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TPA Phase 2

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INITIAL ENTRY

TITLE: TPA

PARTICIPANTS: Ron Janetzke
Sitakanta Mohanty

OBJECTIVES:

The Total System Performance Assessment Computer (TPA) code is designed to estimate the Complimentary Cumulative Distribution Function (CCDF) of the future performance of a geologic repository. The CCDF is called for in the EPA standard (40 CFR Part 191) as the primary performance measure for a geologic repository. Other performance measures such as dose to man may also be calculated. To be capable of analyzing a variety of scenarios, the TPA computer code consists of many modules, some performing very general functions and others performing very specific functions. See Section 2.8 of "TSPA & Technical Integration" in the CNWRA Operations Plans for a further description of the objectives.

TECHNICAL APPROACH:

The executive module of the TPA is that part of the computer code that controls flow of information between different parts of the TPA and does the final processing to produce the CCDF. The design of the executive module and its relationship to other modules of the TPA is explained in CNWRA 91-009, "Total System Performance Assessment Computer Code: Description of Executive Module". Appendix A of this document contains the Software Requirements Document for the TPA code.

CONFIGURATION MANAGEMENT STATUS: controlled

PLATFORM: Cray/SUN

LANGUAGE: FORTRAN 77

COMPILER: Cray/cft77, SUN/f77

HISTORY

The development of the TPA code began in 1991 on the Central Computing Facility VAX/VMS system. It was designed to run on either the CRAY at INEL or the VAX. Parallel instances of the code resided on the VAX and the CRAY. The only difference between the codes were in the invocation mechanism for system functions. This configuration was maintained until it was clear that the VAX was not fast enough to participate in the production runs of the Phase 2 analysis. The development then shifted to the CRAY. Changes were then made to the SEISMO module which could not be duplicated on the VAX version. Development on the VAX was then terminated, and the remaining files were nearly identical to the final CRAY version. The files that were used for the production runs on the CRAY were in the /u4/zke directory. These files were transmitted to /lan/ps/rjanetzke/zke at the CNWRA.

They were then modified to run on the SUN/SUNOS system on 'scratchy' in /home/scratchy/janetzke/zke. This again only required minor modification to the invocation of the system functions. It was found that in order to obtain exactly the same results as the CRAY the code needed to be compiled with the -r8 switch of the f77 compiler on the SUN system. This code was stored in /home/scratchy/janetzke/zke and is the source for the material used for the AUDIT96 code.

The AUDIT96 code was developed in /home/scratchy/janetzke/audit96. The executive and SOTEC modules were modified and a new module call CORPROXY was developed to sit in the SEISMIC directory as a mechanism to introduce random corrosion failure times for the canisters in a given zone, appearing as scenario failures to SOTEC. A feature of the SOTEC algorithm is that if corrosion failures occurred before scenario failures then the scenario failures

were ignored. This was altered to permit the scenario failures coming from CORPROXY to always dictate failure times independent from normal corrosion.

On Aug 10, 1996 a base case run was completed on SIERRA which used the TPA Phase

2 input file for the LHS module name 'lhs20n.inp'. It also used the executive input file 'tpa.inp' modified to supply correct path names for the file specifications. The number of vectors was also modified to 200. The scenario type was OS00 which simulated a base case of 0000 using the CORPROXY module.

The following items should be verified or performed when preparing a run of the system.

Remove scn* files from the scenario directory.

Set 'maxnuc' & 'maxvec' parameters in tpa.pre and recompile if necessary.

File flowmod.inp should be a copy of flow000020n.inp for non-climate runs.

File flowmod.inp should be a copy of flowc00020n.inp for climate runs.

File tpa.inp should refer to flomap0000.dat for non-climate runs.

File tpa.inp should refer to flomapc000.dat for climate runs.

File sotsei.dat should be regenerated if a new base case has been prepared.

Set LHS parameters in lhs20n.inp.

Issue the 'clear' command before starting a run.

Remove any core files from the scenario directory.

Remove lhs0000.out before running a scenario which will invoke 'lhs'.

Move the desired lhsxxxx.out file to 0000/lhs0000.out for non-base case runs if it has been prepared in advance.

Ron J. 9-9-96

C14

A procedure for running with no C14

in the inventory would include:

in 'tpa.inp' set C14 inventory to $1.e-27$.

in 'sotec.inp' change last 4 Waste, Carbon

values to $1.e-27$.

in 'sotec.nuc' change last value for C14

to $1.e-27$.

Ron J. 9-9-96

DOE Data

The comments on the following pages

are from S. Mohanty. They provide an

introduction to the use of DOE data.

Parameters and variable in the TPA calculations

Container lifetime data (Case 1)

The Case 1 study essentially used the base case input file for the TPA code originally developed for the IPA Phase 2 study. The only modification to the input file was to sample failure time from DOE data in stead of calculating the failure time directly by using SOTEC module built into the TPA code. In using the DOE data, the canister was assumed to have failed when the first pit fully penetrated the canister wall including the cladding. For comparison process, the failure history represented in Figure 5.7-10a of TSPA95 was chosen. This figure represents the exposure time vs. cumulative fractions of waste package with first pit penetration relationship and corresponds to case consisting of a thermal load of 83 MTU/acre, high infiltration, with backfill, and with RH-dependent corrosion initiation. The concerned figure was digitized and a histogram of failure time was constructed for sampling purposes. All failure times beyond 10,000 years were assigned to the last bin consisting of failure time. This figure shows that no more than nearly 84% canisters failed. Therefore, the cumulative fraction of the failed waste packages was normalized before the failure times were sampled by using LHS sampling program. The original distribution and sampled values are presented in Figure 1. For each vector, seven values were sampled independently for seven zones. The number of parameters to be sampled was reduced to nearly 199 and therefore sampling 200 vectors was considered adequate for the TPA runs.

Modifications to TPA base case data to reflect DOE data

Because of the time limitations, only the data thought to be favoring conservatism was considered for Case 2 simulation. Of the two total system modeling approaches (i.e., M&O approach and Buscheck et al. approach), the results from M&O approach were selected for failure time distribution because of the built-in conservatism in the M&O approach compared to the Buscheck et al. approach. Any DOE data whose incorporation required modifications to the NRC's TPA code was not incorporated and IPA phase 2 data was retained in stead. For example, the DOE sampled Uranium solubility from a logbeta distribution. Because the TPA code did not have provision to sample from a logbeta distribution, the sampling was therefore maintained at IPA Phase 2 base case value which was a loguniform distribution. However, the minimum and maximum of the distributions were kept same as that of the DOE's data. It is assumed that the reader has access to the IPA phase 2 base case input data. The parameters in the TPA input file that were changed to reflect DOE data are presented in the following tables.

Infiltration

New Distribution	Old
5 .0E-4 to 2.0E-3	Loguniform 1.e-4 to 5.e-3

Matrix permeability

Layers	New data	Distribution	Old data
Tsw	3.167 E - 20 to 5.313E-16 m2	Lognormal	3.6e-19 to 1.2e-18
CHv	5.21 E - 20 to 2.963E-14 m2	Lognormal	3.9e-15 to 2.0e-14
CHn	2.452 E - 21 to 3.167E-16 m2	Lognormal	1.3e-20 to 6.7e-19

Fracture permeability

Layers	New		Old	
Tsw	1.839E-12	Constant	1.1 E - 16 to 1.9E-16	Lognormal
Chv	5.578E-13	Constant	7.166E-12 to 5.805E-11	Lognormal
Chn	1.226E-13	Constant	6.2 E - 16 to 9.9e-16	Lognormal

Matrix Porosity

Tsw	0.004 to 0.48	Uniform
Chv	0.097 to 0.51	Uniform
Chn	0.141-0.47	Uniform

Fracture porosity

Tsw	0.001	Constant
Chv	0.001	Constant
Chn	0.001	Constant

Beta for Unsaturated Zone Matrix

Tsw	1.155 to 5.363	Lognormal
Chv	1.249 9.888	Lognormal
Chn	1.184 to 5.914	Lognormal

Beta for Unsat. Zone Matrix

Tsw	5.0	Constant
Chv	5.0	Constant
Chn	5.0	Constant

Solubility

Radionuclides	Range	New distribution
Cm	1.2E-9 to 1.2e-7	loguniform
U	2.4e-6 to 2.4 e0	loguniform
AM	2.4e-8 to 2.4e-4	uniform
Np	1.2e-3 to 2.4e0	loguniform
Pu	2.4e-6 to 2.4e-4	uniform
Th	2.3e-8 to 2.3e-5	loguniform
Ra	2.3e-7 to 2.3e-3	loguniform
Pb	2.1e-6 to 2.1e-3	loguniform
Cs	1.0	constant
Tc	1.0	constant
Ni	5.9e-5 to 5.9e0	loguniform
Se	1.0	constant
Nb	9.3e-8 to 9.3e-6	loguniform
Sn	1.2e-9 to 1.2e-5	uniform
Zr	9.1e-11 to 9.1e-6	loguniform
Sr	8.e-2	constant

Saturated zone travel time

In order to make the saturated zone travel time in the NRC model compatible to the travel time in the DOE model, only CHv layer was assumed to be connecting the repository legs to the accessible environment. This modification to the saturated zone properties was incorporated by changing the values presented in Table 4-6 of IPA Phase 2 report (NUREG-1464). Consequently, the length of other hydrologic units were forced to be zero in the saturated zone and those lengths were summed and added to the length of CHv.

Other parameters

—A fracture travel time in the saturated zone connecting the seven repository legs to the accessible zone was of the order of 1000 years. The DOE data indicates a mean travel time of 2.5 years. This was inferred from the reported mean darcy flux of 2 m/yr, a selected head gradient of 0.0003, and a fracture porosity of 0.001.

—No changes to K_d values for matrix; assumed no retardation in fracture

—Mixing length in the saturated zone was 500 m compared to a maximum of 30 m used in the IPA phase 2 calculations.

—Discharge area: The discharge area was calculated from the dimensions of the mixing zones presented on page 7-27 of the TSPA95. The discharge area was calculated to be $4.6E3 \times 0.48E3 \text{ km}^2 = 2.208E6 \text{ m}^2$. which is nearly twice as much as used in the IPA Phase 2 base case calculation.

9-20-96

OOE Run

SOTEC.pre

For all runs a modified version of the SOTEC code was used. This version requires the module 'corproxy' to run in the 'seismo'slot. Scenario 0500 must be selected. The following page contains the output of the 'diff' command which shows the changes made to SOTEC relative to the IPA 2 version.

RJ

Listing for Ron Janetzke

Fri Sep 20 10:21:02 1996

```

1c1
< *cpu cray
---
> *cpu sun
1405a1406,1407
>     iscon(nc)=mcon(nc)
>     ncont(nc)=0
1409c1411,1414
<     do 520 itype = 1, 3
---
> C-rwj 03-20-96 Restrict to corrosion only which appears as type 2 due to
> C     the proxy seismic code seisot.dat file.
> C
>     do 520 itype = 2, 2
1532,1534c1537,1539
<     if(ibin.le.10) then
< C       write(*,*) 'sc14, ibin = ',sc14(ibin), ibin
<     endif
---
>     if(ibin.le.10) then
> C       write(*,*) 'sc14, ibin = ',sc14(ibin), ibin
>     endif
1617a1623,1624
> C-rwj 9-12-96 Add c14 curies/yr to fracre for release to neftran.
>     ibin = 2
1619a1627,1633
> C-rwj 9-12-96
> C       Keep gaseous times tbin(ibin) in sync with aqueous times.
> 1589     CONTINUE
>         IF (ibin .LT. MAXBIN .AND. tbin(ibin) .LT. itim*bt) THEN
>             ibin = ibin+1
>             go to 1589
>         END IF
1662a1677,1680
>         IF (namall(ichns,iiso) .EQ. 'C14') THEN
> C-rwj 9-12-96
> C       Add c14 curies/yr to fracre for water release to
> C       neftran input file.
1665,1666c1683,1689
<             goto 569
<         endif
---
>         &                                     + (sumc14(ibin-1)+sumc14(ibin))/2.
>         ELSE
>             fracre(ichns,iiso,itim,nc) = fracre(ichns,iiso,itim,nc)
>         &                                     + tmp
>         END IF
>         goto 569
>     endif

```

9-20-96

TPA.PRE

The following pages show The changes made to the tpa.pre file to convert it from a Cray version to a SUN version.

The listing is output from the 'diff' command, and is relative to the CRAY version used in phase 2, and the SUN version used in Aud. 796.

Listing for Ron Janetzke

Fri Sep 20 16:18:25 1996

```

7a8
> *note: *    sun
9c10
< *cpu cray
---
> *cpu sun
19a21,22
> *fragment sunid
>         cpuid = 'sun'
54c57
<         PARAMETER (maxvec=50)
---
>         PARAMETER (maxvec=200)
617a621,626
> *note: *
> *note: *    SUN cpu specific fragments.
> *note: *    sdate1
> *note: *    sdate2
> *note: *    stime1
> *note: *    stime2
658a668,689
> *fragment sdate1
> CCCCCC
> C        /SDATE1/
> C
> C        string = calendar date in SUN Day Mon dd hh:mm:ss yyyy format.
> C
> C        This fragment is declared separate from the one containing the
> C        actual call to 'date' in order to facilitate placement in
> C        different sections of the target subroutine.
> CCCCCC
> C        CHARACTER*24 string
> C        CHARACTER*9 cdate
> *fragment sdate2
> C        CALL fdate(string)
> C        cdate = string(5:11)//string(23:24)
> *fragment stime1
> CCCCCC
> C        /STIME1/
> C
> C        ctime = time of day in SUN hh:mm:ss format.
> CCCCCC
> C        CHARACTER*8 ctime
> *fragment stime2
> C        ctime = string(12:19)
675a707,711
> *fragment lhssys
> CCCCCC
> C        This fragment is for SUN only.
> CCCCCC
> C        istat = system ('$HOME/audit96/lhs2/lhs.e <'//lhsgbl)
686a723,727
> *fragment temsys
> CCCCCC
> C        This fragment is for SUN only.
> CCCCCC
> C        istat = system ('$HOME/audit96/temper/cant2.e > cant2.lu6')
696a738,742
> *fragment ditsys
> CCCCCC
> C        This fragment is for UNICOS only.
> CCCCCC
> C        istat = ishell ('$HOME/ditty/ditty.e > '//ditout)
1045a1092,1101
> *fragment dirsyst
> CCCCCC Begin fragment dirsyst1 for SUN only.
> C        CHARACTER*90 syscom

```



```

> INTEGER spstat
> CCCCCC End fragment dirsyst1.
> *fragment dirsyst2
> CCCCCC Begin fragment dirsyst2 for SUN only.
>   syscom = 'ls -ls '//filnam//' >'//finfo
>   spstat = system(syscom)
> CCCCCC End fragment dirsyst2
1149a1206
> *insert/sun cumrel
1153a1211
> *insert/sun sdate1
1155a1214
> *insert/sun stime1
1158a1218
> C   opnmsg = error message from 'opnfil'.
1160a1221
>   CHARACTER*80 opnmsg
1200a1262
> *insert/sun sunid
1203a1266
> *insert/sun sdate2
1206a1270
> *insert/sun stime2
1732a1797
>   INTEGER system
1756a1822
> *insert/sun temsys
1788a1855
>   INTEGER system
1833a1901
> *insert/sun copenlis
1845a1914
> *insert/sun lhssys
4670a4740
> *insert/sun sdate1
4676a4747
> *insert/sun sdate2
4884a4956
>   print *, 'sotec',vector,lcompl
4909a4982
>   print *, 'volcano',vector,lcompl
4974a5048
>   print *, 'aircom',vector,lcompl
4991a5066
>   print *, 'c14',vector,lcompl
5007a5083
>   print *, 'flowmod',vector,lcompl
5025a5102
>   print *, 'ditty-air',vector,lcompl
5042a5120
>   print *, 'ditty-water',vector,lcompl
5060a5139
>   print *, 'ditty-food',vector,lcompl
5076a5156
>   print *, 'neftran',vector,lcompl
5101a5182,5183
> *insert/sun sdate1
> *insert/sun stime1
5107a5190,5191
> *insert/sun sdate2
> *insert/sun stime2
5178a5263
>   INTEGER system
5257a5343
> *insert/sun ccl4opli
5308a5395,5407

```

```

> *fragment c14sys
> CCCCCC
> C   Invoke C14 for SUN only.
> CCCCCC
>   spstat = system('$HOME/audit96/c14h/c14h.e')
>   IF (spstat .ne. 0) THEN
>     WRITE (code,'(i10)') spstat
>     CALL errmsg ('C14EXC','C14 status code = '//code)
>     CALL logmsg ('Stopping in C14EXC.')
>     lcompl = .false.
>     GO TO 999
>   END IF
> *insert/sun c14sys
5351a5451
>   INTEGER system
5408a5509
> *insert/sun csotopli
5476a5578,5590
> *fragment sotsys
> CCCCCC
> C   Invoke SOTEC for SUN only.
> CCCCCC
>   spstat = system('$HOME/audit96/sotec/sotec.e')
>   IF (spstat .ne. 0) THEN
>     WRITE (code,'(i10)') spstat
>     CALL errmsg ('SOTEXC','SOTEC status code = '//code)
>     CALL logmsg ('Stopping in SOTEXC.')
>     lcompl = .false.
>     GO TO 999
>   END IF
> *insert/sun sotsys
5519a5634
>   INTEGER system
5576a5692
> *insert/sun cvolopli
5643a5760,5773
> *fragment volsys
> CCCCCC
> C   Invoke VOLCANO for SUN only.
> CCCCCC
>   spstat = system('$HOME/audit96/volcano/volcano.e')
>   IF (spstat .ne. 0) THEN
>     WRITE (code,'(i10)') spstat
>     CALL errmsg ('VOLEXC','VOLCANO status code = '//code)
>     CALL logmsg ('Stopping in VOLEXC.')
>     lcompl = .false.
>     GO TO 999
>   END IF
>   spstat = system('cat volsot.dat >> scnvol.dat')
> *insert/sun volsys
5685a5816
>   INTEGER system
5725a5857
> *insert/sun cseiopli
5772a5905,5918
> *fragment seisisys
> CCCCCC
> C   Invoke SEISMO for SUN only.
> CCCCCC
>   spstat = system('$HOME/audit96/seismic/seismo.e')
>   IF (spstat .ne. 0) THEN
>     WRITE (code,'(i10)') spstat
>     CALL errmsg ('SEIEXC','SEISMO status code = '//code)
>     CALL logmsg ('Stopping in SEIEXC.')
>     lcompl = .false.
>     GO TO 999

