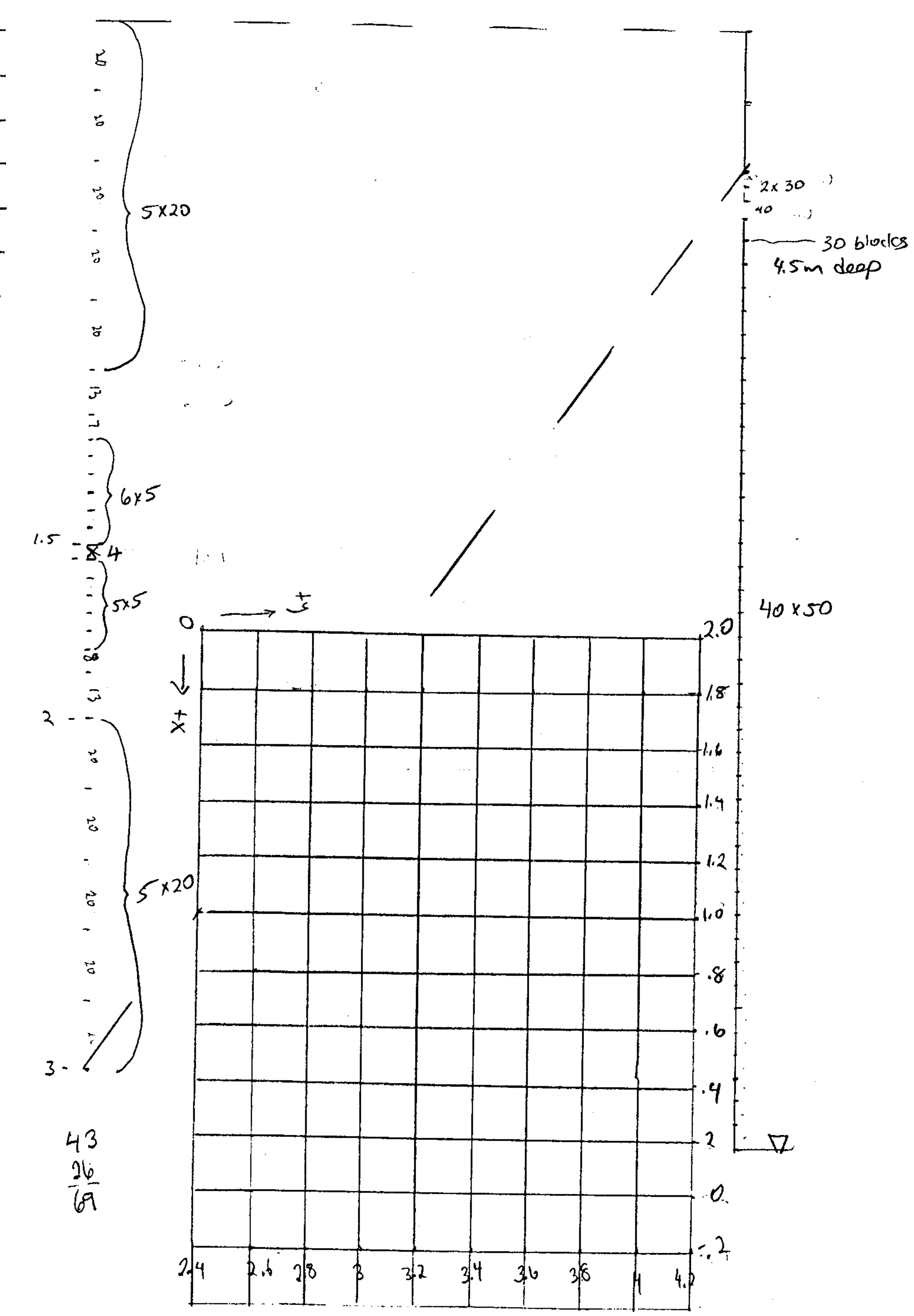
1-D Grid

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Jan 6 2000

Project No. 1402-871
TITLE RT Book No. 305

From Page No.



