SCIENTIFIC NOTEBOOK

170-5E

SCIENTIFIC NOTEBOOK No. 170-5e

by

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J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e

INITIAL ENTRIES

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Participants: Ron Janetzke
Jose M. Menchaca

Sep 16, 1999 - Modification and testing of interpolation module

Received two files by mail from Ron Janetzke, test.f and test1.f

The file test1.f is a test program to exercise the old ainterl function found in the tpa module array.f. The file test.f is a similar test program intended to exercise the new binary search interpolate function.

Results this day were hampered by the fact that there is a unix command called test. When I compiled test.f with Makefile_test, which generated an executable named test, and then executed it, no output would be generated.

Sept 17, 1999 - Modification and testing of interpolation module (continued)

After discovering the unix test command name conflicted with the test executable that

I was generating I was able to verify that the two functions were giving identical results. Using a modulus command to periodically print the output of the controlling program to a file, I then compared the two files with a diff command and found no differences in the two files. The time savings was significant for these tests. What took the old test1.f 122 seconds to complete only required 3.2 seconds for the test program. These tests were conducted in the directory /home/jmench/interpolate.

Modified array.f by replacing the ainterl function with the new method. Ran comparison tests for 1 vector base case and 50 vector base case. Outputs from the two runs was identical with only the time stamp in the header information being different. The time savings here is not as apparent. These experiments were conducted in /home/jmench/runs/tpa33.

Sept 20, 1999 - Modification and testing of interpolation module (continued)

The results from Sept 17, were confusing. therefore a longer run (250 vectors) was conducted to see how the change from LINEAR search to BINARY search affected the execution time of the TPA code.

Sept 21, 1999 - Modification and testing of interpolation module (continued)

Results from the Sept 20th run were analyzed showing a reduction in time for the new BINARY search interpolation module. The 250 vector run using the BINARY search interpolation module was almost 3 minutes faster than the LINEAR module, this out of a total run time of nearly three hours. Results are detailed in /home/jmench/rusn/tpa33/990921RJmessage.txt.

After further study it was noticed that there was a variance of 7.7 seconds from running two identical tpa runs that used the same LINEAR search function. Another tpa run with the BINARY search interpolator was conducted to check its variance.

Sept 22, 1999 - Testing of the interpolation module (continued)

The results from the run of Sept. 21 were analyzed and it was found that there is a variance of 1 minute and 22 seconds for two identical tpa runs using the the new BINARY interpolation function. The results of the test are inconclusive, i.e. there seems to be no real time savings using the new BINARY search interpolation function. Results are detailed in /home/jmench/runs/tpa33/990922RJmessage.txt

Sept 22, 1999 - Preparing for transfer to CD.

After discussing the final storage of all the interpolation testing with Ron Janetzke, I have decided to move and rename some subdirectories and files. Here are the changes made:

- All of the Test1 tests were performed in a subdirectory labeled /home/jmench/interpolate. I have created a subdirectory labeled Test1 under the interpolate subdirectory and moved all of the test files related to conducting Test 1 as described in test plan PA-SCR-281, including source files, executable files and output files, to this new subdirectory.

- I created a new subdirectory labeled Test2 under the interpolate subdirectory and moved all of the files related to conducting Test 2 as described in test plan PA-SCR-281 to this new subdirectory.

- I created a new subdirectory labeled Test3 under the interpolate subdirectory and moved all of the files related to conducting Test 3 as described in test plan PA-SCR-281 to this new subdirectory.

- In the subdirectory Test3, I have moved new250vectors/badrun to a subdirectory of Test3 labeled old250vectors_run2, since new250vectors/badru was not actually a bad run but run intended to use the new interpolation algorithm but mistakenly invoked with the tpa exex containing the old interpolation algorithm.

- I have changed the pathnames in the various diff text files to reflect the changes made above.

Sept 23, 1999 - Preparing for transfer to CD (continued)

Continued to move and rename files pertinent to PA-SCR-281 into the single subdirectory named interpolate. The name changes is for consistency in naming the output of the unix diff utility.

- I have changed the diff text filenames to the following format subdir1VsSubdir2NNvectors.txt where the NN is replaced by the number of vectors that were used in the comparison (either 50 or 250).

- I have moved the /home/jmench/tpa33 subdirectory which contained the old tpa33 exec which uses the LINEAR search interpolation routine into a subdirectory of interpolate.

- I have moved the /home/jmench/tpa33NewAinterl subdirectory, which contained the new tpa33 exec which uses the BINARY search interpolation routine into a subdirectory of interpolate.

Sept. 23, 1999 - LHS random seed investigation.

This problem surfaced when conducting a 4 parameter tpa run to investigate the effect of using a different lhs.out file as input to the mrrslhs sensitivity analysis program code. Changing the random seed that generates the input lhs.out had no effect on two parameters, one of which has a uniform distribution, the other a loguniform distribution.

Let's revisit this problem using a different set of parameters.

Created a subdirectory called /home/jmench/rsTests to run some test out of.

Passing this effort on to Rob Rice.

Sept. 24, 1999 - Changes to invent.f

Began working on changing invent.f. Familiarized myself with the INVENT manual by reading the TPA user manual. Wrote test plan and SCR for changing invent.f.

Sept. 24, 1999 - Miscellaneous administrative activities.

Created a CD of the interpolate subdirectory.
Backed up the entire /home/jmench subdirectory on tape.

Sept. 24, 1999 - Rerun of the 4 parameter test using snllhs compiled with -r8 -o3 option.

After discussions with R. Rice and S. Mohanty it was determined that the problem with duplicate parameters with different random seeds was a result of compiling the snllhs.f module with the -o4 option.

Created a new directory called new4Param to run 4 Morris type runs.

Created a sourceCodes subdirectory under new4Param with which to hold the stand alone snllhs.e program.

Sept. 25, 1999 - 4 Parameter Morris runs.

Launched 4 tpa.e runs each with a different random seed.

The random seeds used were the following:
183310452
183310254
188910452
188910254

Sept. 27, 1999 - 4 Parameter Run Analysis

Under each of the subdirectories containing the different random seeds, 10 subdirectories were created for different 'r' sets of 10, 20, ..., 100 sets. Data was grep'd out for each parameter and plotted using Kaleidagraph.

Sept. 28, 1999 - Revising American Nuclear Society paper.

Oct. 19, 1999 Revised test plan PA-SCR-281

Oct. 20, 1999 Continuing work on invent.f

On /home/jmench/invent made the following subdirectory 43nucs.
Copied all the contents of /net/scratchy1/export/home/janetzke/tpa/test/43nucs to /home/jmench/invent/43nucs.

On /home/jmench/invent made a basecase1 subdirectory and copied /home/jmench/invent/tpa323/tpa.inp to it.

On /home/jmench/invent made a basecase2 subdirectory and copied /home/jmench/invent/43nucs/tpa.inp to it.