```



```

> END IF
> spstat = system ('cat seisot.dat >> scnsei.dat')
> *insert/sun seisys
5814a5961
> INTEGER system
5870a6018
> *insert/sun cdrlopli
5916a6065,6078
> *fragment drlsys
> CCCCCC
> C Invoke DRILLO1 for SUN only.
> CCCCCC
> spstat = system ('$HOME/audit96/drill/drillo1.e')
> IF (spstat.ne. 0) THEN
> WRITE (code,'(i10)') spstat
> CALL errmsg ('DR1EXC','DRILLO1 status code = '//code)
> CALL logmsg ('Stopping in DR1EXC.')
> lcompl = .false.
> GO TO 999
> END IF
> spstat = system ('cat drlsot.dat >> scndrl.dat')
> *insert/sun drlsys
5959a6122
> INTEGER system
6001a6165
> *insert/sun cdr2opli
6062a6227,6239
> *fragment dr2sys
> CCCCCC
> C Invoke DRILLO2 for SUN only.
> CCCCCC
> spstat = system ('$HOME/audit96/drill/drillo2.e')
> IF (spstat.ne. 0) THEN
> WRITE (code,'(i10)') spstat
> CALL errmsg ('DR2EXC','DRILLO2 status code = '//code)
> CALL logmsg ('Stopping in DR2EXC.')
> lcompl = .false.
> GO TO 999
> END IF
> *insert/sun dr2sys
6114a6292
> INTEGER system
6228a6407,6419
> *fragment airsys
> CCCCCC
> C Invoke AIRCOM for SUN only.
> CCCCCC
> spstat = system ('$HOME/audit96/aircom/aircom.e')
> IF (spstat.ne. 0) THEN
> WRITE (code,'(i10)') spstat
> CALL errmsg ('AIREXC','AIRCOM status code = '//code)
> CALL logmsg ('Stopping in AIREXC.')
> lcompl = .false.
> GO TO 999
> END IF
> *insert/sun airsys
6274a6466
> INTEGER system
6395a6588
> *insert/sun cditopli
6494a6688,6700
> *fragment diasys
> CCCCCC
> C Invoke DITTY for SUN only.
> CCCCCC
> spstat = system ('$HOME/audit96/ditty/ditty.e')

```

```

> IF (spstat.ne. 0) THEN
> WRITE (code,'(i10)') spstat
> CALL errmsg ('DIAEXC','DITTY_A status code = '//code)
> CALL logmsg ('Stopping in DIAEXC.')
> lcompl = .false.
> GO TO 999
> END IF
> *insert/sun diasys
6536a6743
> INTEGER system
6656a6864
> *insert/sun cditopli
6756a6965,6977
> *fragment diwsys
> CCCCCC
> C Invoke DITTY for SUN only.
> CCCCCC
> spstat = system ('$HOME/audit96/ditty/ditty.e')
> IF (spstat.ne. 0) THEN
> WRITE (code,'(i10)') spstat
> CALL errmsg ('DIWEXC','DITTY_W status code = '//code)
> CALL logmsg ('Stopping in DIWEXC.')
> lcompl = .false.
> GO TO 999
> END IF
> *insert/sun diwsys
6796a7018
> INTEGER system
6868a7091
> *insert/sun cditopli
6964a7188,7200
> *fragment difsys
> CCCCCC
> C Invoke DITTY for SUN only.
> CCCCCC
> spstat = system ('$HOME/audit96/ditty/ditty.e')
> IF (spstat.ne. 0) THEN
> WRITE (code,'(i10)') spstat
> CALL errmsg ('DIFEXC','DITTY_F status code = '//code)
> CALL logmsg ('Stopping in DIFEXC.')
> lcompl = .false.
> GO TO 999
> END IF
> *insert/sun difsys
7007a7244
> INTEGER system
7080a7318
> *insert/sun cfloopli
7149a7388,7400
> *fragment flosys
> CCCCCC
> C Invoke FLOWMOD for SUN only.
> CCCCCC
> spstat = system ('$HOME/audit96/flowmod/flowmod.e <'//floop)
> IF (spstat.ne. 0) THEN
> WRITE (code,'(i10)') spstat
> CALL errmsg ('FLOEXC','FLOWMOD status code = '//code)
> CALL logmsg ('Stopping in FLOEXC.')
> lcompl = .false.
> GO TO 999
> END IF
> *insert/sun flosys
7182a7434
> *insert/sun cumrel
7195a7448
> INTEGER system

```


7322a7576,7588
 > *fragment nefsys
 > CCCCCC
 > C Invoke NEFMKS for SUN only.
 > CCCCCC
 > spstat = system ('\$HOME/audit96/neftran/nefmks.e')
 > IF (spstat.ne. 0) THEN
 > WRITE (code,'(i10)') spstat
 > CALL errmsg ('NEFEXC','NEFTRAN status code = '//code)
 > CALL logmsg ('Stopping in NEFEXC.')
 > lcompl = .false.
 > GO TO 999
 > END IF
 > *insert/sun nefsys
 7354a7621
 > *insert/sun cumrel
 7447a7715
 > *insert/sun nefexc1
 7512a7781
 > *insert/sun cumrel
 7636a7906
 > *insert/sun cumrel
 7764a8035
 > *insert/sun cumrel
 9549a9821
 > *insert/sun dirsyst1
 9559a9832
 > *insert/sun dirsyst2
 10071a10345
 > *insert/sun cray1
 10098a10373
 > *insert/sun cray2
 10122a10398
 > *insert/sun cray3
 10137a10414,10416
 > *fragment sun4
 > OPEN (UNIT=unit, FILE=filnam, STATUS='OLD',
 > + ACCESS='APPEND')
 10139a10419
 > *insert/sun sun4
 10147a10428
 > *insert/sun cray5

Final runs

The final DOE run was made on

snowwhite. The 'audit96' directory tree
 from 'randall' on snowwhite is on tape

'Audit96 DOE RUN' at the back of this

book. IT is a 'tar' tape.

The LHS seed for this run was -162791.

The final baseline run was made on

Sierra. The 'audit96' directory tree from

'randall' on sierra is on tape 'Audit96 Baseline

Run' at the back of This book. The

LHS seed for this run was -162791.

Ron J.

9-23-96

Detailed Review

A new task is underway to perform a detailed review as described in a 9/11/96 memo from Rex Wescott. See next page.

A major difference between these runs and those of the Audit96 set, is that all runs must have uncorrelated container failure times, whereas for Audit96 all 200 vector runs ~~use~~ used the same set of failure times. 2 sets of 200 vectors each will be used to make up a 400 vector scenario.

The 'corlts' program will be run once for each 200 vector set to obtain new failure times for all runs.

Even though the baseline + DOE runs from Audit96 used the same corlts.out file, they will be used as a starting point for

Revised 9/11/96

NOTE TO: KTI TEAM LEADS

FROM: Rex Wescott
Bob Baca

SUBJECT: DETAILED REVIEW OF DOE TSPA-95 AND SENSITIVITY AND IMPORTANCE ANALYSIS

At the last meeting of the KTI Leads for review of DOE TSPA 95 (July 17, 1996), teams were requested to submit short write-ups of analyses to be performed for the purpose of evaluating DOE TSPA 95 methodology. These descriptions have been received and have been reformatted to clearly state the objective, approach, and expected output. Attached is a brief description of the analyses in this format.

Also, the TSPA&I KTI Team has developed a strategy for combining the technical tasks of review of DOE TSPA 95 with the continuing development of an independent technical assessment capability (IPA Phase 3). Because of recent questions about the separate progress of these programs, we are presenting our milestones with brief explanations to show how review of TSPAs and development of technical assessment capability are combined.

RJ
11/27/96 Phase 1 Sensitivity Analyses (Input to Detailed review of TSPA 95): The phase 1 sensitivity analyses which will be performed during November 1996 will directly compare total system performance assessment results using NRC and DOE subsystem models. Runs will be made using the TPA code (the DOE RIP code is unavailable). A separate run will be made for each alternative conceptual subsystem model using the total system code. Each run will change only one model at a time. The results of these runs will form a bases to determine the relative importance to performance of technical differences arising from the various focused review areas. Faulting and Igneous activity will be incorporated into the analyses as external or auxiliary analyses. Alternative conceptual models and other information are expected to be directly incorporated in the focused areas of: (1) infiltration/percolation, (2) container lifetime and source term (with hydrothermal input), (3) dilution, (4) revised hydrostratigraphy, (5) matrix diffusion, and (6) near-field chemistry. The offline analyses planned for faulting and volcanism are for the purpose of determining effect on compliance from a dose perspective and identification of key parameters through limited sensitivity analyses. This Phase 1 sensitivity analysis is expected to provide some preliminary information regarding relative importance of various KTIs.

The detailed review. All succeeding runs however will have new 'corlhs.out' files.

The nomenclature for the various runs of the detailed Review is given in the 9-19-96 memo/e-mail from R. Mantecufel. See next page. Several files will be archived from each run, and are listed here.

tpa.inp

lhs20n.inp

corlhs.out

ccdf.fmt

pathre.fmt

scnrel.fmt

lhs0000.out

RJ 9-23-96

Author: Randall Manteufel at CNWRA
 Subject: Phase 1 Sens IM
 Date: 09/19/96 Time: 16:44:49
 To: ronald janetzke at CNWRA-SUN
 To: Robert Baca at CNWRA-OS2
 Cc: Gerry Stirewalt at CNWRA-OS2

***** MESSAGE CONTENTS *****

Ron Janetzke, Randy Manteufel, and Rob Rice had a brief meeting on Thursday, 9/19/96 to discuss work on Phase 1 Sensitivity Analyses (IM due 11/27/95). Below are main points:

1) Rob will be leaving CNWRA this friday. He will provide copies of input files to Randy to help understand work in audit review.

2) We will consider "doe" runs in audit review as new baseline for sensitivity runs. These runs were closest to TSPA-95 CCDF. In the audit review, two runs were completed:

"doe" = no gas, no disruption, DOE WP lifetime, DOE data (input by Rob)

"olddata" = no gas, no disruption, DOE WP lifetime, IPA-2 data

ipa2 Rg 9-23-96

3) Ron will give new seed to doe & olddata runs, and rerun. This will provide sufficient input to Randy to perform parameter sensitivity studies. In the future, Ron will try to make 2 LHS-200 runs for any conceptual model case.

4) Randy will contact Gerry Stirewalt and get input about Center's best hydrostratigraphy model to use in TPA code. Will need data for 7 zones. These runs will be known as "hydro" runs.

"hydro" = doe & revised hydrostratigraphy

5) Rob will work-up new set of runs to test importance of matrix diffusion conceptual model. Rob will increase all zone matrix hydraulic conductivities to be greater than greatest percolation rate. This will make all water flow in matrix. This will be known as "matrix" run.

"matrix" = doe & Km,sat > qinfil for all unsat layers

6) Will discuss in future how can make other runs, but these will require more work.

wpfail = all Zones fail at same Time. Rg 9-25-96

"ebspac" = doe & EBSPAC code

"perc" = doe & 7 independent PDFs for percolation

"volcfault" = doe & new VOLCANISM and FAULTING modules.

-Randy

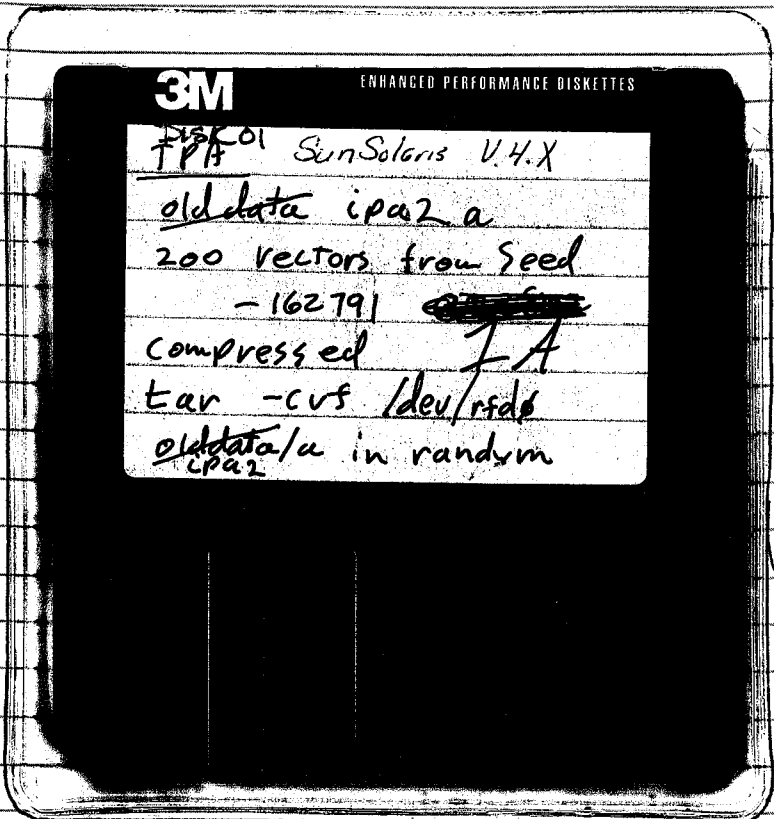
The disk labeled 'ipa2' contains the archive files from the 200 vector run formerly known as The Audit96 baseline. See next page.

The disk labeled 'DOE' contains the archive files from the 200 vector run formerly known as The Audit96 DOE run. See next page.

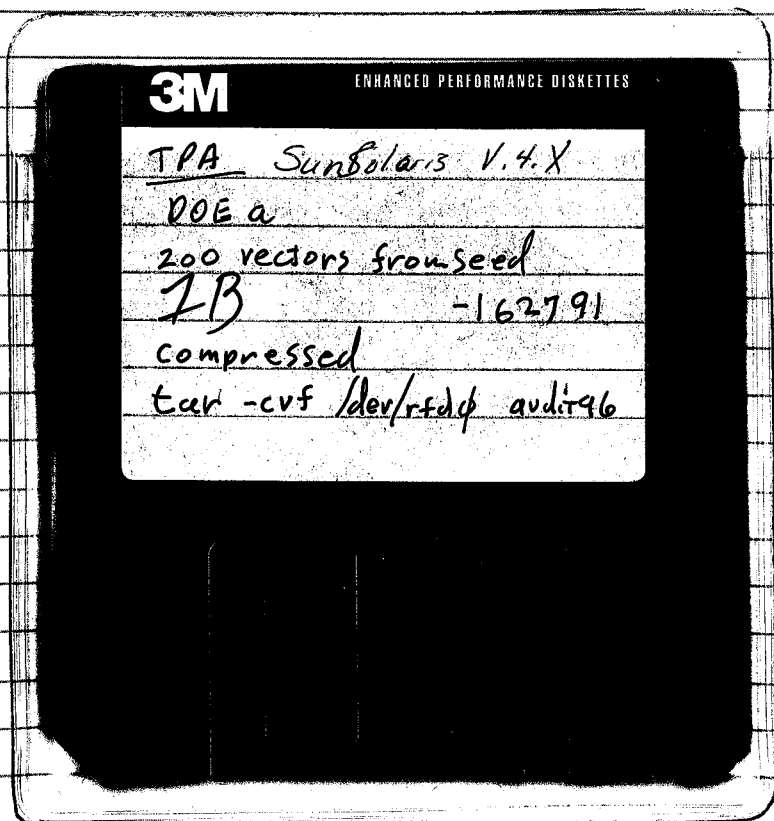
Ron J

9-23-96

ipa2
a



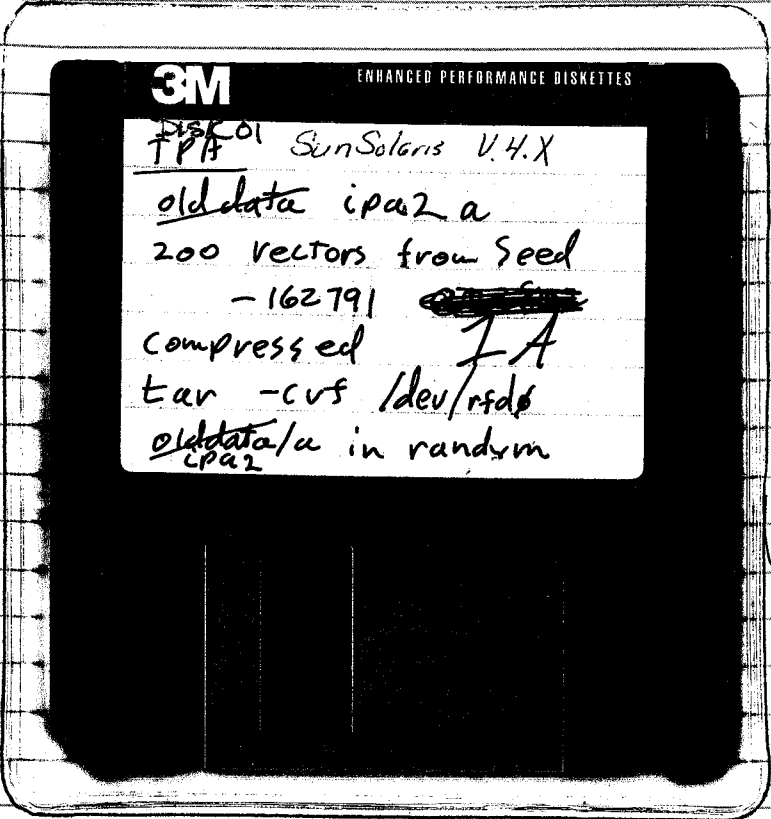
DOE
a



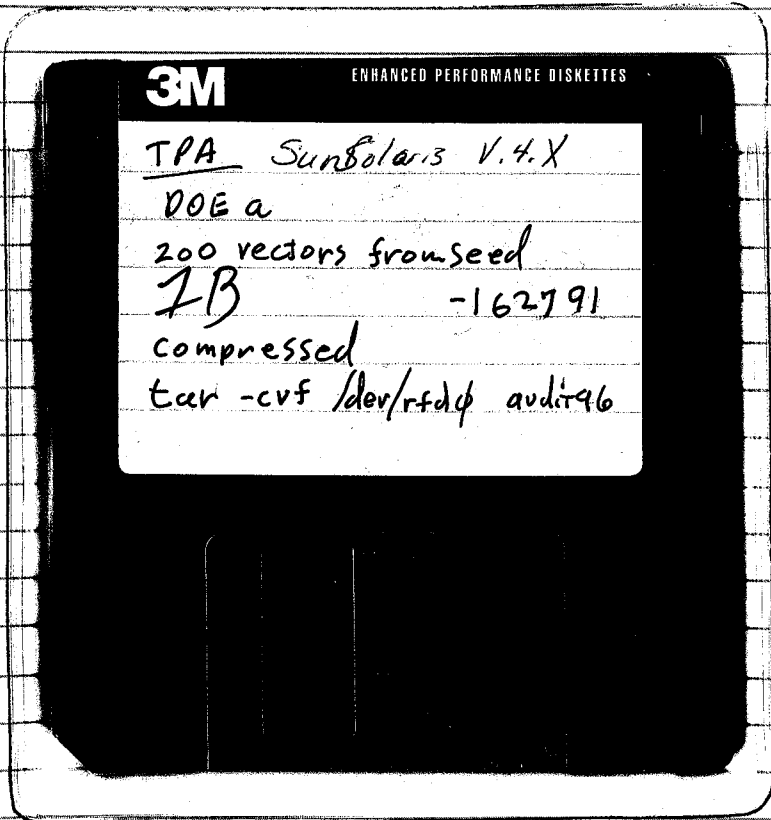
ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK #: 190

Document Date:	09/09/1996		
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:	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright		
Date Generated:	09/23/1996		
Operating System: (including version number)	Sun Solaris Version 4.X; UNIX		
Application Used: (including version number)	NA		
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	2 - 3 1/2 disks		
File Types: (.exe, .bat, .zip, etc.)	Various		
Remarks: (computer runs, etc.)	Disks contain: Archive files from the 200 victor run formerly know as the Audit96 baseline: compressed tar—cvf/dev/rfd0, ipa2/a in random; and archive files from the 200 vector run formerly known as the Audit96 DOE run: compressed tar—cvf/dev/rdf0 audit96		

ipa2
a



DOE
a



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Date Generated:	09/23/1996		
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Application Used: (including version number)	NA		
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File Types: (.exe, .bat, .zip, etc.)	Various		
Remarks: (computer runs, etc.)	Disks contain: Archive files from the 200 victor run formerly know as the Audit96 baseline: compressed tar—cvf/dev/rfd0, ipa2/a in random; and archive files from the 200 vector run formerly known as the Audit96 DOE run: compressed tar—cvf/dev/rdf0 audit96		

Detailed Review Runs

The general procedure for making detailed review runs is:

Adjust LHS seed in corlhs.inp.