To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Jan 6 1999

Project No. 1402-871
Book No. 305 TITLE RT

From Page No.

DH — # Jan 6 2000

Debra.3o

--- Distribution of Aqueous Species ---

Species	Molality	Log molality	Log gamma	Log activity
Na+	9.9494E-03	-2.0022	-0.0487	-2.0509
Cl-	7.7363E-03	-2.1115	-0.0465	-2.1580
HCO3-	1.7033E-03	-2.7687	-0.0450	-2.8138
SO4--	4.7220E-04	-3.3259	-0.1852	-3.5111
O2(aq)	2.5149E-04	-3.5995	0.0012	-3.5983
SiO2(aq)	1.0016E-04	-3.9993	0.0000	-3.9993
K+	9.9750E-05	-4.0011	-0.0502	-4.0513
Ca++	9.5246E-05	-4.0212	-0.1816	-4.2028
Mg++	9.3063E-05	-4.0312	-0.1719	-4.2032
CO2(aq)	3.3879E-05	-4.4701	0.0012	-4.4689
NaSO4-	2.0095E-05	-4.6969	-0.0450	-4.7420
NaHCO3(aq)	1.9474E-05	-4.7106	0.0000	-4.7106
CO3--	1.0890E-05	-4.9630	-0.1796	-5.1426
NaCl(aq)	1.0330E-05	-4.9859	0.0000	-4.9859
MgSO4(aq)	4.9827E-06	-5.3025	0.0000	-5.3025
CaSO4(aq)	2.4961E-06	-5.6027	0.0000	-5.6027
HSiO3-	1.2390E-06	-5.9069	-0.0450	-5.9520
CaHCO3+	1.1991E-06	-5.9211	-0.0487	-5.9698
MgHCO3+	1.1681E-06	-5.9325	-0.0487	-5.9812
OH-	1.1253E-06	-5.9487	-0.0465	-5.9953
CaCO3(aq)	9.5888E-07	-6.0182	0.0000	-6.0182
NaHSiO3(aq)	4.4223E-07	-6.3544	0.0000	-6.3544
MgCO3(aq)	4.2971E-07	-6.3668	0.0000	-6.3668
MgCl+	3.5696E-07	-6.4474	-0.0487	-6.4961
NaCO3-	2.3227E-07	-6.6340	-0.0450	-6.6791
KSO4-	2.3031E-07	-6.6377	-0.0450	-6.6827
CaCl+	9.8246E-08	-7.0077	-0.0487	-7.0564
KCl(aq)	1.9776E-08	-7.7039	0.0000	-7.7039
H+	1.1027E-08	-7.9576	-0.0424	-8.0000
NaOH(aq)	1.4261E-09	-8.8459	0.0000	-8.8459
CaOH+	9.9028E-10	-9.0042	-0.0487	-9.0529
CaCl2(aq)	6.8806E-10	-9.1624	0.0000	-9.1624
HSO4-	3.2590E-10	-9.4869	-0.0450	-9.5320
KOH(aq)	3.0802E-11	-10.5114	0.0000	-10.5114
H2SiO4--	1.6810E-11	-10.7744	-0.1852	-10.9596
HCl(aq)	1.4859E-11	-10.8280	0.0000	-10.8280
H6(H2SiO4)4--	3.5216E-14	-13.4533	-0.1852	-13.6384
KHSO4(aq)	1.7835E-15	-14.7487	0.0000	-14.7487
ClO-	9.6927E-20	-19.0136	-0.0450	-19.0586
H4(H2SiO4)4----	6.4707E-20	-19.1890	-0.7494	-19.9384
HClO(aq)	3.2404E-20	-19.4894	0.0000	-19.4894
CuCl2-	7.2636E-21	-20.1388	-0.0450	-20.1839
H2SO4(aq)	2.9379E-21	-20.5320	0.0000	-20.5320
Cu+	2.2887E-21	-20.6404	-0.0487	-20.6891
CuCl3--	4.4771E-22	-21.3490	-0.1852	-21.5342
HO2-	8.7859E-23	-22.0562	-0.0450	-22.1013
Mg4(OH)4++++	1.4711E-24	-23.8324	-0.7310	-24.5633
ClO3-	1.6933E-25	-24.7713	-0.0450	-24.8163
ClO4-	9.6124E-26	-25.0172	-0.0465	-25.0637
ClO2-	1.5162E-29	-28.8193	-0.0450	-28.8643
HSO5-	2.8072E-31	-30.5517	-0.0450	-30.5968
HClO2(aq)	2.0207E-34	-33.6945	0.0000	-33.6945
Formate	1.6788E-44	-43.7750	-0.0450	-43.8201
H2(aq)	4.9110E-45	-44.3088	0.0012	-44.3077
S2O8--	7.3134E-48	-47.1359	-0.1852	-47.3211
Formic acid(aq)	8.5693E-49	-48.0671	0.0000	-48.0671
SO3--	7.0619E-49	-48.1511	-0.1852	-48.3363