Ran tpa323 from basecase1 and from basecase2.

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Sept. 25, 1999 - 4 Parameter Morris runs.

Launched 4 tpa.e runs each with a different random seed.

The random seeds used were the following:
183310452
183310254
188910452
188910254

Sept. 27, 1999 - 4 Parameter Run Analysis

Under each of the subdirectories containing the different random seeds, 10 subdirectories were created for different 'r' sets of 10, 20, ..., 100 sets. Data was grep'd out for each parameter and plotted using Kaleidagraph.

Sept. 28, 1999 - Revising American Nuclear Society paper.

Entries into Scientific Notebook No. 170 for pages 3-7 have been made by Jose M. Menchaca. Jose M. Menchaca October 19, 1999

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Jose M. Menchaca October 19, 1999

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Examined differences between basecase1/tpa.inp and basecase2/tpa.inp

Besides the obvious addition of the nuclide information, the following differences were found between basecase1/tpa.inp and basecase2/tpa.inp:

Header claims "Test for fsv1r7a10k10y 9-7-99"
VolcanismDisruptiveScenarioFlag is changed from 0 to 1.
FaultingDisruptiveScenarioFlag is changed from 0 to 1.
NumberOfTimeStepsAfterCompliancePeriod is changed from 0 to 100.
RatioOfLastToFirstTimeStepAfterCompliancePeriod is changed from 0.0 to 100.0.
DistanceToReceptorGroup is changed from 20.0 to 10.0.

Oct. 22, 1999 Results of the basecase1 and basecase2 runs.

In both the basecase1 and the basecase2 runs, we have two occurrences where we get the "*** NEFTRAN is skipped ..." message, in subareas 4 and 7.

In both the basecase1 and the basecase2 runs, we have 3 occurrences of "There is no SZ release", in subareas 2, 5, and 6 of both basescases.

Because of this Ron J. suggests running 5 realizations each and select a run that has the most release.

Created a subdirectory named run01 under basecase1. Moved all the files of the latest run in basecase1 to the new subdirectory run01.

Created a new subdirectory named run02 under basecase1. Copied the tpa.inp from run01 subdirectory to run02 subdirectory. Modified the tpa.inp to execute 5 realizations and ran it.

Created a subdirectory named run01 under basecase2. Moved all the files of the latest run in basecase2 to the new subdirectory run01.

Created a new subdirectory named run02 under basecase2. Copied the tpa.inp from run01 subdirectory to run02 subdirectory. Modified the tpa.inp to execute 5 realizations and ran it.

The results of the run02 experiments for both basecase1 and basecase2 were that the first three realizations had multiple cases of "no EBS/UZ/SZ release" and/or "NEFTRAN is skipped ..." messages. Realizations 4 had "NEFTRAN is skipped ..." messages in subareas 3, 4, and 7 and realization 5 had "NEFTRAN is skipped ..." messages in subareas 1, 2, 3, 4 and 7. Neither had any "There is no EBS/UZ/SZ release" messages.

Created a new subdirectory named run03 under basecase1. Copied the tpa.inp from run02 subdirectory to run03 subdirectory. Modified the tpa.inp to start and stop at realization 4 of the previous 5 realization run and ran it.

Created a new subdirectory named run03 under basecase2. Copied the tpa.inp from run02 subdirectory to run03 subdirectory. Modified the tpa.inp to start and stop at realization 4 of the previous 5 realization run and ran it.

Began creating nuclide.dat by extracting the pertinent information from invent.f.

Oct. 25, 1999 Developing nuclides data file and file reader.

With the help of script files, I rearranged the nuclide information into 9 columns of names and data for each nuclide. This resulted in 43 rows of nuclide data.

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Jon M. M January 4, 2000

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e
Jan 26, 2001 PA-SCR-332

PA-SCR-332 deals with the new tpameans.out file. The goal of this task is to verify that the tpameans.out file indeed contains the mean values of the sampled parameters.

Instead of verifying the correctness of each parameter, a simple check of a parameter from each distribution function will be checked.

Two parameters from each distribution type were checked using either a hand calculator or spreadsheet calculation. All of the parameters were indeed the mean value of the minimum and maximum input values according to their distribution.

Additionally, a mean value run using the tpameans.out file as the tpa.inp file was successful.

Jan 29, 2001 PA-SCR-331

PA-SCR-331 deals with the new pkmndose.out file. The pkmndose.out file is an implementation of the getTimePeakMean.f program I wrote for Sitikanta Mohanty.

To verify that the pkmndose.out file is giving the desired output I will take a basecase run of 350 vectors, run the getTimePeakMean.e program on totdose.res and compare the result to pkdmndose.out.

There were no differences in the two output files, pkmndose.out and doseatmeanpeak.out which is the output file of getTimePeakMean.e.

Jan 30, 2001PA-SCR-330

PA-SCR-330 is a comparison of the use of Latin Hypercube sampling and Monte Carlo sampling. The comparison will be made by running two runs, one a tpa4.1 run and the other a tpa4.1d run. Both will have the Latin Hypercube Sampling (LHS) flag

set to 0. A comparison of the sp.tpa output files should yield different results for each run.

Repeating the runs, but with the LHS flag set to 1 for each case should yield identical lhs.out files.

Passed on both tests.

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Jose M. Menchaca April 4, 2001

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Jun. 8, 2001 Morris Results

The results of the Morris run are stored in
/net/spock/home/jmench/tpa41j/newYMR-TC/morris
The PostProcessing subdirectory is needed to combine the seven 'r' sets that make up the complete morris run.

Aug 21, 2001 Combining probability weighted igneous activity run with basecase ground water dose.

A method was needed to combine the output from D. Codell's cvolc.f output with a basecase tpa run. The problem, cvolc.out is formatted at 1001 points from 5 to 10005 in 10 unit increments and the groundwater dose as written in nucdose100k_allnuc.plt is formatted with 301 steps with varying step sizes from 0 to 10,000 years and a uniform 900 year step size from 10,000 to 100,000 years. Nowhere in the period from about 4,000 years to 10,000 years does the nucdose data coincide with the cvolc.out data. A quick interpolation routine was needed to produce a plot with the combined ground water and ground surface outputs.

Instead of producing a fortran code that would do this, both the ground water data and the ground surface data were read into an excel spreadsheet. The bottom portion of this spreasheet is reproduced below.