Remove corlhs.out.

Run lhs.e with TPA-LHS.LGD as stdin in seismic.

Adjust LHS seed in lhszon.inp in os00.

Remove *.fmt

Remove *.cum

./clear

Run tpa/tpa.e < tpa.inp +

Recover archive files.

Ron J 9-25-96

Matrix Runs

The matrix runs are based on
the following e-mail from Randy M.

cc:Mail for: randall manteufel

Subject: matrix runs
From: Randall Manteufel 9/24/96 8:55 AM
To: ronald janetzke at CNWRA-SUN

Ron,

For the "matrix" runs, change the following 3 parameters:

perm (1)
perm (2)
perm (3)

Change to:

CONSTANT
1.0e-16

Thanks.
-Randy

9-25-96

ipa2

a

corlhs seed = -162791

lhszon seed = -162791

b

corlhs seed = -273802

lhszon seed = -273802

doe

a

corlhs seed = -162791

lhszon seed = -162791

b

corlhs seed = -384913

lhszon seed = -273802

matrix

a

corlhs seed = -162791

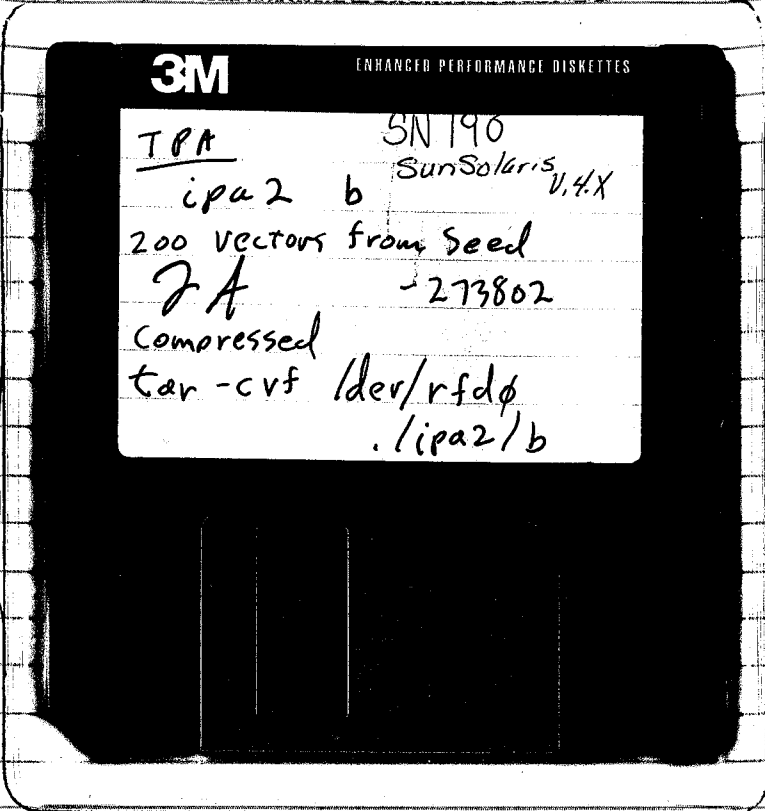
lhszon seed = -162791, perm(1..3) = 1.e-16

b

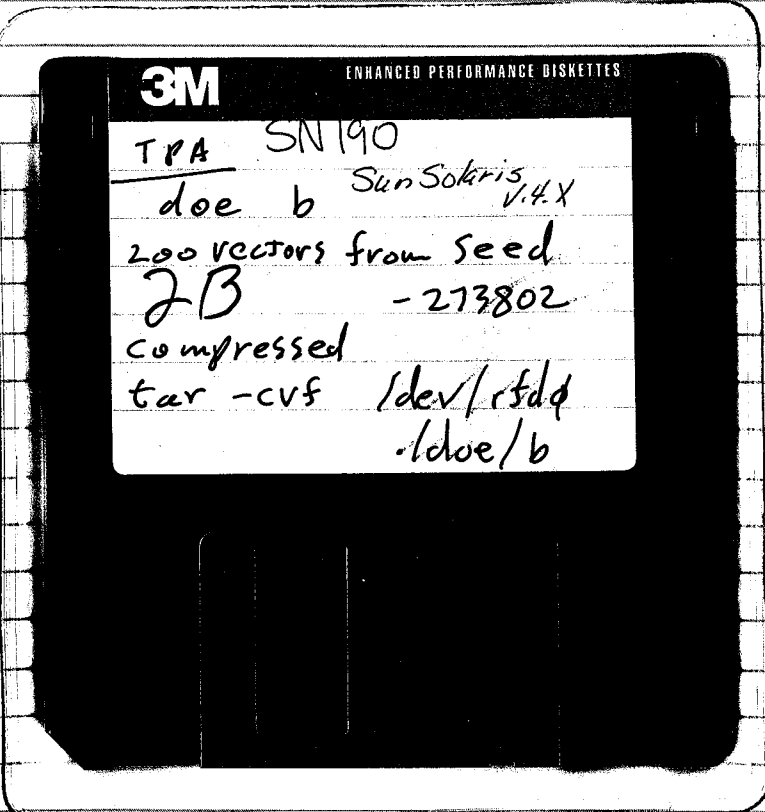
corlhs seed = -384913

lhszon seed = -273802, perm(1..3) = 1.e-16

Randy 9-25-96



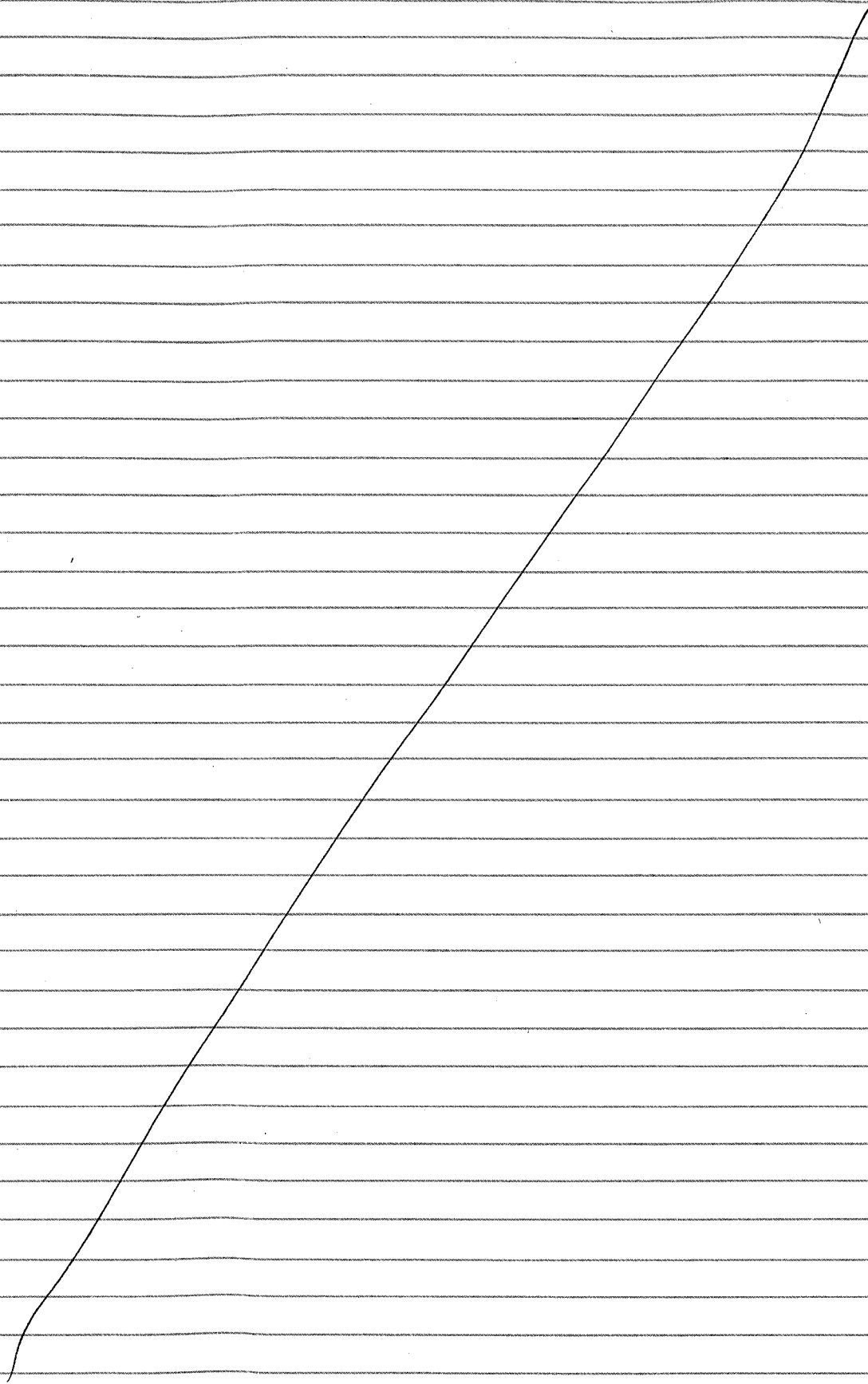
ipa2
b

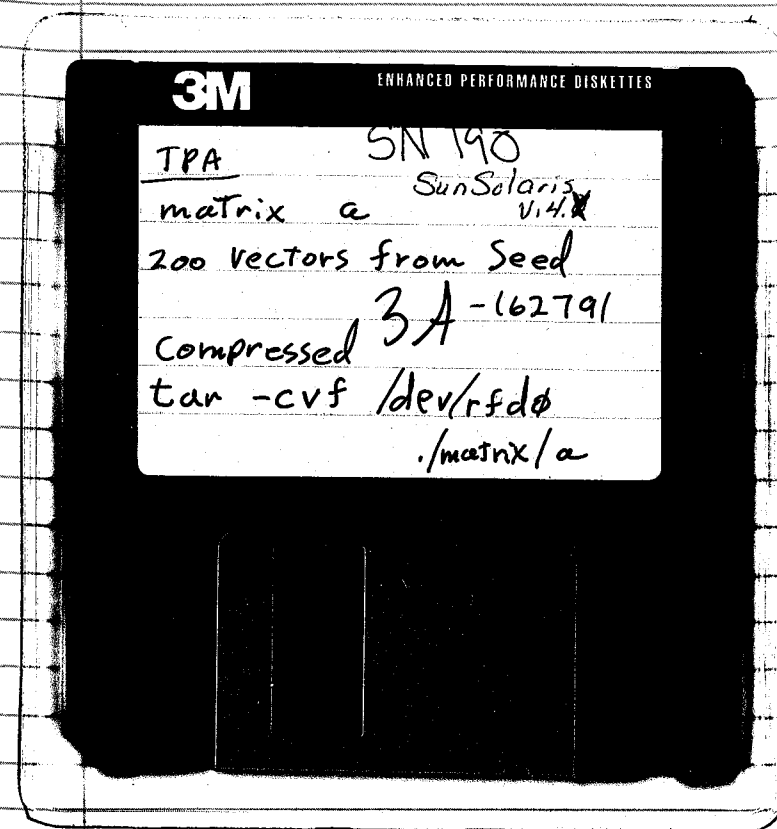


DOE
b

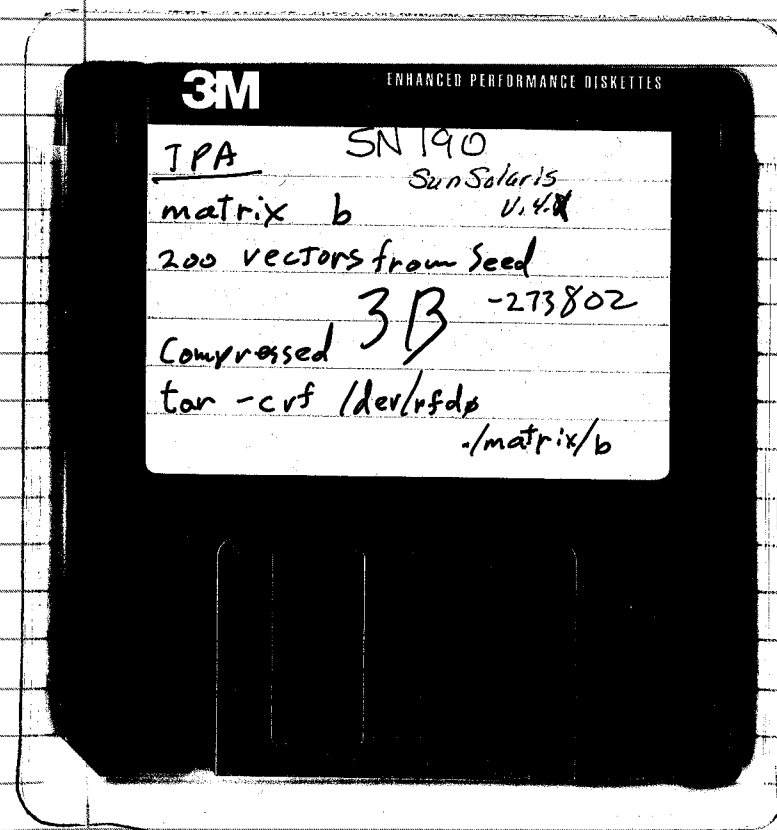
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Application Used: (including version number)	NA
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	2 - 3 1/2 disks
File Types: (.exe, .bat, .zip, etc.)	Various
Remarks: (computer runs, etc.)	Disks contain: Compressed tar—cvf/dev/rfd0/ipa2/b, 200 vectors from seed 273802; and compressed tar—cvf/dev/rfd0/doe/b



matrix

a



b

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Data Sensitivity:	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright
Date Generated:	09/30/1996
Operating System: (including version number)	Sun Solaris Version 4.X; UNIX
Application Used: (including version number)	NA
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	2 - 3 1/2 disks
File Types: (.exe, .bat, .zip, etc.)	Various
Remarks: (computer runs, etc.)	Disks contain: Compressed tar—cvf/dev/rfd0/matrix/a, 200 vectors from seed 162791; and compressed tar—cvf/dev/rfd0/matrix/b, 200 vectors from seed 273802

wpfail

one of the 'corlhs.out' files was edited
 To duplicated the first failure time for
 each vector to each of the remaining
 6 positions. The resulting file then
 had the same canister failure times
 for all 7 zones. This file was
 used for input to the 'wpfail'
 scenario.

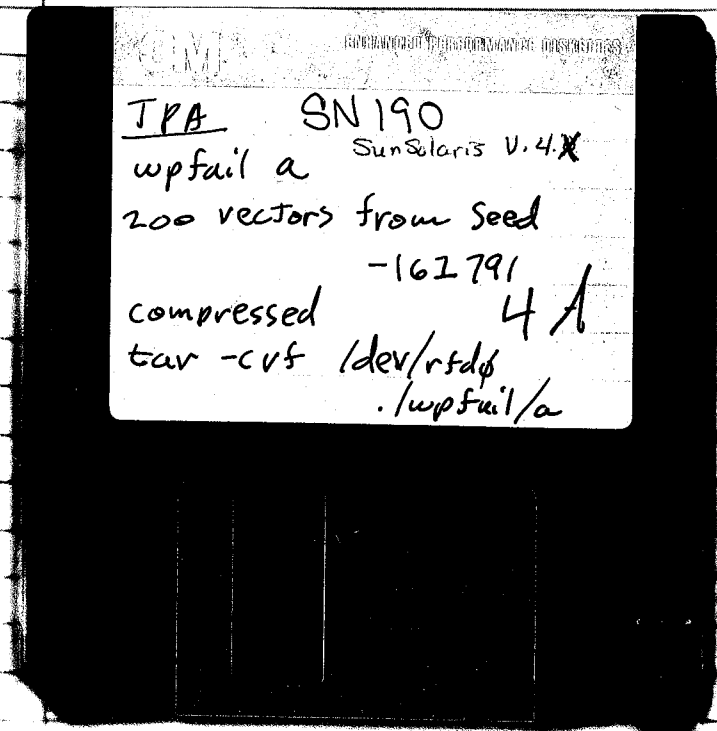
a

corlhs file = wpfaillhs.out
 lhs file = lhszon.inp
 seed = -162791

b

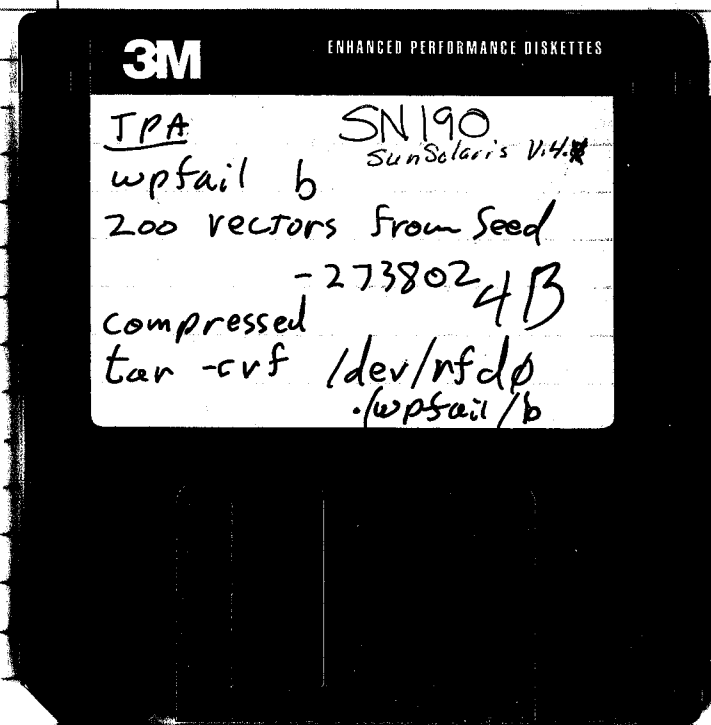
corlhs file = wpfaillhs.out
 lhs file = lhszon.inp
 seed = -273802