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Jan 6 2000

TITLE RT Project No. 1402-871
Book No. 305

From Page No.

DH # Jan 6 2000

HSO3-	8.2069E-50	-49.0858	-0.0450	-49.1309
CO(aq)	1.9289E-51	-50.7147	0.0000	-50.7147
H2SO3(aq)	7.5325E-56	-55.1231	0.0000	-55.1231
SO2(aq)	5.3641E-56	-55.2705	0.0000	-55.2705
S2O6--	3.4867E-73	-72.4576	-0.1852	-72.6428
Formaldehyde(aq)	1.6297E-94	-93.7879	0.0000	-93.7879
S2O5--	1.2768-103	-102.8939	-0.1852	-103.0791
Methanol(aq)	4.7741-124	-123.3211	0.0000	-123.3211
S2O4--	1.2715-136	-135.8957	-0.1852	-136.0809
HS-	2.6012-143	-142.5848	-0.0465	-142.6314
H2S(aq)	2.2716-144	-143.6437	0.0000	-143.6437
S--	4.1564-148	-147.3813	-0.1852	-147.5665
Methane(aq)	1.7440-148	-147.7585	0.0000	-147.7585
S2O3--	6.6133-150	-149.1796	-0.1852	-149.3648
Acetate	7.3237-154	-153.1353	-0.0450	-153.1803
NaCH3COO(aq)	4.6280-156	-155.3346	0.0000	-155.3346
MgCH3COO+	8.7965-157	-156.0557	-0.0487	-156.1044
HS2O3-	4.9462-157	-156.3057	-0.0450	-156.3508
CaCH3COO+	3.9491-157	-156.4035	-0.0487	-156.4522
Acetic acid(aq)	3.7748-157	-156.4231	0.0000	-156.4231
KCH3COO(aq)	3.1954-158	-157.4955	0.0000	-157.4955
CuCH3COO(aq)	2.8866-174	-173.5396	0.0000	-173.5396
S3O6--	5.5477-182	-181.2559	-0.1852	-181.4411
Acetaldehyde(aq)	1.0020-201	-200.9991	0.0000	-200.9991
Ethyne(aq)	9.6393-223	-222.0160	0.0000	-222.0160
Ethanol(aq)	1.0610-235	-234.9743	0.0000	-234.9743
Ethylene(aq)	3.6324-240	-239.4398	0.0000	-239.4398
S2--	2.4588-254	-253.6093	-0.1852	-253.7945
Ethane(aq)	2.9042-264	-263.5370	0.0000	-263.5370
Propanoate	1.4920-267	-266.8262	-0.0450	-266.8713
Propanoic acid(aq)	1.0246-270	-269.9895	0.0000	-269.9895
S4O6--	7.1122-275	-274.1480	-0.1852	-274.3332