	A	B	C	D	E	F	G	H
976	5560.00	0.004071		9755	6.72E-05	6.72E-02	0.020540	8.77E-02
977	5700.00	0.004283		9765	6.55E-05	6.55E-02	0.020554	8.61E-02
978	5830.00	0.004245		9775	6.39E-05	6.39E-02	0.020551	8.44E-02
979	5970.00	0.004067		9785	6.22E-05	6.22E-02	0.020533	8.27E-02
980	6110.00	0.004079		9795	6.05E-05	6.05E-02	0.020515	8.11E-02
981	6260.00	0.004172		9805	5.89E-05	5.89E-02	0.020496	7.94E-02
982	6410.00	0.004196		9815	5.72E-05	5.72E-02	0.020478	7.77E-02
983	6560.00	0.004450		9825	5.56E-05	5.56E-02	0.020460	7.60E-02
984	6720.00	0.005147		9835	5.39E-05	5.39E-02	0.020441	7.44E-02
985	6870.00	0.006505		9845	5.23E-05	5.23E-02	0.020423	7.27E-02
986	7040.00	0.008578		9855	5.06E-05	5.06E-02	0.020405	7.10E-02
987	7210.00	0.010875		9865	4.90E-05	4.90E-02	0.020386	6.94E-02
988	7380.00	0.013254		9875	4.73E-05	4.73E-02	0.020368	6.77E-02

989	7550.00	0.014374	9885	4.57E-05	4.57E-02	0.020350	6.60E-02
990	7730.00	0.014825	9895	4.40E-05	4.40E-02	0.020331	6.44E-02
991	7910.00	0.014897	9905	4.24E-05	4.24E-02	0.020313	6.27E-02
992	8100.00	0.014450	9915	4.07E-05	4.07E-02	0.020295	6.10E-02
993	8290.00	0.013563	9925	3.91E-05	3.91E-02	0.020277	5.94E-02
994	8490.00	0.013443	9935	3.74E-05	3.74E-02	0.020258	5.77E-02
995	8690.00	0.014215	9945	3.58E-05	3.58E-02	0.020240	5.60E-02
996	8900.00	0.015548	9955	3.42E-05	3.42E-02	0.020222	5.44E-02
997	9110.00	0.017210	9965	3.25E-05	3.25E-02	0.020203	5.27E-02
998	9320.00	0.019041	9975	3.09E-05	3.09E-02	0.020185	5.11E-02
999	9540.00	0.020251	9985	2.92E-05	2.92E-02	0.020167	4.94E-02
1000	9770.00	0.020561	9995	2.76E-05	2.76E-02	0.020148	4.77E-02
1001	10000.00	0.020139	10005	0.00E+00	0.00E+00	0.020130	2.01E-02

Columns A and B are from the first 201 data lines of nucdose100K_allnuc.plt. Columns D and E are from the cvolc.out file. Column F is 1000.0 times each cell in column E to express cvolc.out data in millirems/year. Column G is the interpolated nucdose output. Column H is the sum of columns F and G which was the desired output.

To demonstrate the interpolation formula, the formula from cell G1000 is displayed below:

=B$1001-(((A$1001-D1000)/(A$1001-A$1000))*(B$1001-B$1000))

What this formula does is take the ratio of the desired time (A$1001-D1000) to the time spanned (A$1001-A$1000), multiply this by the expected dose spanned (B$1001-B$1000) and subtracts it from the larger of the expected dose difference (B$1001). The $ signs are anchors to keep the span distances current until a new span is needed. For instance the A$1001-A$1000 was used until G977 at which time the time span swithced to A$1000-A$999.

Aug 24, 2001 Problems running 350 vector alternate transport model 9_noretardpuamth and the solution.

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In running the alternative transport model of "No Retardation of Pu, Am and Th" I ran into problems of the lhs.out not being written to. The problem stems from changing all the retardation parameters for Pu, Am and Th from PDF's to constants. Each retardation parameter that is changed must be removed from the correlation table at the end of the tpa.inp in order to get a successful run.

Aug. 29, 2001 Running 9a_noretardpuamthByFreezing.

Because of a failure in vector 182, 9_noretardpuamth never yielded a Peak Mean Dose reading. Several attempts to discover what caused the failure (NaN type errors) were fruitless. Instead of making all of the sampled parameters responsible for retardation constants, I limited their range.

Sept. 12, 2001 Running morris on tpafunc

Kept running into problems running mrrslhs on the 100,000 vector lhs.out that I had run on Sept. 11, 2001. The problem was that I was getting numbers out of their domain range. Running at 100,000 vectors gave many negative numbers, but all of the variables I am using in tpafunc.inp are between 00 and 1.0 for non-log parameters and 1.0e-3 to 1.0 for log parameters.

The solution was to use a smaller lhs.out. There is no need to run 100,000 vectors, only as many vectors as there will be number of sets. For this case I ran a 300 vector run and got no negative parameters.

Sep. 17, 2001 Basecase Results

The results of the basecase run for tpa 4.1j with new Yucca Mountain Rock Thermal Conductivity are in subdirectory
/net/spock/home/jmench/tpa41j/newYMR-TC/basecaseRuns/bcrWithAppendFiles2

The plot files ending with file extension plt are generated using the following files:

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ccdfOfTotdose.f
multiVectorMakeplot.f
read_500kyr_totdose.f
read_allreleaserate.f
read_totdose.f
Which are found in subfolder /net/spock/home/jmench/tpa41j/

Sept. 26, 2001 running multi vector morris runs to determine when convergence occurs.

Problem 1: Parameters were ending up outside the min and max values specified in the lhs.inp file. Ron Janetzke determined that it was a resolution problem. The problem was resolved by using the following line to compile snllhs.f

```
f77 -r8 -O3 snllhs.f zportunx.o -o snllhs.e
```

Problem 2: The postprocessing program checkres kept crashing. The problem ended up being a dimensioning problem. In the tpa4.1 checkres, ydata is dimensioned as

```
double precision  ydata(maxvec * maxvar)
```

with maxvec and maxvar set to 7 and 350 respectively.

Within the program ydata is used as follows:

```
      do i = 1, nvec * (nvar + 1)
        ydata(i) = gwout(i, 2)
      enddo
```

This never produced a problem in the past since the actual number of variables used was much less than the 350 specified for maxvar.

When I adapted checkres.f to the tpafunc software I used exact dimensions of maxvec and maxvar of 100 and 10 respectively, so that ydata was dimensioned to exactly 1000 data points when actually 100 * (10 +1) = 1100 data points are needed. The

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From

double precision bmat(maxvec * maxvar, maxvar)

to

double precision bmat(maxvec * (maxvar+1), maxvar)

Additionally, I had to make the same change to bmat_old in efftlhs.out.

Found one more problem. In several of the efftlhs.f files there is a 3500 hardcoded into the dimension statements. These all need to be changed to maxvec * (macvar+1).

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Jose M. Menchaca October 4, 2001

parameter nvec was being overwritten since the ydata array was too small. The solution was to dimension ydata as shown below:

```
double precision  ydata(maxvec * (maxvar + 1))
```

which is in keeping with the way it is used in the program.

Sept. 27, 2001 running multi vector morris runs to determine when convergence occurs.

Had failures running the 500 vector morris run. Even though I had trouble understanding the problem, a similar fix to yesterdays fixed the problem.