Ron Jr. 9-30-96



wpfail

a



b

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK #: 190

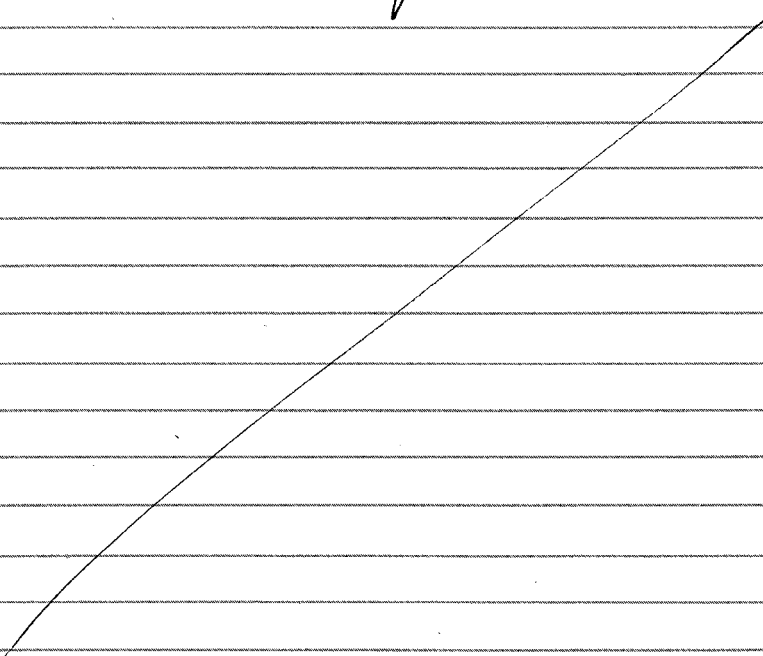
Document Date:	09/09/1996
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Data Sensitivity:	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright
Date Generated:	10/04/1996
Operating System: (including version number)	Sun Solaris Version 4.X; UNIX
Application Used: (including version number)	NA
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	2 - 3 1/2 disks
File Types: (.exe, .bat, .zip, etc.)	Various
Remarks: (computer runs, etc.)	Disks contain: Compressed tar—cvf/dev/rfd0/wpfail/a, 200 vectors from seed 162791; and compressed tar—cvf/dev/rfd0/wpfail/b, 200 vectors from seed 273802

nettran

a new nefmks.e was generated on scratchy which will be used for all runs from now on. The new module appends all 'watrel.in' files from all vectors into one large file. This probably precludes its use as an input file to DITTY, Therefore DITTY should not be run as part of The System. The 'clear' file was also changed to remove 'watrel.in'.

Ron G

OCT-4-1996



flowmod7inf

A separate version of Flowmod was created for the 'perc' runs. This version accommodates 7 distinct sampled infiltration values, one for each zone. This requires a corresponding change in the 'flowmod/flomaf7inf.dat' file and the 'lhf7inf.inp' file.

Ron J 10-4-96

perc a

a test run of 200 vectors was initiated on scratchy. This involved creating a new 'corlhf.out', and 'tpa.inp', and 'clear'. 'tpa.inp' was changed to point to 'flowmod/flomaf7inf.dat' and 'lhf7inf.inp'.

lhf seed = -162791

We await final PDF's for the 7 infiltrations.

Ron J 10-14-96

perc b

The following files were transferred
from scratchy to geomat in
preparation for the 'perc b' run.

seismic/cor/hs.out

TPainp

flowmod/flowmap7int.dat

lhs7inp.inp

clear

flowmod/flowmod.e

nettran/netmks.e

Ran J 10-4-96

Risk

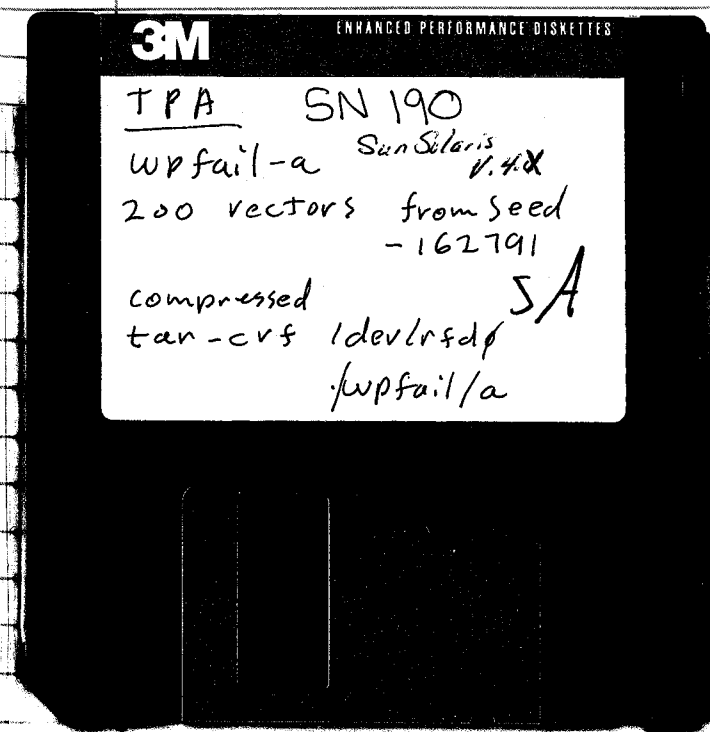
R. Mantel announced today that all
Detailed Review runs must be re-done.

He wishes that all runs be performed
with the new 'netmks.e' file which
will provide input for risk analysis.

Ran J. 10-8-96

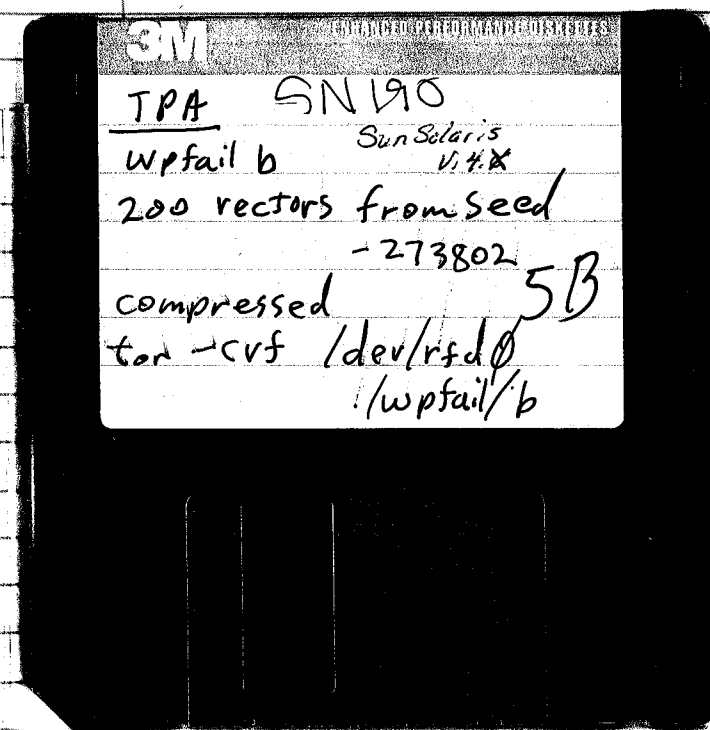
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Data Sensitivity:	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright
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Operating System: (including version number)	Sun Solaris Version 4.X; UNIX
Application Used: (including version number)	NA
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	6 - 3 1/2 disks
File Types: (.exe, .bat, .zip, etc.)	Various
Remarks: (computer runs, etc.)	Disks contain: Compressed tar—cvf/dev/rfd0/wpfail/a, 200 vectors from seed 162791; and compressed tar—cvf/dev/rdf0/wpfail/b, 200 vectors from seed 273802; compressed tar: cvf/dev/rfd0/doe/a, 200 vectors from seed 162791; compressed tar: cvf/dev/rfd0/doe/b, 200 vectors from seed 273802; compressed tar: cvf/dev/rfd0/matrix/a, 200 vectors from seed 162791; compressed tar: cvf/dev/rdf0/matrix/b, 200 vectors from seed 273802

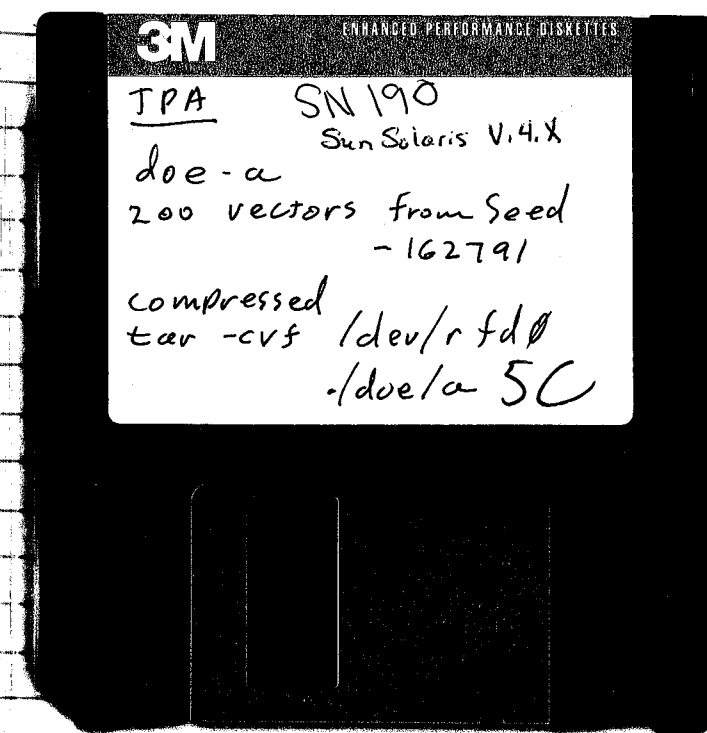


wpfail

a

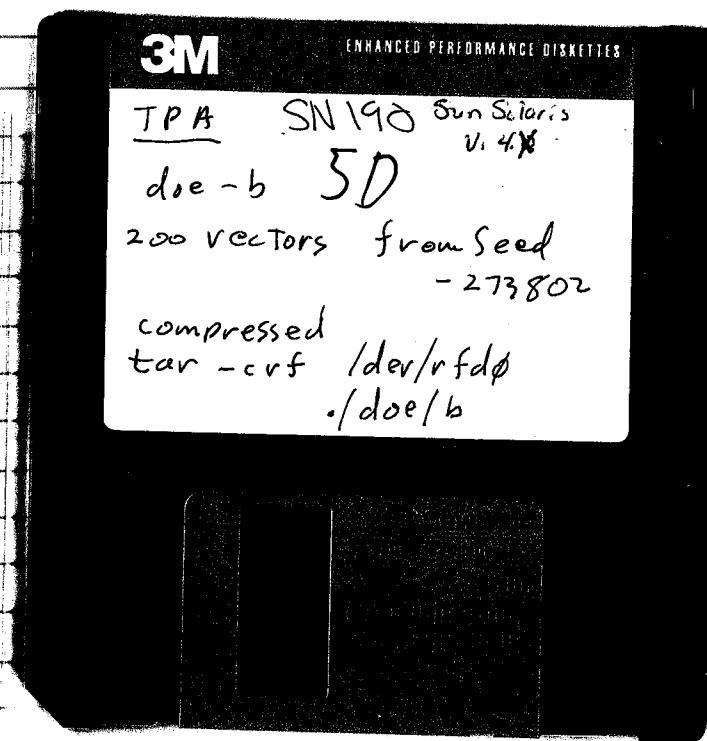


b



doe

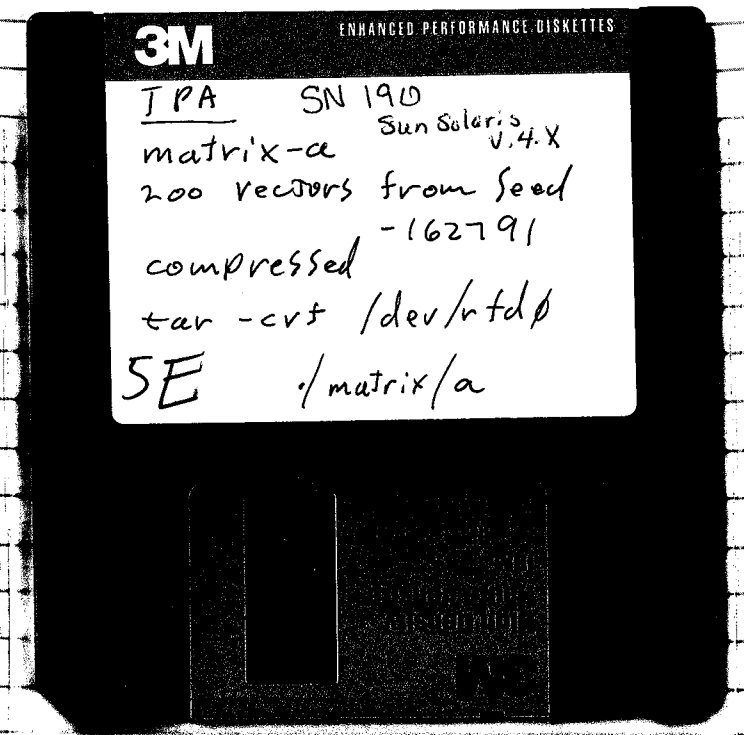
a



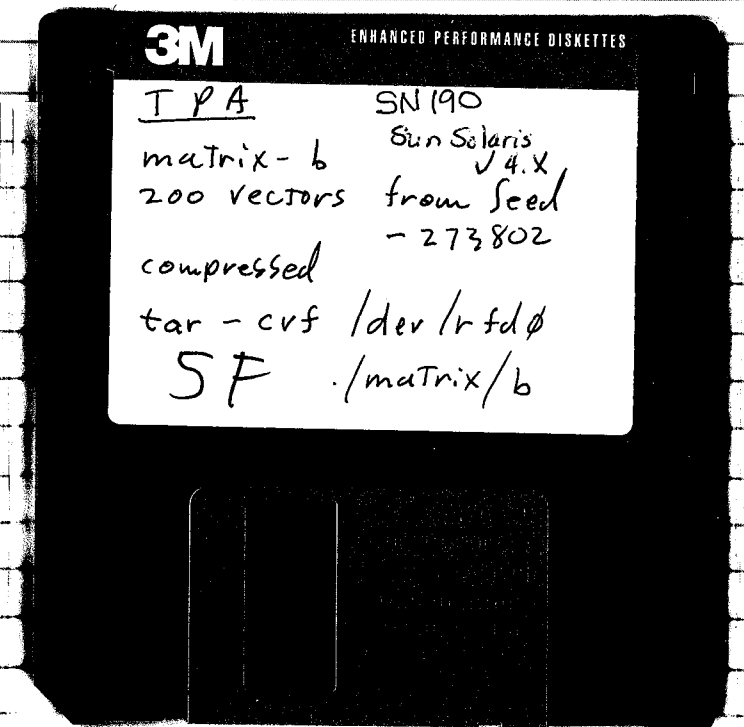
b

Matrix

a



b



THIS will
 REMAIN Empty.
 No diskette
 included.
 Sun 12/23/99

Author: Randall Manteufel at CNWRA
 Subject: "hydro7inf" runs
 Date: 10/10/96 Time: 16:44:40
 To: ronald janetzke at CNWRA-SUN

***** MESSAGE CONTENTS *****

Ron,

Instead of running "hydro" only runs, please make "hydro7inf" runs.

I've modified the appropriate files and they can be found at:

/home/scratchy/randalld/randym/hydro7inf/lshydro7inf.inp
 /home/scratchy/randalld/randym/hydro7inf/tpa.inp

You should use same TPA code as modified for "perc" runs.

In summary, we should have the following runs:

doe
 ipa2data
 matrix
 perc
 wpfail
 hydro7inf
 geochem <- this is new, I will give you files asap
 ebispac <- will need input from Sitakanta or Gustavo, may not get done.

This should complete our set of runs for the phase 1 sensitivity analyses.

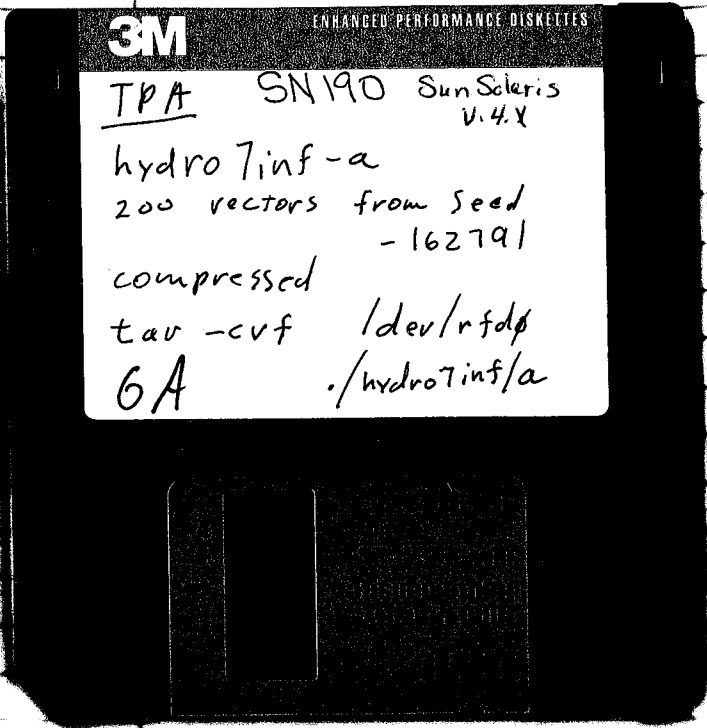
-Randy

Ron Jr.