Ca(CH3COO)2(aq)	3.7119-309	-308.4304	0.0000	-308.4304
Mg(CH3COO)2(aq)	3.0033-309	-308.5224	0.0000	-308.5224
Na(CH3COO)2-	1.4094-309	-308.8510	-0.0450	-308.8960
Acetone(aq)	1.2489-310	-309.9035	0.0000	-309.9035
K(CH3COO)2-	7.1805-312	-311.1438	-0.0450	-311.1889
Propanal(aq)	0.0000E+00	-314.1329	0.0000	-314.1329
Cu(CH3COO)2-	0.0000E+00	-326.7042	-0.0450	-326.7492
1-Propyne(aq)	0.0000E+00	-331.6680	0.0000	-331.6680
1-Propanol(aq)	0.0000E+00	-348.6065	0.0000	-348.6065
1-Propene(aq)	0.0000E+00	-350.9024	0.0000	-350.9024
S3--	0.0000E+00	-359.9154	-0.1852	-360.1006
Propane(aq)	0.0000E+00	-377.5380	0.0000	-377.5380
Butanoate	0.0000E+00	-381.0009	-0.0450	-381.0459
Butanoic acid(aq)	0.0000E+00	-384.2227	0.0000	-384.2227
Ethylacetate(aq)	0.0000E+00	-392.9382	0.0000	-392.9382
S5O6--	0.0000E+00	-395.9206	-0.1852	-396.1058
2-Butanone(aq)	0.0000E+00	-423.7923	0.0000	-423.7923
Butanal(aq)	0.0000E+00	-429.6637	0.0000	-429.6637
1-Butyne(aq)	0.0000E+00	-445.8355	0.0000	-445.8355
1-Butanol(aq)	0.0000E+00	-463.4483	0.0000	-463.4483
1-Butene(aq)	0.0000E+00	-465.2530	0.0000	-465.2530
S4--	0.0000E+00	-466.4415	-0.1852	-466.6267
n-Butane(aq)	0.0000E+00	-491.5946	0.0000	-491.5946
Pentanoate	0.0000E+00	-495.0657	-0.0450	-495.1108
Pentanoic acid(aq)	0.0000E+00	-498.2656	0.0000	-498.2656
2-Pentanone(aq)	0.0000E+00	-538.0989	0.0000	-538.0989
Phenol(aq)	0.0000E+00	-543.0657	0.0000	-543.0657
Pentanal(aq)	0.0000E+00	-543.5012	0.0000	-543.5012
1-Pentyne(aq)	0.0000E+00	-559.9881	0.0000	-559.9881
S5--	0.0000E+00	-573.1874	-0.1852	-573.3726
Benzene(aq)	0.0000E+00	-575.3968	0.0000	-575.3968
1-Pentanol(aq)	0.0000E+00	-576.3109	0.0000	-576.3109