I changed bmat dimension as follows:

From

double precision bmat(maxvec * maxvar, maxvar)

to

double precision bmat(maxvec * (maxvar+1), maxvar)

Additionally, I had to make the same change to bmat_old in efftlhs.out.

Found one more problem. In several of the efftlhs.f files there is a 3500 hardcoded into the dimension statements. These all need to be changed to maxvec * (macvar+1).

October 12, 2001 Running cvolc.e to get probability weighted dose.

To produce a plot like figure 3-50 of the System-Level Repository Sensitivity Analysis Using TPA Version 3.2 Code requires the following steps.

1. Generate twelve basecase tpa runs with the following conditions:

a. VolcanismDisruptiveScenarioFlag set to 1 (TRUE)
b. DirectReleaseOnlyFlag set to 1 (TRUE)
c. TimeOfNextVolcanicEventinRegionOfInterest set to a constant value in the following increments:

100 years
500 years
1000 years
2000 years
3000 years
4000 years
5000 years
6000 years
7000 years
8000 years
9000 years
10000 years
11000 years
12000 years

Note: For the runs of October 10, 2001 an additional change was made. The VolcanoModel was changed from the normal basecase of 1, Geometric, to 2, Distribution.

2. Once the 12 runs have completed, run combinev.e on each. An example interactive session of running combinev.e is shown below. Please note that the entries that the user makes are bolded.

```
~rjanetz/tpa41aprod/combinev.e
 enter num. vectors(typ. 400)
350
  enter number of time intervals (typ. 201)
301
  enter file name
combine.out
 Note: IEEE floating-point exception flags raised:
    Inexact;  Underflow;
 See the Numerical Computation Guide, ieee_flags(3M)
```

3. Once combinev.e has been run for each of the event times, cvolc.e must be run. The program cvolc.e assumes the presence of a file named vnames.inp which contains the following.

```
12
.0000001
ETGW01/combine.out
ETGW02/combine.out
ETGW03/combine.out
ETGW04/combine.out
ETGW05/combine.out
ETGW06/combine.out
ETGW07/combine.out
ETGW08/combine.out
ETGW09/combine.out
ETGW10/combine.out
ETGW11/combine.out
ETGW12/combine.out
```

The first parameter is the number of files to be read in. The next parameter is the probability weighting. The following 12 lines contains the file names to be retrieved by cvolc.e. Once vnames.inp has been created in the working directory where cvolc.e will be run, cvolc is invoked by simply typeing cvolc.e. No command line parameters are needed.

4. Once cvolc.out has been created and converted to dos type text it can be read in by Kaleidagraph and plotted.

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e
Oct. 15, 2001 Correction to read_allrealeaserate.f

I was getting very high average values for Tc99 release for ebs, uz and sz. The problem was that I was summing over all areas and dividing by 350 (i.e. the number of realizations for this run.)

The solution was to add a test to see if we were reading subarea 1, and only then adding to the Tc99 total dosage.

The change is noted in read_allreleaserate.f.

Oct. 16, 2001 Creating Figure 3-48 faulting present.

Did not have a complete rgwsa.tpa for faulting run. However I did have a complete totdose.res file for a 350 basecase run with faulting. Using read_totdose.e I was able to get the same data as rgwsa.tpa.

NOTE: The expdose.plt file produced when running read_totdose.e on a totdos.res produces the same output as rgwsa.tpa except that expdose.plt is expressed in mrem/yr and rgwsa.tpa is expressed in rem/yr.

Oct. 22, 2001 Generating ccdf's for frozen parameters.

Nov. 13, 2001 Finding subarea streamtube lengths.

Run each subarea by itself and view nefii.inp for each subarea.
Add the lengths of Leg # 1, 2, and 3 found in nefii.inp.

Nov. 15, 2001 Problems running 962 vectors

One problem was that some of the subarea thicknesses, especially for Subarea 10 were set to 0.0, 1.0. This caused problems. Changed all occurences of 0.0, 1.0 to 80.0, 120.0.

The next problem was the uniform TimeStepForClimate[yr] ranging from 400.0 to 600.0. This has to be a constant at 500.0.

Nov. 16, 2001 Creating a samplpar.res file from a "split" run.

Write the first 7 lines of the first set's samplpar.res file to header.txt with the following command while in a vi session of that samplpar.res:

:1,7 w header.txt

Open the original unsplit lhs.out file, read in header.txt using the following command:

:r header.txt

Be sure that the 7 lines just read are at the very top of the file. (:r always attaches the new text below the current line.

Nov. 29, 2001 Backfill and ventilation relationship

In tpa4.1j there is no backfill. More specifically backfill thickness is 0.0 meters which is the same as saying there is no backfill. However the ventilation stop time is related to the TimeOfBackfillEmplacement.

Dec. 10, 2001 Differential Analysis Problems

This is a recurring problem when doing differential analysis. We currently have 330 parameters, but when we run the differential analysis we end up with 329 parameters.

The offending parameter is NumberOfMagmaInducedMechanicalFailuresRemainingInDrift.

that has o

from 20010409.hst:

Got the average of the diffAn runs by copying each sens.out file into an excel spreadsheet, averaging the columns and then sorting the absolute value of the resulting averages. Results are in softbd[c:\jmench\diffAn\tpa41f results.xls]

Problem with NumberOfMagmaInducedMechanicalFailuresRemainingInDrift.

Increased each value of NumberOfMagmaInducedMechanicalFailuresRemainingInDrift by 1 unit in its 5th place after the decimal point.

Dec. 12, 2001 top 20 Codell Parameters

Took the basecase tpameans.out file and replaced the top 20 paremeters as listed by Codell with their original distribution types and min and max values from the basecase tpa.inp file.

Dec. 14, 2001 Revised script file to get ccdf's of tpa runs.

I revised the method used to generate ccdf's of tpa runs. In the past it would take several steps of first copying the gwpkdos.res to gwpkdos.txt, deleting the first 8 lines (the title, header, and column heading lines) from gwpkdos.txt and running the ccdf script file. The process would be repeated for the gwpkds_c.res file. It is now done all at once with the new getccdfFor100Vectors.scr file. The only change that would now need to be made is the base number and the multiplier of NR to get the probabilities, (hence the specific name of the script file).

```
#!csh
echo Processing 100kyr case.
awk ' NR>8 { printf "%12.8f \n", $3*1000.  } ' gwpkdos.res > unsorted.asc
sort unsorted.asc > sorted.asc
awk ' { printf " %12.8f, %12.8f \n", $1, ((1.01) - (NR * 0.01)) } ' sorted.asc > ccdf.asc
unix2dos ccdf.asc ccdf.txt
/bin/rm unsorted.asc sorted.asc ccdf.asc
echo Processing 10kyr case.
awk ' NR>8 { printf "%12.8f \n", $3*1000.  } ' gwpkds_c.res > unsorted_c.asc
sort unsorted_c.asc > sorted_c.asc
awk ' { printf " %12.8f, %12.8f \n", $1, ((1.01) - (NR * 0.01)) } ' sorted_c.asc > ccdf_c.asc
unix2dos ccdf_c.asc ccdf_c.txt
/bin/rm unsorted_c.asc sorted_c.asc ccdf_c.asc
```

Feb. 1, 2002 Plotting Areal Annual Temperature (AAT.plt)

To produce AAT.plt, vi dcagw.ech and execute the following command:

:42,344w AAT.plt

This selects out that portion of the file that deals with temperature.