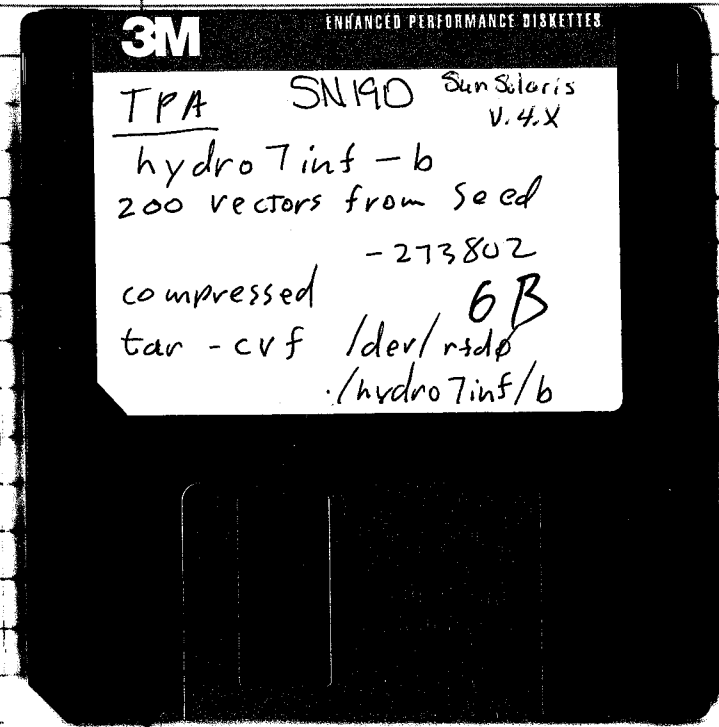
10-11-96

hydro7inf

a



b



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Date Generated:	10/04/1996
Operating System: (including version number)	Sun Solaris Version 4.X; UNIX
Application Used: (including version number)	NA
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	2 - 3 1/2 disks
File Types: (.exe, .bat, .zip, etc.)	Various
Remarks: (computer runs, etc.)	Disks contain: Compressed tar—cvf/dev/rfd0/hydro7inf/a, 200 vectors from seed 162791; and compressed tar—cvf/dev/rfd0/hydro7in/b, 200 vectors from seed 273802

hydro7inf + Perc

This listing shows the changes made to
'flowmod.pre' in 'diff' output format!

Listing for Ron Janetzke

Fri Oct 4 17:47:58

```

9601c9601,9606
<      CALL opnfil (29,'watrel.in','replace',.true.,errnum,errmsg)
-----
> C-rw] 10-4-96
> C      Adjust file attributes to open in appedn moe to capture all vector
> C      output for 'watrel.in' for Detailed Review.
> C
> C      CALL opnfil (29,'watrel.in','replace',.true.,errnum,errmsg)
> C      CALL opnfil (29,'watrel.in','append',.true.,errnum,errmsg)

```



This listing shows the changes made to

'flowmap0000.dat' in 'diff' output format!

Listing for Ron Janetzke

Mon Oct 14 14:34:54

```

1c1
< TITLE: FLOWMOD map file for undisturbed sampled variables from LHS.
-----
> TITLE: FLOWMOD map file for infiltrations sampled for each area.
13a14
> AINFIL      446      7

```



10-14-96

Rwp

This listing shows the changes made to
 'hs20n.inp' in 'diff' output format to
 accomodate the Perc runs!

Listing for Ron Janetzke

Mon Oct 14 14:37:41

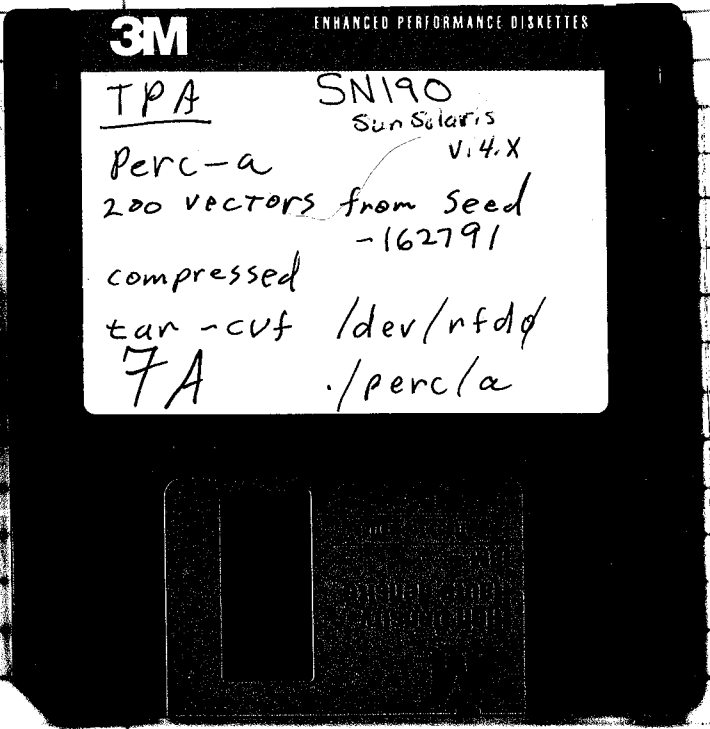
```

1c1
< TITLE - oooo20n, AUDIT96 DOE values by Rob Rice.
---
> TITLE -oooo20n, AUDIT96 DOE values, detailed perm, & zonal infiltrations.
893c893,907
< LOGUNIFORM      infiltration (DOE-disturbed) FLOWMOD infiltration rate (M/yr)
---
> LOGUNIFORM      infiltration (DOE-disturbed) FLOWMOD infiltration rate (M/yr)
> 5.0E-4          2.0e-3
> UNIFORM         infiltration Area #1
> 5.0E-4          2.0e-3
> UNIFORM         infiltration Area #2
> 5.0E-4          2.0e-3
> UNIFORM         infiltration Area #3
> 5.0E-4          2.0e-3
> UNIFORM         infiltration Area #4
> 5.0E-4          2.0e-3
> UNIFORM         infiltration Area #5
> 5.0E-4          2.0e-3
> UNIFORM         infiltration Area #6
> 5.0E-4          2.0e-3
> UNIFORM         infiltration Area #7
  
```

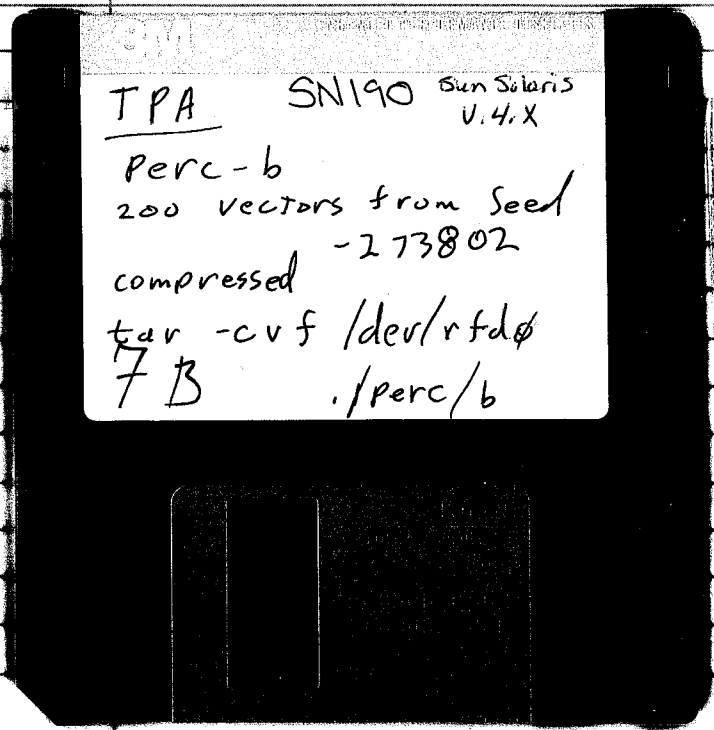
Ron J.

10-14-96

perc



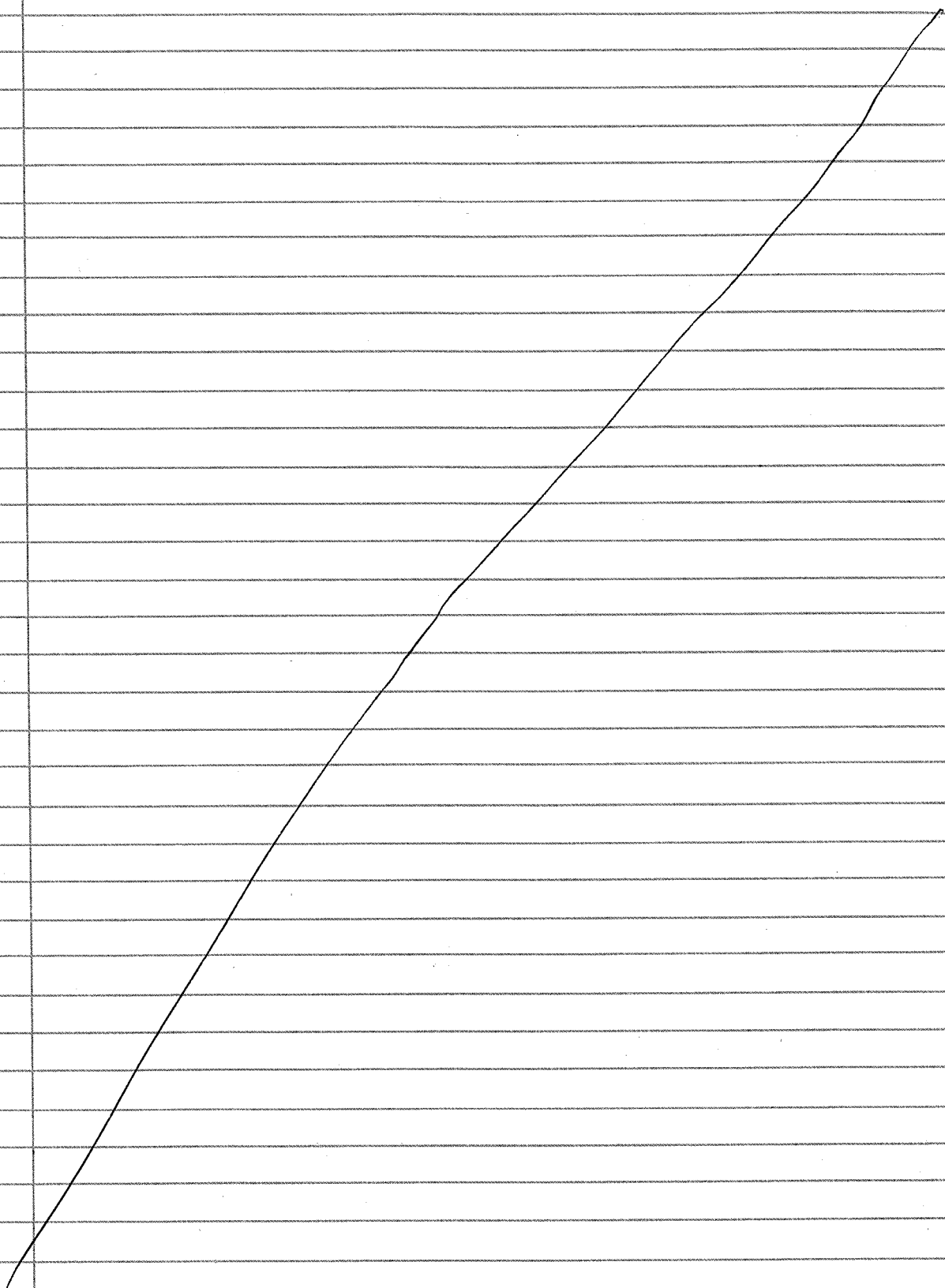
a



b

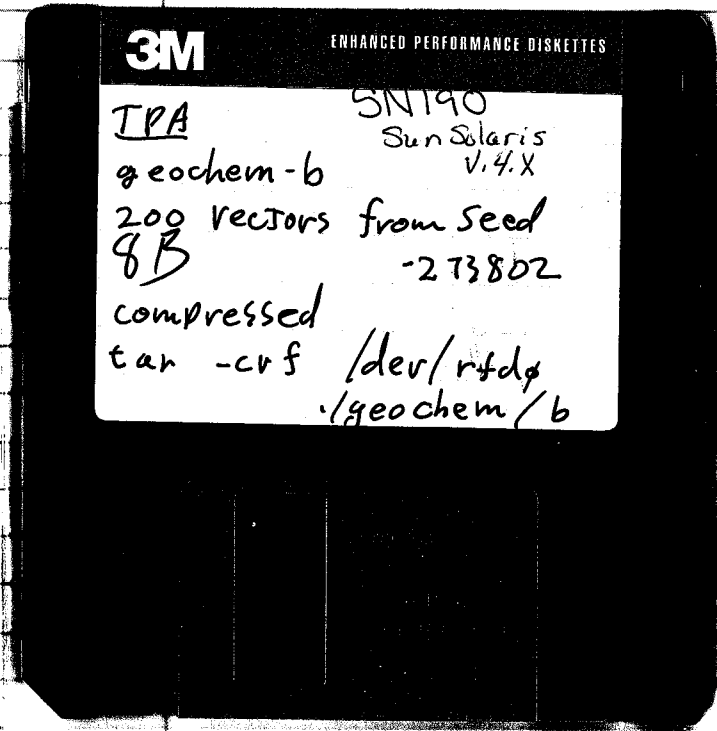
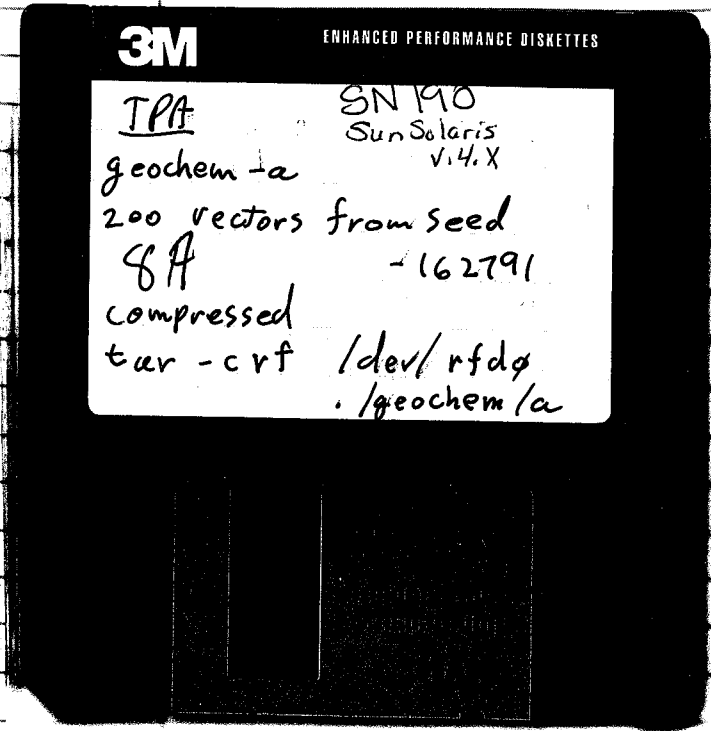
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Contact:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, TX 78228-5166 Attn.: Director of Administration 210.522.5054
Data Sensitivity:	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright
Date Generated:	10/14/1996
Operating System: (including version number)	Sun Solaris Version 4.X; UNIX
Application Used: (including version number)	NA
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	2 - 3 1/2 disks
File Types: (.exe, .bat, .zip, etc.)	Various
Remarks: (computer runs, etc.)	Disks contain: Compressed tar—cvf/dev/rfd0/perc/a, 200 vectors from seed 162791; and compressed tar—cvf/dev/rfd0/perc/b, 200 vectors from seed 273802



geochem

a



b

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK #: 190

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Data Sensitivity:	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright
Date Generated:	10/18/1996
Operating System: (including version number)	Sun Solaris Version 4.X; UNIX
Application Used: (including version number)	NA
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	2 - 3 1/2 disks
File Types: (.exe, .bat, .zip, etc.)	Various
Remarks: (computer runs, etc.)	Disks contain: Compressed tar—cvf/dev/rfd0/geochem/a, 200 vectors from seed 162791; and compressed tar—cvf/dev/rfd0/geochem/b, 200 vectors from seed 273802

Curium (Cm):

DOE
log triangular g/m³ mol/L
Min: log(1.2e-6) log(4.9e-12)
Max: log(1.2e-4) log(4.9e-10)
Mean/Peak: log(1.2e-5) log(4.9e-11)
Source: Jardine (1991)

NRC
triangular
Min: 1.2e-6
Max: 1.2e-4
Mean/Peak: 1.2e-5
Source: DOE values.

Recommended
uniform g/m³ mol/L
Min: 2.4e-5 1.0e-10
Max: 2.4e-1 1.0e-6
Mean/Peak: 1.2e-1 5e-7
Rationale: Analogy with Am³⁺ (see Fuger, 1992; 1993)

Uranium:

DOE
log beta g/m³ mol/L
Min: log(2.4e-3) log(1.0e-8)
Max: log(2.4e+3) log(1.0e-2)
Mean/Peak: log(7.6) log(3.2e-5)
Source: Elicitation

NRC
triangular
Min: 2.4e-3
Max: 2.4e+3
Mean/Peak: 7.6
Source: DOE values.

Recommended
triangular
Min: 2.4e-3
Max: 2.4e+3
Mean/Peak: 7.6
Rationale: Keep current values, which compare well with literature data.

Americium:

DOE
uniform g/m³ mol/L
Min: 2.4e-5 1.0e-10
Max: 2.4e-1 1.0e-6
Mean/Peak: 1.2e-1 5e-7
Source: Elicitation. (Note: biased towards 10⁻⁶ M)

NRC
uniform
Min: 2.4e-5
Max: 2.4e-1
Mean/Peak:
Source: DOE values.

Recommended
uniform
Min: 2.4e-5
Max: 2.4e-1
Mean/Peak:
Rationale: Keep current values, which compare well with literature data.

Neptunium:

DOE
log beta g/m³ mol/L
Min: log(1.2) log(5e-6)
Max: log(2.4e+3) log(1.0e-2)
Mean/Peak: log(3.4e+1) log(1.4e-4)
Source: Elicitation

NRC
triangular
Min: 1.2
Max: 2.4e+3
Mean/Peak: 3.4e+1
Source: DOE values.

Recommended
triangular
Min: 1.2
Max: 2.4e+3
Mean/Peak: 3.4e+1
Rationale: Keep current values, which compare well with literature data.

Plutonium:DOE

<i>uniform</i>	g/m^3	mol/L
Min:	$2.4\text{e-}3$	$1.0\text{e-}8$
Max:	$2.4\text{e-}1$	$1.0\text{e-}6$
Mean/Peak:	$1.2\text{e-}1$	$5.1\text{e-}7$
Source:	Elicitation. (Note: biased towards 10^{-6} M).	

NRC

<i>uniform</i>	
Min:	$2.4\text{e-}3$
Max:	$2.4\text{e-}1$
Mean/Peak:	
Source:	DOE values.

Recommended

<i>uniform</i>	
Min:	$2.4\text{e-}3$
Max:	$2.4\text{e-}1$
Mean/Peak:	

Rationale: Keep current values, which compare well with literature data.