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DH	Jan 6 2000

From Page No. ____

VD Jan 6 2000

1-Pentene(aq)	0.0000E+00	-579.4277	0.0000	-579.4277
o-Phthalate	0.0000E+00	-586.1704	-0.1852	-586.3556
Na(o-Phthalate)-	0.0000E+00	-587.6614	-0.0450	-587.7065
Ca(o-Phthalate)(aq)	0.0000E+00	-588.1383	0.0000	-588.1383
H(o-Phthalate)-	0.0000E+00	-588.9025	-0.0450	-588.9476
o-Phthalic acid(aq)	0.0000E+00	-593.9976	0.0000	-593.9976
n-Pentane(aq)	0.0000E+00	-605.7210	0.0000	-605.7210
Hexanoate	0.0000E+00	-609.2330	-0.0450	-609.2780
Hexanoic acid(aq)	0.0000E+00	-612.4182	0.0000	-612.4182
2-Hexanone(aq)	0.0000E+00	-652.0904	0.0000	-652.0904
Hexanal(aq)	0.0000E+00	-657.6832	0.0000	-657.6832
1-Hexyne(aq)	0.0000E+00	-674.2362	0.0000	-674.2362
Toluene(aq)	0.0000E+00	-686.7127	0.0000	-686.7127
1-Hexanol(aq)	0.0000E+00	-691.0867	0.0000	-691.0867
1-Hexene(aq)	0.0000E+00	-693.4118	0.0000	-693.4118
n-Hexane(aq)	0.0000E+00	-719.9909	0.0000	-719.9909
Heptanoate	0.0000E+00	-723.3344	-0.0450	-723.3795
Heptanoic acid(aq)	0.0000E+00	-726.4244	0.0000	-726.4244
2-Heptanone(aq)	0.0000E+00	-766.1845	0.0000	-766.1845
Heptanal(aq)	0.0000E+00	-772.7375	0.0000	-772.7375
1-Heptyne(aq)	0.0000E+00	-788.5208	0.0000	-788.5208
Ethylbenzene(aq)	0.0000E+00	-800.9021	0.0000	-800.9021
1-Heptanol(aq)	0.0000E+00	-806.2362	0.0000	-806.2362
1-Heptene(aq)	0.0000E+00	-807.5279	0.0000	-807.5279
n-Heptane(aq)	0.0000E+00	-834.0850	0.0000	-834.0850
Octanoate	0.0000E+00	-837.4285	-0.0450	-837.4735
Octanoic acid(aq)	0.0000E+00	-840.2985	0.0000	-840.2985
2-Octanone(aq)	0.0000E+00	-880.2785	0.0000	-880.2785
Octanal(aq)	0.0000E+00	-886.1939	0.0000	-886.1939
1-Octyne(aq)	0.0000E+00	-902.6736	0.0000	-902.6736
n-Propylbenzene(aq)	0.0000E+00	-914.7616	0.0000	-914.7616
1-Octanol(aq)	0.0000E+00	-920.1104	0.0000	-920.1104
1-Octene(aq)	0.0000E+00	-921.7832	0.0000	-921.7832
n-Octane(aq)	0.0000E+00	-948.2230	0.0000	-948.2230

```
****************************************************************************
|-----------------------------------------------------------------|
|Version level= 7.2  (xcon3)                                      |
|EQ3NR input file name= Debra.3i                                  |
|                                                                 |
|Akrotiri Water Composition                                       |
|Computations by Lauren Browning 6-29-99                          |
|                                                                 |
|-----------------------------------------------------------------|
|Temperature (C)          | 25.00        |Density(gm/cm3)|  1.00000 |
|-----------------------------------------------------------------|
|Total Dissolved Salts    |              | mg/kg | mg/l  |*not used |
|-----------------------------------------------------------------------|
|Electrical Balancing on |Cl-                   | code selects | not performed|
|-----------------------------------------------------------------------|
| SPECIES                | BASIS SWITCH/CONSTRAINT| CONC/ETC  | UNITS OR TYPE |
|-----------------------------------------------------------------------|
|redox                   |                      |-.7        |Logfo2         |
|H+                      |                      |8.0        |pH             |
|Ca++                    |                      |1e-4       |molality       |
|Mg++                    |                      |1e-4       |molality       |
|Na+                     |                      |0.01       |molality       |
|SiO2(aq)                |Quartz                |           |mineral        |
|HCO3-                   |CO2(g)                |-3         |log fugacity   |
|Cl-                     |                      |1e-2       |molality       |
|K+                      |                      |1e-4       |molality       |
|SO4--                   |                      |5e-4       |molality       |
|Cu+                     |                      |1e-20      |molality       |
|-----------------------------------------------------------------------|
```

To Page No. ____

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by DJ	Jan 6 2000

From Page No. ____

To Page No. ____

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	

From Page No.

DJ Jan 6 2000

Step # 40 Xi = 0.4000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 6.077 log fO2 = -0.800
Eh = 0.8577 volts pe = 14.4995
Ionic strength = 0.009563
Activity of water = 0.999687
Solvent mass = 1.000039 kg
Solution mass = 1.000672 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.008968 molal
Dissolved solids = 633 mg/kg sol'n

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
Atacamite	3.000	2.000	854.3	113.6

Minerals in system	moles	log moles	grams	volume (cm3)
Atacamite	1.999	0.301	854.0	113.6
Malachite	0.0001840	-3.735	0.04068	0.01009
Tenorite	0.001985	-2.702	0.1579	0.02426
(total)			854.2	113.6