Then do a unix2dos conversion and read it into Kaleidagraph.

Define a kaleidagraph function as follows

c5 = (c3-32)/1.8

Also added value for Well Pumping Rate which is constant over the entire TPI.

This will convert Fahrenheit to Celsius.

Feb. 1, 2002 To find UZ retardation factors

UZ retardation factors are stored in nefiiuz.inp in the bottom table under the column heading MOBIL RD

Feb. 4, 2002 To get surface area of SF available for dissolution

To get surface area of SF available for dissolution look in echorel.out and search for sareat.

Feb. 5, 2002 Kaleidagraph Layouts

Saved a six pane Kaleidagraph layout at
~/jmench/tpa41j/newYMR-TC/plots/meanvalueplots/SixPaneKGLayout.QPL

To plot six plots on a single Kgraph layout:

1. Open the files to be pasted into the layout.

2. Load the graphs onto the layout in the order that they will appear beginning with the upper left hand image, then the upper right hand image, then the middle left hand image, etc. In other words, left to right, top to bottom.

3. Print the layout.

Note: The layout with the six images can not be saved. To reproduce a layout, you call in SixPaneKGLayout.QPL and repeat steps 1, 2, and 3 listed above.

Feb. 6, 2002 Freezing FractionOfCondensateTowardRepository

FOCTR was not one of the parameters that I got in my analysis so I had not done a ccdf of it yet. Here is the output for freezing the parameter.

```
~/ccdfRuns/freezeParam
 Enter the minimum value for this parameter.
.05
 Enter the maximum value for this parameter.
1.
 5.25000000E-01
 5.23100000E-01, 5.26900000E-01
```

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e
Feb. 7, 2002 Creating Sensitivity Analysis Report Appendix D.

File is stored in softbd at
D:\jmench\TPA Sensitivity\TPA 4.1 Sensitivity Analysis Appendix D.wpd

I used samplpar.alphaOrder.txt found in
~/jmench/tpa41j/newYMR-TC/basecaseRuns/bcrWithAppendFiles2
as an auxiliary file.

Feb. 19, 2002 Running tpa 4.2 to test outpout.

Running in ~jmench/tpa4.2/basecaseRuns/bcrWithNoAFs
which stands for basecase run with no append files.

Feb.19, 2002 Number of Sampled and Constant Parameters

Here is the email that I sent to S. Mohanty in answer to the question of how many sampled parameters and how many constant parameters there are.

```
From:      "Jose M. Menchaca " <jose.menchaca@swri.org>
Sent:      Tuesday, February 19, 2002 10:19 am
To:        Sitakanta Mohanty <smohanty@swri.org>
Subject:   Number of Sampled and Constant Parameters.
Attachments:  TheseIConsiderConstants.txt 7K

Looking at the sp.tpa file of the constants as sampled parameters run,
we were able to sample 961 parameters.

Looking at the cp.tpa file there are 129 constant parameters but only
87 of those I consider "constants".

961 + 87 = 1048

The following constants that appear in cp.tpa I do not consider true
constants to be counted.  In you judgement there may be more or less to
be included.  I am including the list of those that were counted
as "true" constants.
 0 = ImportanceAnalysisFlag(yes=1,no=0)
 0 = SubsystemNaturalStudy
 0 = BarrierBiosphereStudy
 0 = ComponentPrecipitationStudy
 0 = BarrierUpperUnsaturatedZoneStudy
 0 = ComponentTivaCanyonStudy
 0 = BarrierLowerUnsaturatedZoneStudy
 0 = ComponentTSwStudy
 0 = ComponentCHnvStudy
 0 = ComponentCHnzStudy
 0 = ComponentPPwStudy
 0 = ComponentUCFStudy
```

```
 0 = ComponentBFwStudy
 0 = BarrierSaturatedZoneStudy
 0 = Component_STFF_SAV_Study
 0 = BarrierReceptorGroupStudy
 0 = ComponentWellWaterStudy
 0 = SubsystemEngineeredStudy
 0 = BarrierDriftStudy
 0 = ComponentBackfillStudy
 0 = ComponentDripShieldStudy
 0 = BarrierInvertStudy
 0 = ComponentInvertStudy
 0 = BarrierWastePackageStudy
 0 = ComponentInnerContainerStudy
 0 = ComponentOuterContainerStudy
 0 = VolcanismDisruptiveScenarioFlag(yes=1,no=0)
 0 = FaultingDisruptiveScenarioFlag(yes=1,no=0)
 1 = SeismicDisruptiveScenarioFlag(yes=1,no=0)
 0 = StartAtSubarea
10 = StopAtSubarea
 0 = CheckNuclidesAndChains(yes=1,no=0)
 3 = LatinHypercubeSampling(yes=1,no=0)
 1 = NsetLatinHypercubeSampling
500 = NumberOfRealizations
 1 = StartAtRealization
 0 = StopAtRealization
 1 = StartRealizationForSEISMORandomNumber
 0 = OutputMode(0=None,1=All,2=UserDefined)
 1 = UserDefinedLowerRealizationAppended
 1 = UserDefinedUpperRealizationAppended
 0 = SelectAppendFiles

I am putting this memo into the Scientific Notebook for future
reference.

Jose M. "Marty" Menchaca
```

Feb. 21, 2002 Peak expected dose for S. Mohanty's wm2002run 3 and 4.

Received phone call to get the peak expected dose at 10,000 years for runs located on spock at ~smohanty/wm2002run_3 and ~/smohanty/wm2002run_4.

Here are the results:
~/smohanty/wm2002run_3 Peak Mean Dose of 3.98428E-02 mrem/yr occurs at 10000.00 years.
~/smohanty/wm2002run_4 Peak Mean Dose of 5.08299E-02 mrem/yr occurs at 6407.30 years.

Feb. 26, 2002 Testing effect of refluxend.

Statement from S. Mohanty:

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We need to do a calculation to ensure that the 10,000 yr limit on thermal perturbation does not significantly impact the dose results for 100,000yr.

To test this lets modify refluxend in nfenv.f for both reflux2 and reflux3.

In other words change refluxend = 1.0E4 to refluxend = 1.0E5.