Thorium:DOE

<i>log uniform</i>	g/m^3	mol/L
Min:	$\log(2.3\text{e-}5)$	$\log(1.0\text{e-}10)$
Max:	$\log(2.3\text{e-}2)$	$\log(1.0\text{e-}7)$
Mean/Peak:	$\log(7.3\text{e-}4)$	$\log(3.2\text{e-}9)$
Source:	Elicitation	

NRC

<i>log uniform</i>	
Min:	$2.3\text{e-}5$
Max:	$2.3\text{e-}2$
Mean/Peak:	
Source:	DOE values.

Recommended

<i>log uniform</i>	g/m^3	mol/L
Min:	$\log(2.3\text{e-}4)$	$\log(1.0\text{e-}9)$
Max:	$\log(2.3\text{e+}2)$	$\log(1.0\text{e-}3)$
Mean/Peak:	$\log(2.3\text{e-}1)$	$\log(1.0\text{e-}6)$

Rationale: New solubility data in carbonate containing systems (Osthols et al, 1994; Rai et al., 1995)

Radium:

DOE		
log beta	g/m ³	mol/L
Min:	log(2.3e-4)	log(1.0e-9)
Max:	log(2.3)	log(1.0e-5)
Mean/Peak:	log(2.3e-2)	log(1.0e-7)
Source:	Elicitation	

NRC	
triangular	
Min:	2.3e-4
Max:	2.3
Mean/Peak:	2.3e-2
Source:	DOE values.

Recommended	
triangular	
Min:	2.3e-4
Max:	2.3
Mean/Peak:	2.3e-2

Rationale: Keep current values. Consistent with EQ3 and MINTEQ calculated solubility of radium sulfate.

Lead:

DOE		
log beta	g/m ³	mol/L
Min:	log(2.1e-3)	log(1.0e-8)
Max:	log(2.1)	log(1.0e-5)
Mean/Peak:	log(6.6e-2)	log(3.2e-7)
Source:	Elicitation	

NRC	
triangular	
Min:	2.1e-3
Max:	2.1
Mean/Peak:	6.6e-2
Source:	DOE values.

RR

Recommended

triangular

Min: 2.1e-3
Max: 2.1
Mean/Peak: 6.6e-2

Rationale: Keep current values. Consistent with EQ3 solubility calculations using various Pb minerals.

Cesium:

DOE

	<i>log triangular</i>	<i>g/m³</i>	<i>mol/L</i>
Min:	log(1.2)		9.0e-6
Max:	log(2.1e+3)		1.6e-2
Mean/Peak:	log(3.9e+2)		2.9e-3
Source:	Golder (1993); EPRI (1992)		

NRC

triangular

Min: 1.2
Max: 2.1e+3
Mean/Peak: 3.9e+2
Source: DOE values.

Recommended

	<i>constant</i>	<i>g/m³</i>	<i>mol/L</i>
Min:		1.35e+5	1.0
Max:		1.35e+5	1.0
Mean/Peak:			

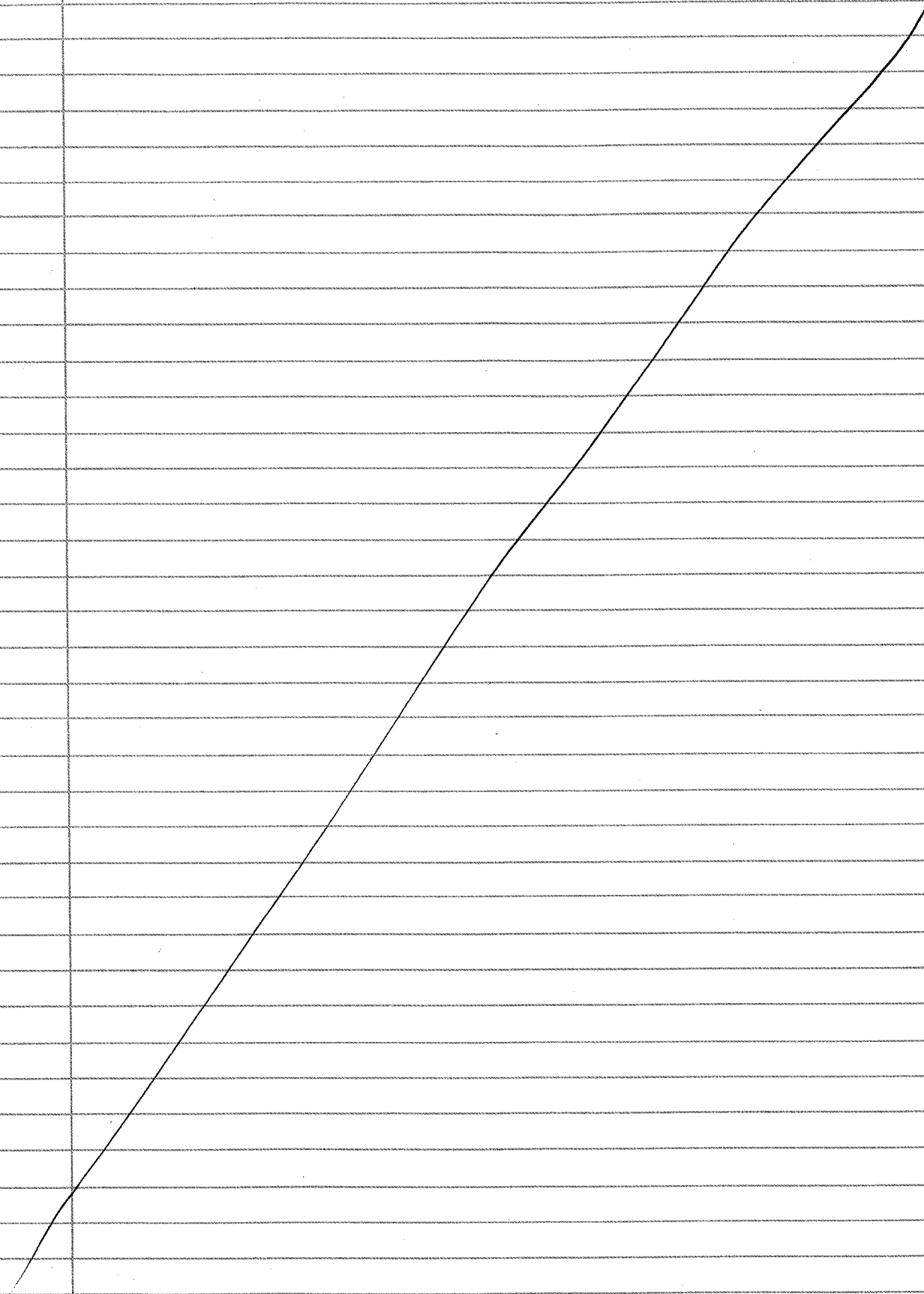
Rationale: No solubility controlling phase. Assume 1.0 mol/L, which converts to 1.35e+5 g/m³ (or 1.35e+2 kg/m³).

Iodine:

DOE

	<i>constant</i>	<i>g/m³</i>	<i>mol/L</i>
Min:			1.0
Max:			1.0
Mean/Peak:			
Source:	Elicitation		

RJ



NRC

constant

Min: 1.0e+3

Max: 1.0e+3

Mean/Peak:

Source: Unknown.

Recommended

constant

Min: 1.29e+5

Max: 1.29e+5

Mean/Peak:

Rationale: No solubility controlling phase. DOE used 1.0 mol/L, which converts to 1.29e+5 g/m³ (or 1.29e+2 kg/m³).

Technetium:

DOE

log triangular g/m³ mol/L

Min: log(3.5e-2) log(3.6e-7)

Max: log(9.9e+5) log(1.0e+1)

Mean/Peak: log(1.0e+2) log(1.0e-3)

Source: Elicitation

NRC

constant

Min: 1.0e+3

Max: 1.0e+3

Mean/Peak:

Source: Unknown.

Recommended

constant

Min: 9.9e+4

Max: 9.9e+4

Mean/Peak:

Rationale: No solubility controlling phase under oxidizing conditions. Assume 1.0 mol/L which converts to 9.9e+4 g/m³ (or 9.9e+1 kg/m³).

Handwritten initials or signature.

Nickel:DOE

<i>log beta</i>	g/m^3	mol/L
Min:	$\log(5.9\text{e-}2)$	$\log(1.0\text{e-}6)$
Max:	$\log(5.9\text{e+}3)$	$\log(1.0\text{e-}1)$
Mean/Peak:	$\log(1.1\text{e+}2)$	$\log(1.8\text{e-}3)$
Source:	Elicitation	

NRC*triangular*

Min:	$5.9\text{e-}2$
Max:	$5.9\text{e+}3$
Mean/Peak:	$1.1\text{e+}2$
Source:	DOE values.

Recommended*triangular*

Min:	$5.9\text{e-}2$
Max:	$5.9\text{e+}3$
Mean/Peak:	$1.1\text{e+}2$

Rationale: Keep current values. EQ3 calculated solubility for Ni_2SiO_4 is much lower than mean value.

Carbon:DOE

<i>constant</i>	g/m^3	mol/L
Min:		1.0
Max:		1.0
Mean/Peak:		
Source:	Elicitation	

NRC*constant*

Min:	$1.0\text{e+}3$
Max:	$1.0\text{e+}3$
Mean/Peak:	
Source:	Unknown.

Recommended
constant

Min: 1.4e+4
Max: 1.4e+4

Mean/Peak:

Rationale: Assumed gaseous release and no solubility controlling phase. DOE used 1.0 mol/L, which converts to 1.4e+4 g/m³ (or 1.4e+1 kg/m³).

Selenium:

DOE

log triangular	g/m ³	mol/L
Min:	log(7.9e+2)	log(1.0e-2)
Max:	log(5.5e+5)	log(7.0)
Mean/Peak:	log(7.9e+3)	log(1.0e-1)
Source:	Golder (1993); EPRI (1992)	

NRC

constant
Min: 1.0e+3
Max: 1.0e+3
Mean/Peak:
Source: Unknown.

Recommended
constant

Min: 7.9e+4
Max: 7.9e+4

Mean/Peak:

Rationale: Assume release of radionuclide is controlled by waste form dissolution. High value of 1.0 mol/L is used for solubility, which converts to 7.9e+4 g/m³ (or 7.9e+1 kg/m³).

Niobium:

DOE

log uniform	g/m ³	mol/L
Min:	log(9.3e-5)	log(1.0e-9)
Max:	log(9.3e-3)	log(1.0e-7)
Mean/Peak:	log(9.3e-4)	log(1.0e-8)
Source:	Elicitation	

NRC*log uniform*

Min: 9.3e-5

Max: 9.3e-3

Mean/Peak:

Source: DOE values.

Recommended*log uniform*

Min: 9.3e-5

Max: 9.3e-3

Mean/Peak:

Rationale: Keep current values. No better solubility data available.

Tin (Sn):DOE*uniform*g/m³

mol/L

Min: 1.2e-6

1.0e-11

Max: 1.2e-2

1.0e-7

Mean/Peak: 6.0e-3

5.0e-8

Source: Elicitation. (Note: biased towards 10⁻⁷ m).NRC*uniform*

Min: 1.2e-6

Max: 1.2e-2

Mean/Peak:

Source: DOE values.

Recommended*uniform*

Min: 1.2e-6

Max: 1.2e-2

Mean/Peak:

Rationale: Keep current values. Low solubility consistent with experimental data.

Zirconium:

DOE
log uniform g/m³ mol/L
Min: log(9.1e-8) log(1.0e-12)
Max: log(9.1e-3) log(1.0e-7)
Mean/Peak: log(2.9e-5) log(3.2e-10)
Source: Elicitation

NRC
log uniform
Min: 9.1e-8
Max: 9.1e-3
Mean/Peak:
Source: DOE values.

Recommended
log uniform
Min: 9.1e-8
Max: 9.1e-3
Mean/Peak:
Rationale: Keep current values. No better data available.

Strontium:

DOE (not considered)
 g/m³ mol/L
Min:
Max:
Mean/Peak:
Source:

NRC
constant
Min: 8.2e+1
Max: 8.2e+1
Mean/Peak:
Source: Unknown.

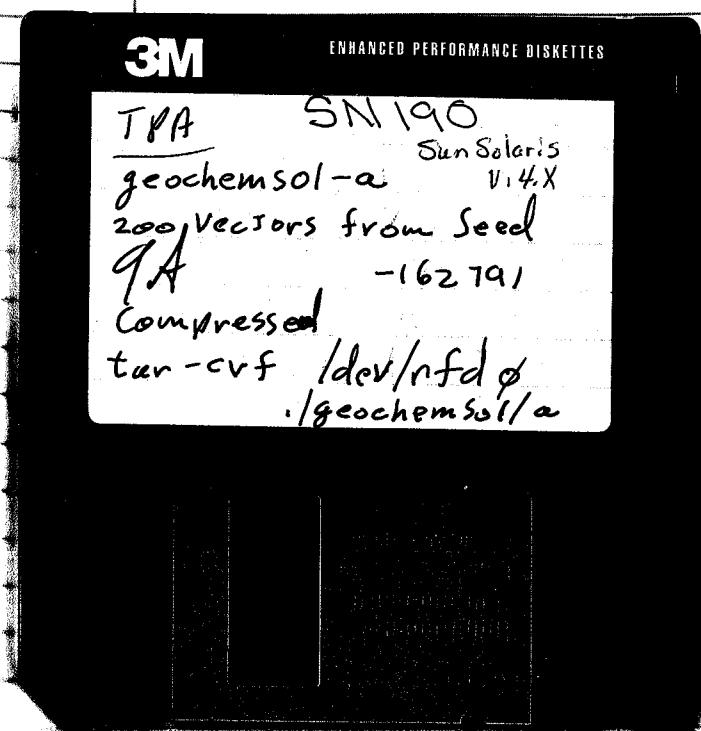
Recommended~~log triangular~~ normalMin: $\log(8.7e-2)$ Max: $\log(8.7e+1)$ ~~Mean/Peak: $\log(2.8)$~~ Rationale: EQ3 calculated solubility of SrCO_3 for a range of solution composition from J-13-type to UE25p#1-type.