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Na+	0.009419	216.4	0.9038	-2.0699
Cl-	0.008955	317.3	0.9011	-2.0931
CO2(aq)	0.0009392	41.31	1.0000	-3.0273
HCO3-	0.0005607	34.19	0.9038	-3.2952
O2(aq)	0.0002003	6.405	1.0000	-3.6983
SiO2(aq)	9.998e-005	6.003	1.0000	-4.0001
Cu++	4.673e-005	2.967	0.6803	-4.4977
NaCl(aq)	1.148e-005	0.6705	1.0000	-4.9400
CuCO3(aq)	8.138e-006	1.005	1.0000	-5.0895
NaHCO3(aq)	6.152e-006	0.5165	1.0000	-5.2110
CuOH+	2.165e-006	0.1743	0.9038	-5.7084
H+	9.151e-007	0.0009217	0.9154	-6.0769
CuCl+	7.764e-007	0.07681	0.9038	-6.1539
CO3--	4.240e-008	0.002543	0.6693	-7.5470
HSiO3-	1.473e-008	0.001135	0.9038	-7.8758
OH-	1.337e-008	0.0002273	0.9025	-7.9183

(only species > 1e-8 molal listed)

Mineral saturation states

To Page No.

Witnessed & Understood by me, | Date | Invented by | Recorded by DH | Date Jan 6 2000

From Page No.

	log Q/K		log Q/K
Malachite	0.0000 sat	Cristobalite(alp	-0.5513
Tenorite	0.0000 sat	Coesite	-0.8108
Atacamite	0.0000 sat	Cristobalite(bet	-0.9948
Quartz	-0.0008	SiO2(am)	-1.2865
Ice	-0.1388	Dioptase	-2.4215
Tridymite	-0.1723	Chrysocolla	-2.5586
Chalcedony	-0.2720		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1585	-0.800
CO2(g)	0.02765	-1.558
H2O(g)	0.02597	-1.586
HCl(g)	3.345e-015	-14.476
Cl2(g)	6.463e-022	-21.190
H2(g)	7.038e-042	-41.153
CO(g)	6.078e-047	-46.216
Cu(g)	6.972e-075	-74.157
Na(g)	1.168e-076	-75.932
CH4(g)	5.412e-144	-143.267
C(g)	3.581e-188	-187.446
Si(g)	5.589e-221	-220.253
C2H4(g)	1.167e-234	-233.933

Jan 6 2000 DJ

To Page No.

Witnessed & Understood by me, | Date | Invented by | Recorded by DH | Date Jan 6 2000

Project No. 1402-871
Book No. 305 TITLE RT

From Page No.____

This notebook has been prepared in accordance with applicable quality assurance procedures. The content is sufficient to allow a technically qualified person to replicate the studies described herein.

Gordon Wittmeyer

5/25/2000

FINAL FINAL (?) ENTRY:

I HAVE reviewed THIS notebook AND find it in compliance with QAP-001. I HAVE improved THE quality of THIS notebook BY retroactively ADDING my initials AND TODAY'S DATE in various places. There is sufficient information in THIS notebook SO THAT ANOTHER qualified individual could repeat THE Activity.

E. C. [signature]
8/24/2000

To Page No.____

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK #: 305

Document Date:	02/05/1999
Availability:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, Texas 78228
Contact:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, TX 78228-5166 Attn.: Director of Administration 210.522.5054
Data Sensitivity:	■"Non-Sensitive" □ Sensitive □"Non-Sensitive - Copyright" □ Sensitive - Copyright
Date Generated:	05/19/2000
Operating System: (including version number)	Windows
Application Used: (including version number)	See listed file types
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	2 Iomega Zip 250s (original) 2 CDs
File Types: (.exe, .bat, .zip, etc.)	tif, ppt, xls, jpg, gif, ASCII, txt, lay, plt, scr. out, inp
Remarks: (computer runs, etc.)	Media contains a variety of files including PowerPoint, Excel, graphics.