Results:

After changing refluxend to 1.0E4, the Seepage Rate did change as expected, i.e. there was no rapid rise in seepage rate at 10kyr. The Peak Expected Dose changed as shown below:

noRefluxTimeLimit:

Peak Mean Dose is 3.68540E-03 rem/yr at 100000.0 yr.

tpa41j/newYMR-TC/meanvalueRuns/basecase :

Peak Mean Dose is 3.78960E-03 rem/yr at 100000.0 yr

There is a slight decrease in Peak Expected Dose for the no reflux time limit run.

Feb. 28, 2002 Slick way to extract a single tar file.

I needed to compare the current gwpkdos.res output with that of a previous run. The problem was that the old run was already tarred off to tape. I tried extracting using wildcards and that didn't work. I did a "man tar" and found a technique for that allows your to extract on 'pattern' matches. The generic example given in the man page is:

```
tar xvf... /dev/rmt/0 `tar tf... /dev/rmt/0 | grep 'pattern' `
```

In my case I was trying to extract both gwpkdos.res and gwpkds_c.res but only those from a basecase run with append files. Here is the command I used:

```
tar xvf /dev/rmt/0 `tar tf /dev/rmt/0 | grep basecaseWithAppendFiles | grep gwpkd`
```

Mar. 1, 2002 Converting from curies to becquerels.

I needed this for verifying information in the TPA 4.1 Sensitivity Analysis report

1 becquerel = 1 disintigration/sec

1 curie = $3.7 * 10^{10}$ disintigrations/second = $3.7 * 10^{10}$ becquerels

This information comes from the www.ymp.gov web page after entering "becquerel conversion" in the search window and clicking on an article titled Secondary Low-Level Waste Treatment Strategy Analysis. In the lines that have the formulas above it quotes the following source, 10 CFR 20.1005 (Section 4.3.1.4)

Mar. 3, 2002 Verification of the FAST methods performed on FAST_c in the July 2001 time frame.

The lhs.out file was split into eight separate lhs.out files of 522 vectors each. Let's verify that the split was performed correctly. Let's merge the eight files into a combined file and compare to the original.

From the ~/tpa41j/newYMR-TC/FAST_c/fast_lhs subdirectory, I executed the following command:

```
cat lhs01.out lhs02.out lhs03.out lhs04.out lhs05.out lhs06.out lhs07.out lhs08.out > lhsCombined.out
```

Then I did a diff on the original lhs.out file and the just created lhsCombined.out file with the following results:

```
/net/spock/home/jmench/tpa41j/newYMR-TC/FAST_c/fast_lhs{23}>diff lhs.out lhsCombined.out
/net/spock/home/jmench/tpa41j/newYMR-TC/FAST_c/fast_lhs{24}>
```

which indicates that there was no difference in the two files consequently indicating that the split was done correctly.

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I did a comparison of the tpa.inp files with the basecase tpa.inp with the following result:

```
/net/spock/home/jmench/tpa41j/newYMR-TC/FAST_c{28}>diff    -C    1    Set1/tpa.inp
~/*j/new*/base*/b*les2/tpa.inp
*** Set1/tpa.inp        Fri Jun  8 18:43:10 2001
--- /net/spock/home/jmench/tpa41j/newYMR-TC/basecaseRuns/bcrWithAppendFiles2/tpa.inp    Tue Jan 15
17:59:41 2002
***************
*** 342,344 ****
  LatinHypercubeSampling(yes=1,no=0)
! 3
  **
--- 342,344 ----
  LatinHypercubeSampling(yes=1,no=0)
! 1
  **
***************
*** 350,352 ****
  NumberOfRealizations
! 522
  **
--- 350,352 ----
  NumberOfRealizations
! 350
  **
***************
*** 360,369 ****
  **
- ** mam 5-21-01 SCR 344
- **     Iterate hazard curve random number for seismo to
- **     catch up with main program using seismostart# - 1.
- iconstant
- StartRealizationForSEISMORandomNumber
- 1
  **
- **
  **          ***>>>  Simulation Times  <<<***
--- 360,362 ----
/net/spock/home/jmench/tpa41j/newYMR-TC/FAST_c{29}>
```

The above is the output with the first set and the basecase tpa.inp files. All the other diffs are the same except for the **********

Mar. 3, 2002 Noticed an error in the morris runs.

While setting up to run a second volcanic2, I noticed and error in the runFirstHalf.scr and runSecondHalf.scr script files. In the second and third lines I have the following:

I discovered a potential problem with the morris run.

In the first two lines of my script files I had the following:

```
Setenv TPA_TEST /home/jmench/tpa41jskip
Setenv TPA_DATA /home/jmench/tpa41jskip
```

The problem with these two lines is that there is no "Setenv" command. What was needed was a setenv command. Consequently the TPA being executed was tpa41j and not tpa41jskip. The tpa41jskip was a special run for running morris with smaller lhs.out files and then reassembling them later so that the runs would not keep crashing (something that happened often with vulcan when we had dimensioned for large realization arrays, i.e. larger that 500.)

Running it again but first let's verify that the lhs.out files are correct.

```
/net/spock/home/jmench/tpa41j/newYMR-TC/morris2{280}>cat Set*/lhs.out > combinedLhs.out
/net/spock/home/jmench/tpa41j/newYMR-TC/morris2{281}>gzip -d ../morris/splitlhs/lhs.out
/net/spock/home/jmench/tpa41j/newYMR-TC/morris2{282}>diff !cat:$ !:$
diff combinedLhs.out ../morris/splitlhs/lhs.out
/net/spock/home/jmench/tpa41j/newYMR-TC/morris2{283}>
```

This indicates that the lhs.out split was successful.

March 4, 2002 Verifying that there were no seismic failures in the first morris run.

I used the following script file to verify that there were no seismic failures in any of the seven sets from the morris run dated May 30, 2001.

```
/net/spock/home/jmench/tpa41j/newYMR-TC/morris{42}>awk '{if($4!=0) print $0}' Set1/wpsfail.res
 Input file tpa.inp as supplied with TPA Version 4.1j Code.
 Base case.
 TPA 4.1j, Job started: Wed May 30 16:25:08 2001
 Number of Failed WPs by Type of Disruptive Event

 Including Time of Event - Values for Each Vector

     vector          time         #corrode       #seismic        #fault         #igact
    unitless          yr          unitless       unitless       unitless       unitless
/net/spock/home/jmench/tpa41j/newYMR-TC/morris{43}
```

Mar. 4, 2002 Adding a listing to nfenv.f for tempsf (Spent Fuel Temperature)

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e
For the Sensitivity Analysis Report we need spent fuel temperature. I modified exec.f to add a list for tempsf. I did this to tpa4.2 since tpa41j was executing at the time.

The results are in ~/tpa4.2/meanvalueRuns/basecaseWithTempSFPrintout

March 5, 2002 Verification of data in Table 3-13 of Sensitivity Analysis Report.