RDM 10/20/96

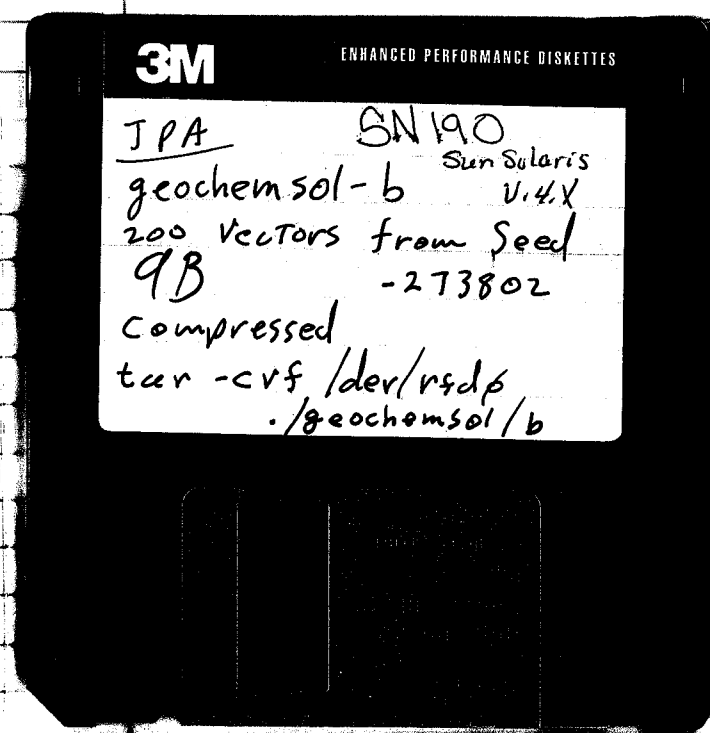
RDM 10-20-96

geochemsol

a

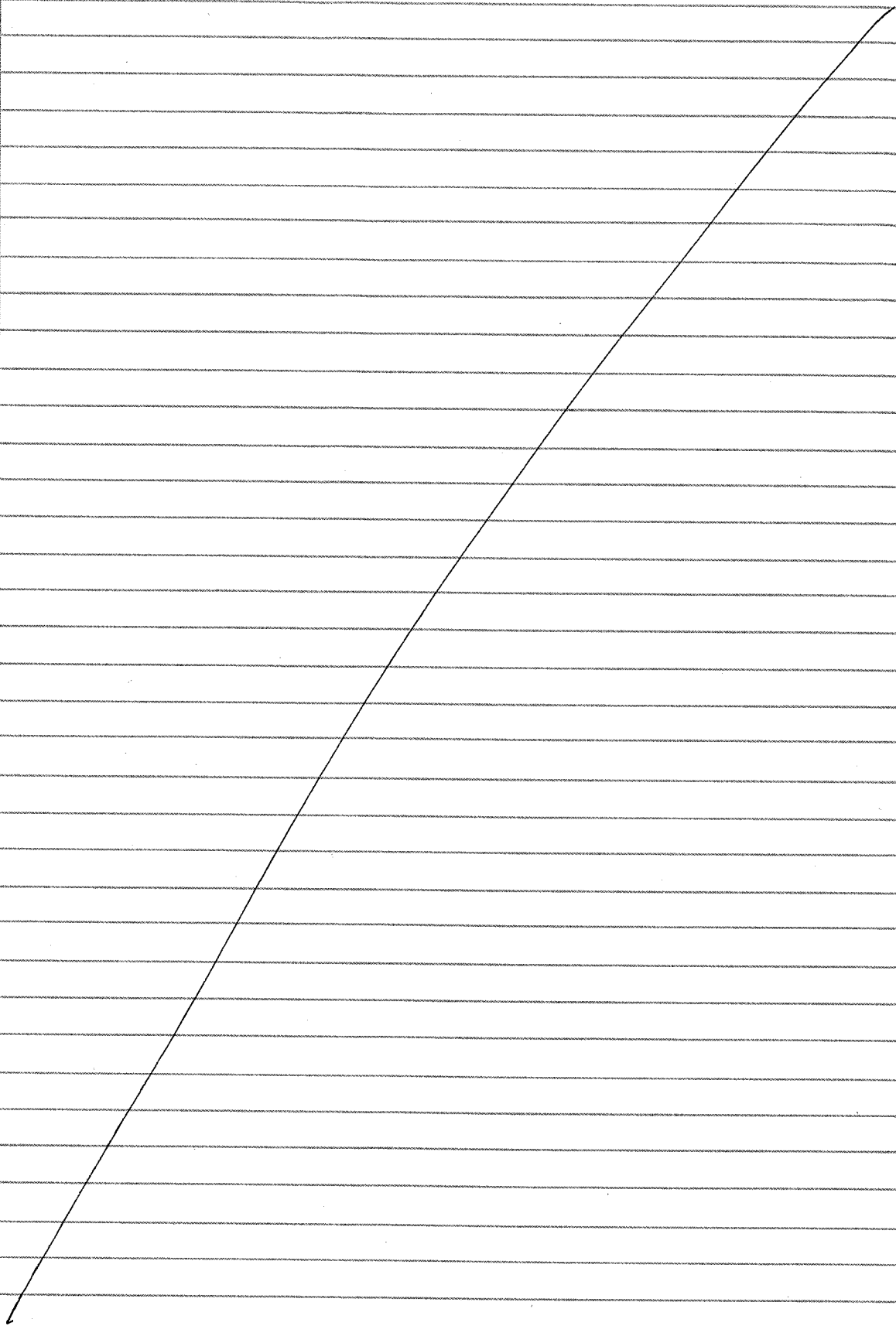


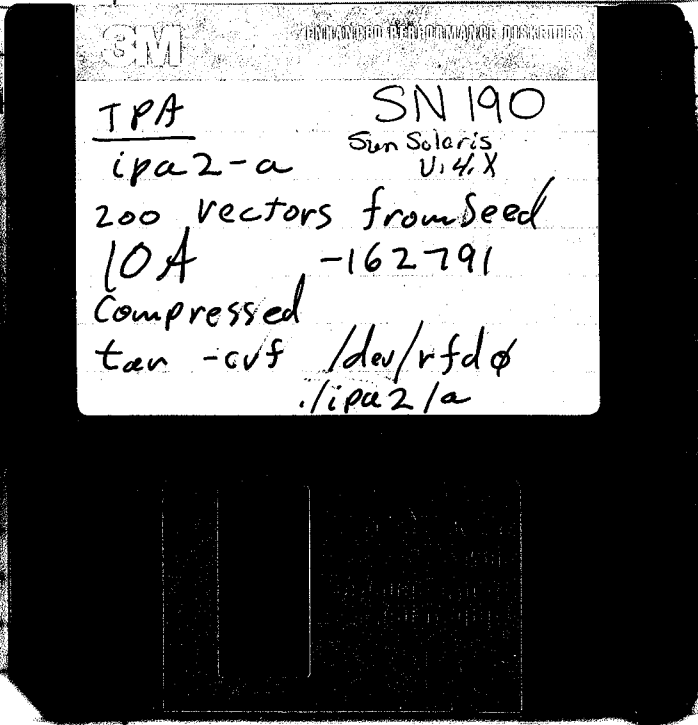
b



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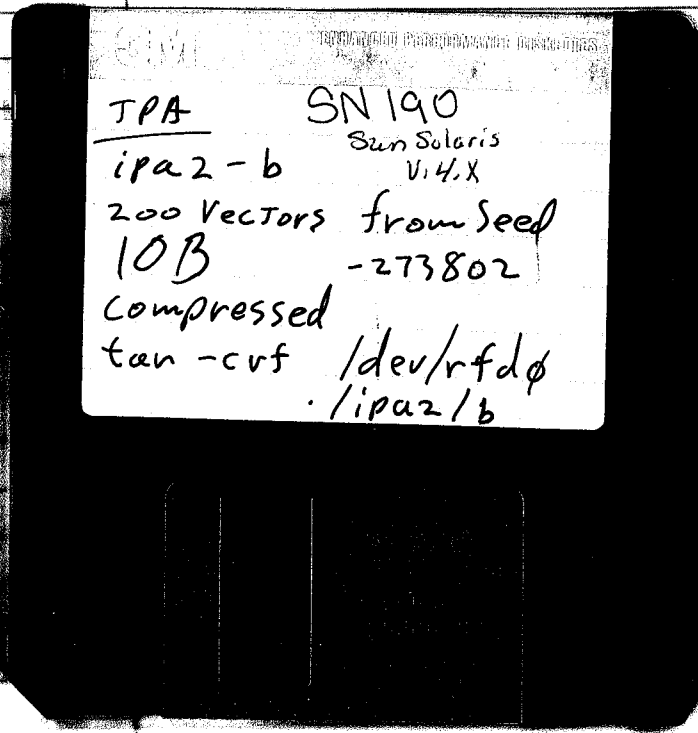
Document Date:	09/09/1996
Availability:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, Texas 78228
Contact:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, TX 78228-5166 Attn.: Director of Administration 210.522.5054
Data Sensitivity:	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright
Date Generated:	10/20/1996
Operating System: (including version number)	Sun Solaris Version 4.X; UNIX
Application Used: (including version number)	NA
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	2 - 3 1/2 disks
File Types: (.exe, .bat, .zip, etc.)	Various
Remarks: (computer runs, etc.)	Disks contain: Compressed tar—cvf/dev/rfd0/geochemsol/a, 200 vectors from seed 162791; and compressed tar—cvf/dev/rfd0/geochemsol/b, 200 vectors from seed 273802





ipa2

a



b

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Data Sensitivity:	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright		
Date Generated:	01/13/1997		
Operating System: (including version number)	Sun Solaris Version 4.X; UNIX		
Application Used: (including version number)	NA		
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	2 - 3 ½ disks		
File Types: (.exe, .bat, .zip, etc.)	Various		
Remarks: (computer runs, etc.)	Disks contain: Compressed tar—cvf/dev/rfd0/ipa2/a, 200 vectors from seed 162791; and compressed tar—cvf/dev/rfd0/ipa2/b, 200 vectors from seed 273802		

I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient technical information so that another qualified individual could repeat the work

PG/Zaca 1/13/97

First Additional Set of Detailed Review Runs

A set of 3 additional runs are requested.

See e-mail on next page. Before this can be done the 'nefmks.e' file

must be reinstated to its phase 2

operational mode, that is the 'watrel.in'

file must NOT be an appended file

but rather a new file for each

Vector. The source file for this

mode is on scratchy in

/home/scratchy/janetke/audit96/neftran/nefmksipar.pre;

Author: Robert Baca at cnwra-os2
 Subject: Re: TPA detailed review runs
 Date: 01/20/97 Time: 14:12:24
 To: Ronald Janetzke at CNWRA-SUN

***** MESSAGE CONTENTS *****

Bob,

Could you send me an e-mail on the purpose of each of the 3 runs we are doing so it can be included in the scientific notebook?

Thanks,
 ron j

=====

Ron:

The purpose of the 3 runs is to produce CCDFs for cumulative release for use in the Detailed Review of TSPA-95. We found in the Audit Review of TSPA-95 that our temperature and relative humidity calculations were different than those presented by DOE in TSPA-95. In two of the TPA runs, we will evaluate the significance of the T & RH histories. The third run will examine the impact of matrix diffusion, by looking at the case where there is only matrix flow.

These results will be documented in our Detailed Review report to NRC which is an IM at the end of February.

Cheers, Bob.

1-22-97

Also, 'flowmod.e' must be returned to its phase 2 mode where one infiltration value is sampled. The source file for this mode is 'home/scratchy/janetzke/audit96/flowmod/flowmodipa2.pre' or the executable 'flowmodipa2.e' may be use directly having the same path. The accompanying map file for this mode is 'flowmap0000.dat'.

SCRATCHY 1

TPA-Audit96 was installed on scratchy1 by using the old taraudit96 file on scratchy. Then the phase 2 versions of 'nefmks.e', 'flowmod.e', 'flowmap.dat' were transferred to scratchy1. Also, 'lhs.e' was transferred to .../seismic/ on scratchy1.

The following 3 runs are defined
with disk directories on scratchy

ebsfail/dae

ebs fail

hydro7mat

ebs fail/dae

The 'corproxy' input file was prepared
by Rob Rice and is called 'tspae.inp'.

'lhs.e' was executed with this file

specified as input in the configuration

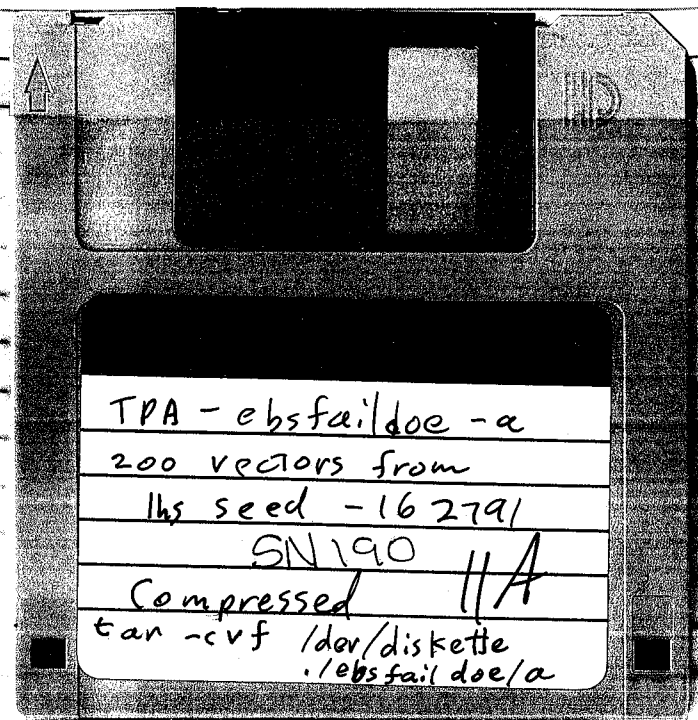
file 'TPA_LHS.LGD'. 200 vectors

were run for the TPA system and

results were stored in .../ebstfail/dae/a.

The 2 yellow notes, 2 graphs, and case
description which follow were received
from Rob Rice.

Ron Jr. 1-22-97



ebsfaildae

a

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Data Sensitivity:	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright	
Date Generated:	01/22/1997	
Operating System: (including version number)	Sun Solaris Version 4.X; UNIX	
Application Used: (including version number)	NA	
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	2 - 3 1/2 disks	
File Types: (.exe, .bat, .zip, etc.)	Various	
Remarks: (computer runs, etc.)	Disks contain: Compressed tar—cvf/dev/rfd0/ebsfail doe/a, 200 vectors from seed 162791	

RJ
 Ron,
 the files are located:

1/16/97

/home2/sierra/baca/albert/plots
 called:
 cor/hs.inp (DOE) - used w/ matrix hydro
 + spa.inp (EBSPAC TSPA) - w/o
 auditrev.inp (EBSPAC audit review) coupling
 Thanks RJ

RJ
 Ron,

UNDER /home2/sierra/baca/albert/plots,

the files → /hs20n.matrixhydro.inp
 → +spa.matrixhydro.inp
 will be used for the 3rd run (matrix hydro)
 Bob wants the infiltration sampled for
 each subarea (i.e., 7 times) - as in the
 hydro7infil case. Thanks RJ

1-22-97

20

Description of TPA 2.0 Cases

Case	Input Source	Waste Package Failure Source	Other Changes
1	TSPA-95 Data (Baseline)	EBSPAC (TSPA-95)	
2	TSPA-95 Data (Baseline)	EBSPAC (Audit Review)	
3	MATRIX Input File	TSPA-95	HYDRO7INFIL hydrostratigraphy and Infiltration

1-22-97

The following files will be archived
after each run:

ccdf.fmt

corlks.out

lks20n.inp

lks0000.out

pathre.fmt

scnrel.fmt

tpa.inp

corlks.inp

Ken J

1-22-97

ebsfail

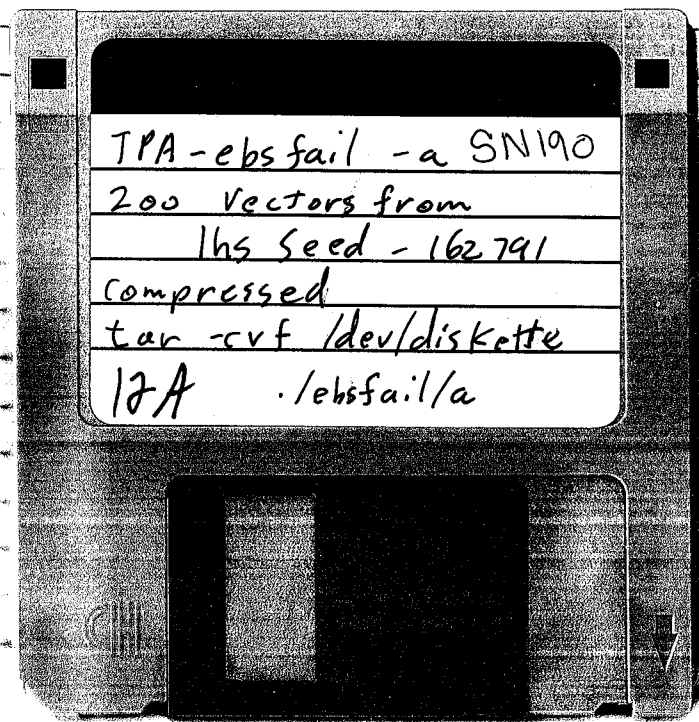
File auditrev.inp was used as input to

lks.e to create corlks.out.

200 Vectors were submitted & run.

Ken J

1-23-97



ebsfail
a

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Data Sensitivity:	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright		
Date Generated:	01/24/1997		
Operating System: (including version number)	Sun Solaris Version 4.X; UNIX		
Application Used: (including version number)	NA		
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	2 - 3 ½ disks		
File Types: (.exe, .bat, .zip, etc.)	Various		
Remarks: (computer runs, etc.)	Disks contain: Compressed tar—cvf/dev/rfd0/ebsfail doe/a, 200 vectors from seed 162791		

hydro7mat

flomap7inf.dat was copied from

1001/janetake/audit96/flowmod to 0500.

flowmod2int.e was also copied from

1001/janetake/audit96/flowmod to flowmod.

tpa.matrixhydro.inp was copied to 0500/tpa.inp.

This file was corrected for a bad

ANALYST data field.

It was also modified to point to

flomap7inf.dat, and to enable post

NEFTXAN modules to run.

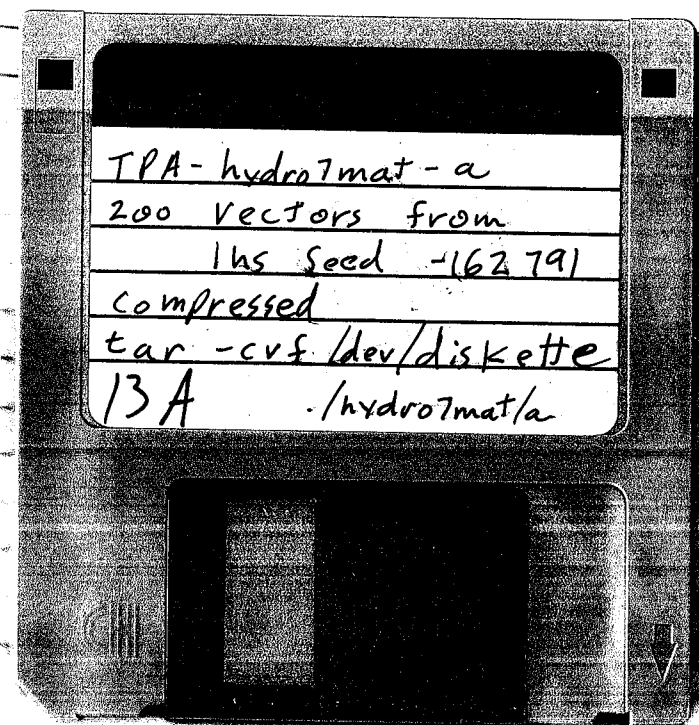
1hs20n.matrixhydro.inp was copied to

0500/1hs20n.inp. This file was

corrected for a bad title line.

Ron J

1-24-97



hydro7mat

a

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK #: 190

Document Date:	09/09/1996
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:	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright
Date Generated:	04/15/1997
Operating System: (including version number)	Sun Solaris Version 4.X; UNIX
Application Used: (including version number)	NA
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	2 - 3 1/2 disks
File Types: (.exe, .bat, .zip, etc.)	Various
Remarks: (computer runs, etc.)	Disks contain: Compressed tar—cvf/dev/rfd0/hydro7mat/a, 200 vectors from seed 162791

CAR-96-01

Installation Test for TPA-2 on SUN
Platform.

A 50 Vector run was performed in
/vphi/scratchy/janetzke/zke/00002phi5phi

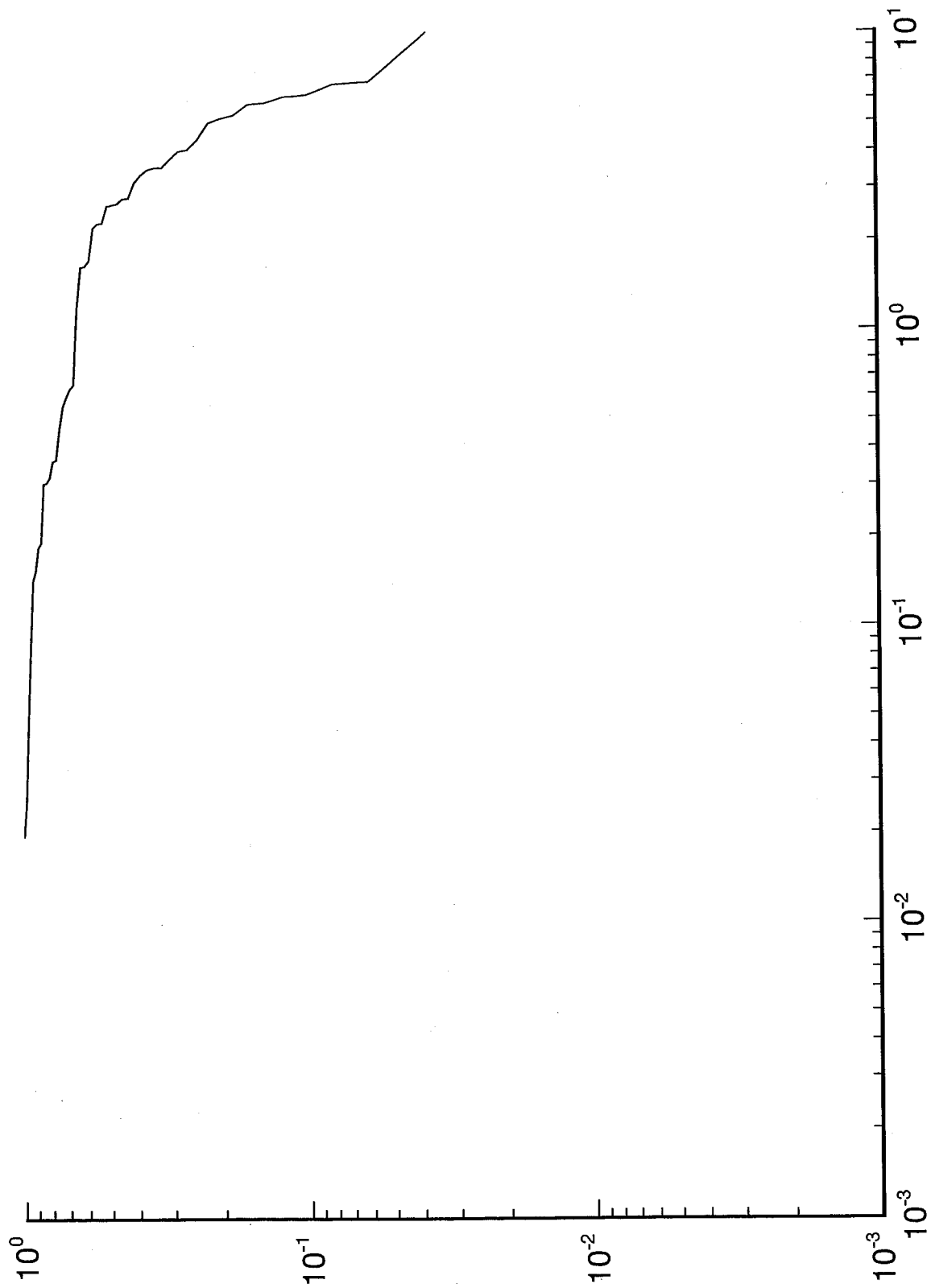
The resulting ccdt was plotted & compared
To The ccdt from The CRAY in
/lan/ra/rjanetzke/zke/00002phi5phi/ccdf5phi.dat.