The values in Table 3-13 are derived from nucdose100k_allnuc.plt

For the 10kyr case the following data is found from running, getTimePeakMean_c.e.
Peak Mean Dose of 2.05106E-02 mrem/yr occurs at 9769.00 years.

Using this information, one can extract the radionuclide contribution at 9,769 years from the nucdose100k_allnuc.plt file.

At the end of the tpa run the following line is seen before the "run successfully completed" statement:
Peak Mean Dose is 9.89872E-03 rem/yr at 100000.0 yr.

Using this information, one can extract the radionuclide contribution at 100,000 years from the nucdose100k_allnuc.plt file.

March 5, 2002 Determining the earliest corrosion failure in a multi-vector tpa run.

The easiest way to determine when the earliest WP corrosion failure time occured is to execute the following command:

```
grep CORROSION tpa.out > corrosionTimes.txt
```

Then read corrosionTimes.txt into and excel file and do a minimum function [min(d1:d3500)] on the year column.

Doing this on the basecase tpa.out revealed that the earliest corrosion failure time is 37,900 years.

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e
March 5, 2002 DCF determination

Ron Janetzke suggested adding up the 6 columns of DCFs in gw_cb_ad.dat to arrive at a single DCF value for use in the Sensitivity Analysis report.

March 8, 2002 Generating the new GWTT CCDFs for each subarea.

I wrote getGWTTCcdf.scr to produce ccdfs of gwtt for the UZ and SZ to produce figures 3-33 and 3-36 for the Sensitivity Analysis report for TPA 4.1j.

Here is a typical line that produces a ccdf of gwtt of the UZ for Subarea 1:

```
echo Processing Subarea 1 uz gwtt.
awk ' NR>8 { printf "%8.2f \n", $2  } ' gwttuzsz.res > unsorted.asc
sort unsorted.asc > sorted.asc
echo 'UZ  gwtt  Subarea01' > SA01uzgwttccdf.txt
awk ' { printf " %8.2f  %8.6f \n", $1, ((1.002857) - (NR * 0.002857)) } ' sorted.asc >> SA01uzgwttccdf.txt
/bin/rm unsorted.asc sorted.asc
unix2dos SA01uzgwttccdf.txt dosFiles/SA01uzgwttccdf.txt
```

This script is repeated for each subarea in both the UZ and SZ and for the average gwtt for each of UZ and SZ.

March 8, 2002 Getting the minimum fail time from 4,000 vector run.

For some reason I was unable to do a min(d1:dXXX) in excel for any XXX that was large. This was occuring when I used the outputs from a "grep -i corrosion tpa.out" command. Instead I used wpsfail.res and did a min(d9:dYYY) where YYY was typically in the 700's. This gave a minimum corrosion fail time of 37,900 years.

March 11, 2002 Getting average of cumulative release of top nuclides.

For the mean value data set this is trivial. These are listed in cumrel.res and cumrel_c.res.

For the 350 vector case, a little more work is needed. I read in cumrel.res and cumrel_c.res into an Excel worksheet and on a new worksheet averaged each nuclide over the 350 vectors. Care was needed to make sure the range of each nuclide was

correct. The first through third nuclide formulas were:
=AVERAGE(cumrel_c!E9:E358)
=AVERAGE(cumrel_c!E359:E708)
=AVERAGE(cumrel_c!E709:E1058)
and so on until the final nuclide formula was:
=AVERAGE(cumrel_c!E6659:E7008)

Note how the subsequent formula's start is 350 counts greater than the previous start count and that the subsequent formula's stop count is 350 greater than the previous stop count.

The top 3 contributors to release for the 10kyr TPI are:
^{99}Tc with 159.04 Ci
^{129}I with 0.43 Ci
^{36}Cl with 0.15 Ci.

The top contributors to release for the 100kyr time period are:
^{99}Tc with 35288.52 Ci
^{237}Np with 439.25 Ci
^{129}I with 130.44 Ci
^{36}Cl with 41.37 Ci.
^{59}Ni with 28.98 Ci.
^{79}Se with24.01 Ci.
^{234}U with 7.46 Ci.

The 2 files used to generate this data are
average cumulative release from cumrel.xls
average cumulative release from cumrel_c.xls
on [softbd]D:\jmench\tpa41j.

March 12, 2002 Presenting Dose curves in milliSieverts.

S. Mohanty needed the dose curves in milliSieverts/yr instead of millirems/yr.

To do this, using Kaleidagraph, I read in the dose curves (figure 3-20a and figure 3-20b), extracted the data and then applied the following formulas with the following Formula Entry button definitions.

F1 => c7 = c2/100
F2 => c8 = c3/100
F3 => c9 = c4/100
F4 => c10 = c5/100
F5 => c11 = c6/100
F6 => c3 = c2/100

Function buttons F1 through F5 worked for both the totdose.plt and ccdfdose.plt since they each have 5 columns of dose data. F6 was used for the expdose.res data.
The same functions were used for the totdos_c.plt, ccdfdos_c.plt and expdos_c.plt data.

March 15, 2002 Error discovered in multiVectorMakeplot.f

Discovered an error in multiVectorMakeplot.f. The subroutine inventory uses a hardcoded value for waste package payload of 9.76 MTU. We now have 7.89 MTUs per waste package. We either need to find a way to read in wastepackage payload or make the WP payload an entry from the user to prevent errors like this from happening again.

Here is the section of code that has caused the error.

```
      wp_payload = 7.89d0

c     area_m2 /4046.9 = area_acres
c     area_acres * 83 MTUs/acres = mtus
c     mtus / 9.76 mtus/wp = avgnwps

      area=0.d0
      do i=bsa,esa
        area = area+saarea(i)
      enddo
      area_acres = area/4046.9d0
      dmtus = area_acres *83.d0

      anumberwps = dmtus / 9.76d0          != 6427.0d0
```

I changed it to the following to get the data that I needed since I know the total

number of waste packages.

```
cjmm  wp_payload = 9.76d0
    wp_payload = 7.89d0

cjmm  1 acre = 4046.9 square meters
c     area_m2 /4046.9 = area_acres
c     area_acres * 83 MTUs/acres = mtus
c     mtus / 9.76 mtus/wp = avgnwps

    area=0.d0
    do i=bsa,esa
      area = area+saarea(i)
    enddo
    area_acres = area/4046.9d0
    dmtus = area_acres *83.d0

cjmm  anumberwps = dmtus / 9.76d0          != 6427.0d0
    anumberwps = 8877
```

After emailing Rob Rice, I got information on the 83 multiplier in equation for dmtus. It is the areal mass loading which used to be a tpa.inp input variable but now is calculated on the fly and can be found in the opening repository design section of the screen output (typically saved as tpa.out).

March 25, 2002 Correlations in morris runs.