The run compares favorably, but is
NOT exact. IT is assumed that the
difference is due to the difference
in precision between the two
machines. See next page.

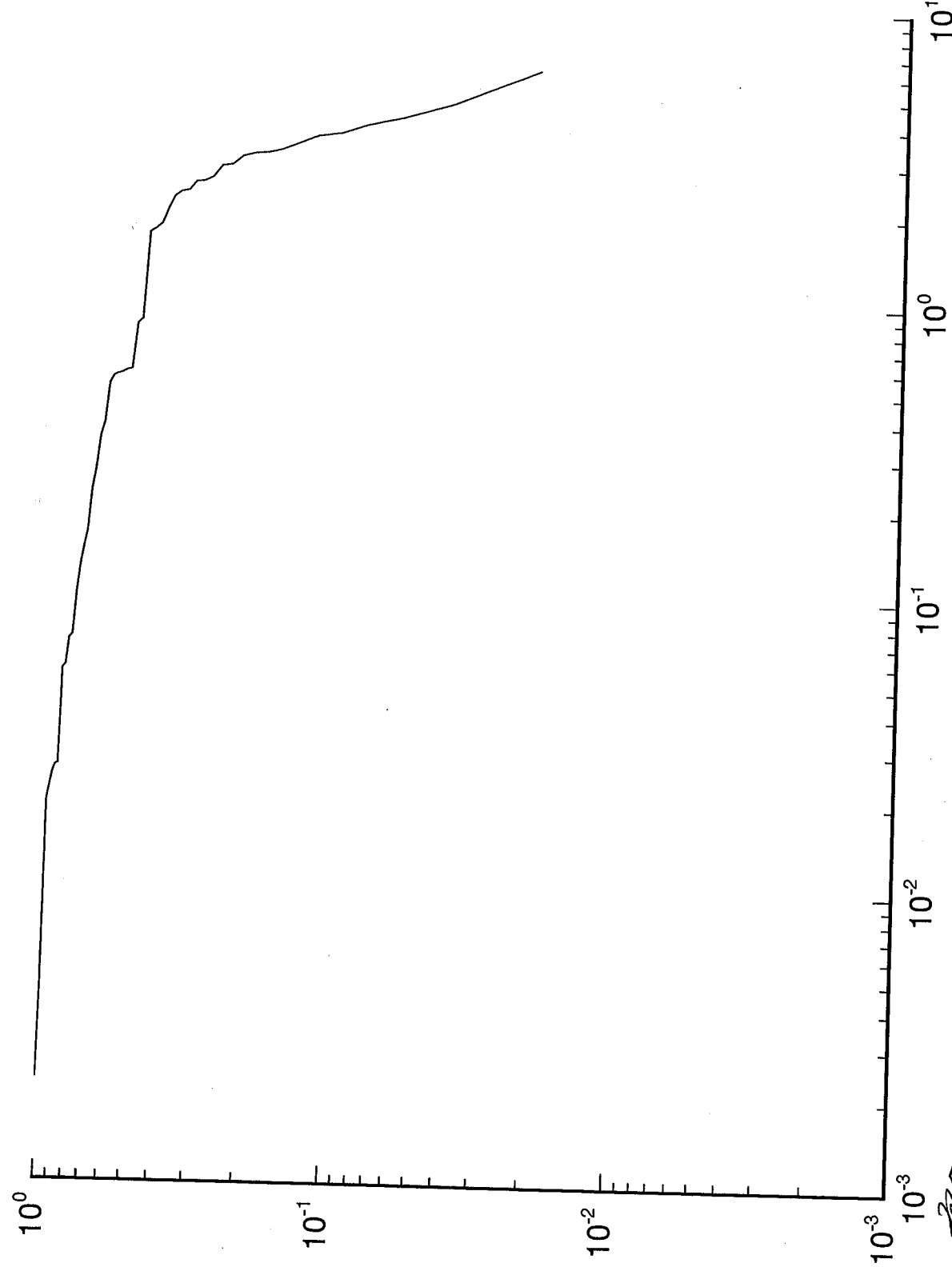
Ron Jr.

4-15-97

4-15-97 rint || 14 Apr 1997 || ccdf50v.plt || Scenario CCDF for 4/23 000020n50v case, DITTY food run, DOSIRR=0.



nt || 14 Apr 1997 || ccdf50vian.plt || Scenario CCDF for 4/23 000020n50v case, DITTY food run, DOSIRR=0.



TPA2 Acceptance Test

The acceptance Test directory was located on scratch1. It is

/V01/scratch/jano1zke/ake/0000

The following files were put on diskette from this directory:

tan -cvt /dev/diskette
 1h5000a.out
 tpa.inp
 ccd.f.dat

Although The Title of these files, usually in line 1, does not reflect

The contents of a 50 vector run, it is obvious from the input data that this run is the same as the 50 vector run on the CRAY.

The SUN test run was performed on July 28, 1995.

The CRAY directory is located in
/lan/pa/rjanetzke/zke/000020n50v

The following files were put on
diskette using 'tar -crf /dev/diskette'

hs0000.out
tpa.inp
ccdf50v.dat

This disk is labeled 'TPA2/CRAY'.

The SUN disk is labeled 'TPA2/SUN'.

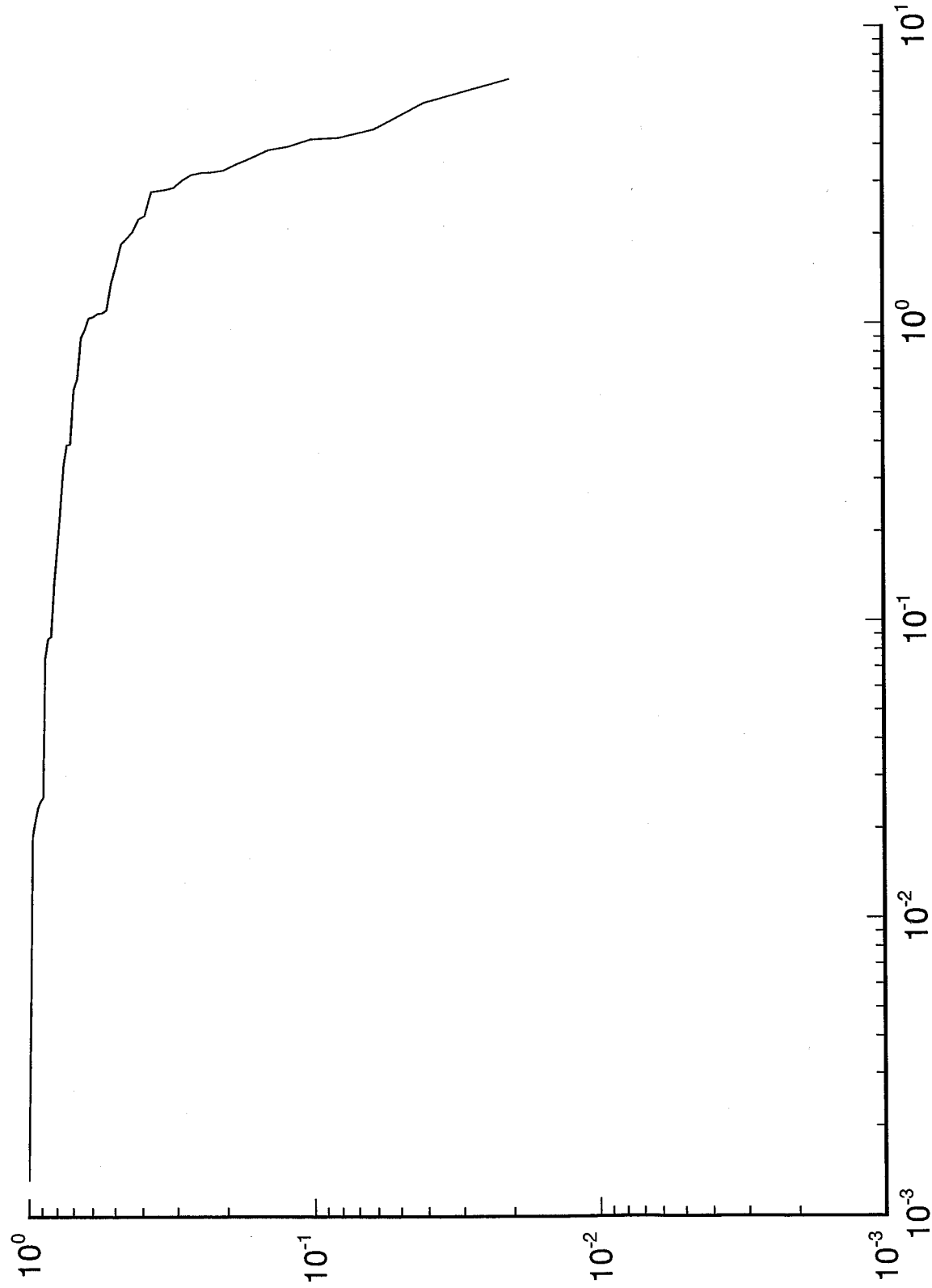
The ccdf plots are presented on the
following pages. The original CRAY
files are dated Apr 23, 1993

The diskettes are included after
the plots.

There are only minor differences in
the curve, and these may be attributed
to the differences in machine
precision.

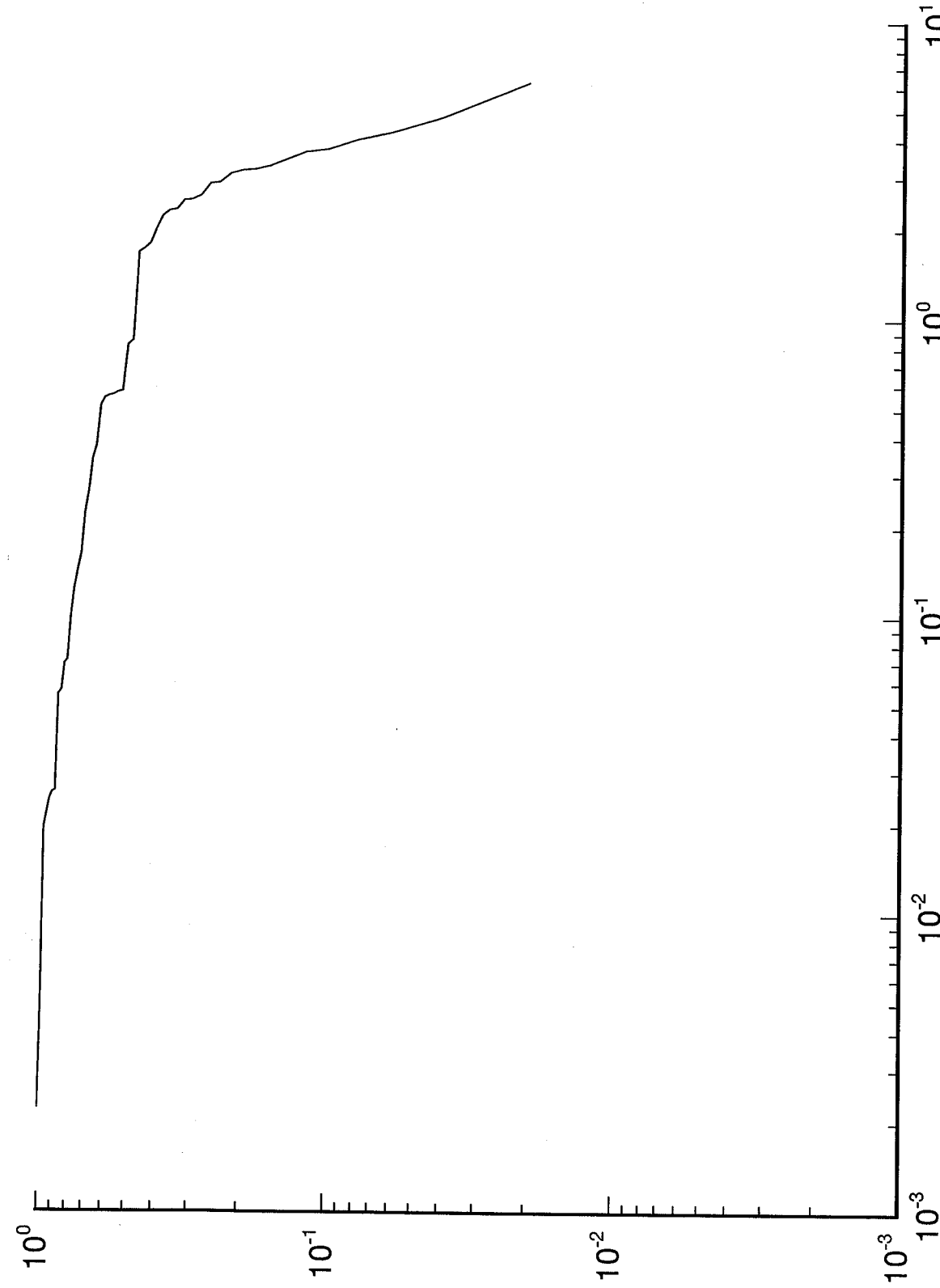
Print || 16 Apr 1997 || ccdf.plt || Scenario CCDF for 000020n2v case, SUN test.

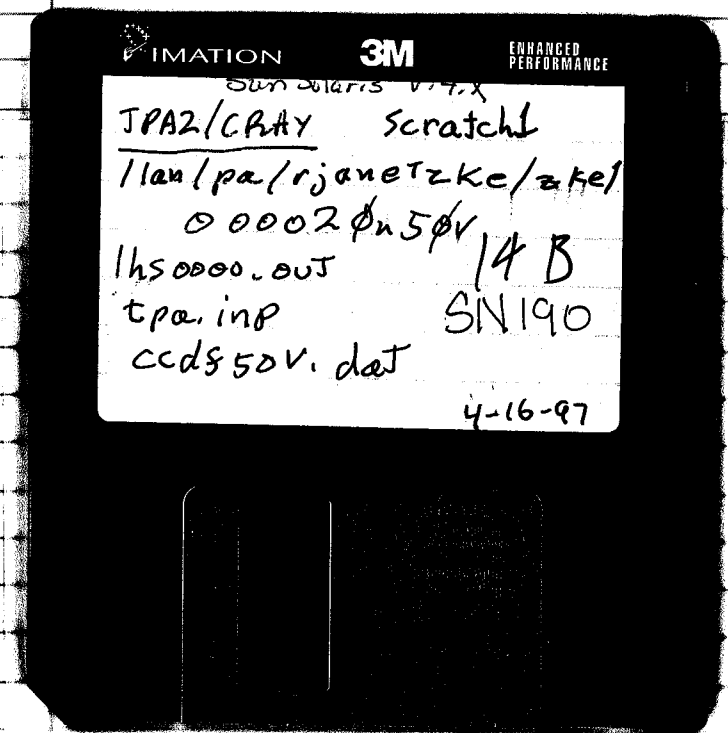
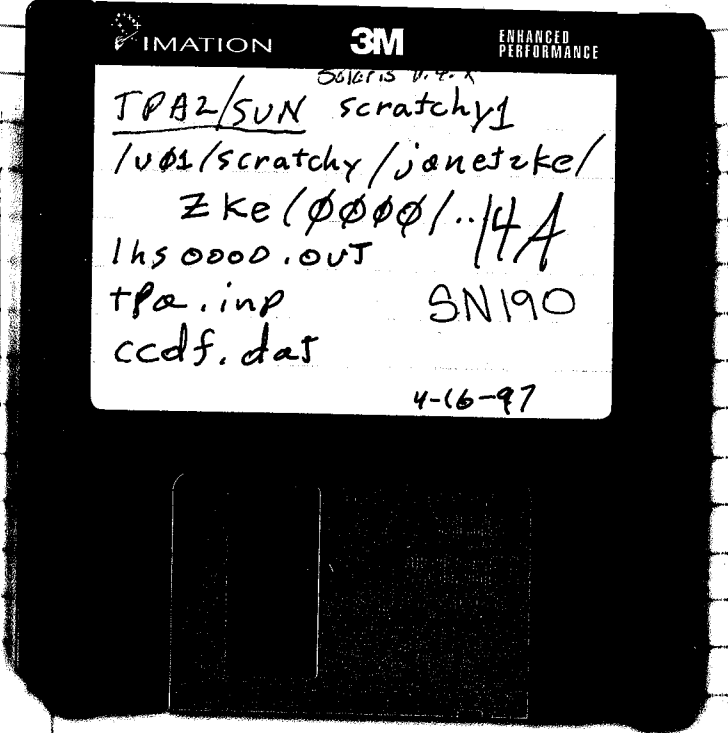
4-16-97



4-16-97

Print || 16 Apr 1997 || ccdf50v.plt || Scenario CCDF for 4/23 000020n50v case, DITTY food run, DOSIRR=0.





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Date Generated:	04/16/1997		
Operating System: (including version number)	Sun Solaris Version 4.X; UNIX		
Application Used: (including version number)	NA		
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	2 - 3 ½ disks		
File Types: (.exe, .bat, .zip, etc.)	Various		
Remarks: (computer runs, etc.)	Disks contain: Input/Output files—TPA2/SUN; TPA2/CRAY		

"I have reviewed the scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding procedures used for conducting tests, acquiring and analyzed data so that another qualified individual could repeat the activity."

Gordon Wittmeyer 2/25/97

(Element Manager signature and date above line,
Name of Element beneath line).

Gordon Wittmeyer

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Date Generated:	01/22/1997
Operating System: (including version number)	Sun Solaris Version 4.X; UNIX
Application Used: (including version number)	NA
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	(2) 8-mm tapes
File Types: (.exe, .bat, .zip, etc.)	Various
Remarks: (computer runs, etc.)	Tapes contain: All files relative to Scientific Notebook 190