A question has arisen in my mind as to whether we are truly testing correlated parameters in our standard way of doing morris. After a discussion with Ron Janetzke I found out that snllhs.e does not truly correlate parameters until the number of realizations exceeds the number of parameters. Currently I set my dummyRun, the run which is used as the source of the morris design matrix, to have only seven vectors. I did this to cause the snllhs.e program to select a sample from each 'bin' in the parameter space for each parameter.

A test is needed to see how differently the lhs.out would look, if I set the number of realizations to 1 more than the number of parameters being sampled. Since a basecase tpa.inp uses 350 realizations, let's start with a comparison of the lhs.out from the basecase run and the 7 vector morris dummyRun1.

The result of a preliminary inspection shows that the two lhs.out files are very

different. Let's use the readsp.e program to read what the values are correlated parameters such as ARDSAVNp and ARDSAVPu which have a correlation value of 0.881.

The readsp.e program requires access to the following four files in order to operate properly:
readsp.inp, a file that names the parameter(s) to be read
samplpar.hdr, the tpa.e output file of the sampled paremters and there abbreviations
samplpar.res, the sampled parameters used for the realizations
gwpkdos.res, the resulting peak dose output file

The results show that the correlation is lost for the seven vector lhs.out

April 4, 2002 NOTE: Error in figure 3-1 showing Mean Annual Precipitation

I just found out from R. Janetzke that the AAP column in dcagw.ech is expressed in inches/yr and not mm/yr. The data will have to be multiplied by 25.4 to get it into mm/yr.

April 5, 2002 Repository Precipitation, Infiltration and Amount of Water hitting Waste Packages.

Need to determine
1. The cumulative precipitation over the repository at 10kyr.
2. The cumulative infiltration that enters the repository at 10kyr.
3. The cumulative amount of water that enters the WPs at 10kyr.

Determining cumulative precipitation:
The dcagw.ech file has a column that has AAP (average annual precipitation) as its heading ...

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e
April 11, 2002 Number of "non-zero" parameters identified by morris method.

Sitakanta asked how many non-zero parameters were identified by morris method. By non-zero, he means parameters that had either a non-zero mean or non-zero standard deviation. Additionally I think it might prove useful to see what parameters were dropped from or added to the list when switching from the noncorrelated lhs.out input file.

10,000 yr morris results.				
Parameter #	abbreviation	Name	rank in uncorrelated method	rank in correlated method
75	SFWt%I7	SFWettedFraction_Initial_7	unranked	40
205	MPrm_PPw	MatrixPermeability_PPw_[m2]	13	unranked
209	FPrm_TSw	FracturePermeability_TSw_[m2]	47	unranked
218	FPrs_CHz	FracturePorosity_CHnz	59	unranked
232	ARDSAVNi	AlluviumMatrixRD_SAV_Ni	unranked	63
269	gen_gitC	GrainIrrigationTimeCB[mo/yr]	unranked	64
274	gen_hfgt	HenFeedGrowTime[day]	unranked	62
298	genKDsNp	KD_Soil_Np[cm3/g]	unranked	50

100,000 yr morris results.				
Parameter #	abbreviation	Name	rank in uncorrelated method	rank in correlated method
67	Solbl-Np	SolubilityNp[kg/m3]	73	unranked
75	SFWt%I7	SFWettedFraction_Initial_7	unranked	72
142	MKDPPwNp	MatrixKD_PPw_Np[m3/kg]	79	unranked
147	MKD_CHvU	MatrixKD_CHnvU[m3/kg]	unranked	64
189	MKDCHvNi	MatrixKD_CHnvNi[m3/kg]	unranked	97
230	ARDSAVPb	AlluviumMatrixRD_SAV_Pb	unranked	104
232	ARDSAVNi	AlluviumMatrixRD_SAV_Ni	unranked	80
269	gen_gitC	GrainIrrigationTimeCB[mo/yr]	unranked	101
299	genKDsTh	KD_Soil_Th[cm3/g]	87	unranked
307	genKDsSe	KD_Soil_Se[cm3/g]	unranked	102

April 11, 2002 Made changes to checkres.f

Two changes were needed to checkres.f. Sitakanta needs the abbreviations on the morris output. Added the abbreviations to checkres.

The sorting of the the mean values needs to be done on the absolute value of the mean. Added that capability.

April 15, 2002 Method for calculating cumulative repository precipitation, infiltration and amount of water entering all wps.

These calculations were actually carried out on April 5, 2002.

Cumulative Repository Precipitation

1. Create a MAP.txt file using the following awk script

   ```
   awk ' {if (NF==4) print $0} ' dcagw.ech > MAP.txt
   ```

   Remove all the lines containing "All" and the first two lines of MAP.txt to run readMAP.e. The program readMAP will generate a file called avgMAP.plt which is a table of the repository mean annual precipitation as a function of time.

2. Read avgMAP.plt into an excel spreadsheet to get the amount of precipitation that has fallen on the repository. To get the amount of precipitation that has fallen during a single time step use the following formula

   (current time step-last time step)*((current rate + last rate)/2)

   The cumulative precipitation (in mm) is the sum of the of each succeeding time

step.

This sum divided by 1000 (to convert to meters) times 4717726 square meters gives the cumulative repository precipitation in cubic meters.

Cumulative Repository Infiltration

1. The multiVectorMakeplot.f program reads in the qm3/yr/sa from the uzflow.rlt file and produces an average repository flow expressed in m^3/yr.

2. Get the amount of flow for the time period step using the following formula:

   (current time step-last time step)*((current rate + last rate)/2)

3. Sum up the time step flow rates to get the cumulative flowrate at the time desiresd.

   For the nominal case, the result is 5.323E+08 cubic meters by year 10,000.

Calculating Total Amount of Water entering WPs.

1. Using multiVectorMakeplot.f, produce a seep10k.plt file which is an average of the seepage flux, i.e, the amount of water in cubic meters that hits a waste package per year per subarea (qm3hit/yr/wp/sa). The amount of water is expressed as a function of the 201 time steps. This data is gathered from ebsrel.ech.

2. Read in seep10k.plt into an excel spreadsheet. Get a repository average by averaging the 10 subarea flow rates.

3. Get the amount of water that has entered a representative waste package during the single time period step using the following formula

   (current time step-last time step)*((current rate + last rate)/2)

The right hand of the formula gets an average flow rate during the time period so as not to favor the beginning or ending flow rate.

4. Multiply the amount of step 3 by 8,877, the number of waste packages in the repository to get the total amount of water that has infiltrated WPs for that time step.

5. Cumulatively add up the amounts from 0 time to 10,000 years.

   Result 3.530E+06 cubic meters of water has entered all the waste packages in the repository by 10,000 years.
   (see "d:\jmench\tpa41j\seep100k to get amt of water entering wp.xls" on softbd)

April 17, 2002 Finding the source file for volcanic plot needed by M. Muller

On April 16, 2002, Mike Muller requested source data for a "hairline" plot of volcanic activity combined with normal gw dose curves. For tpa41j newYMR-TC this data was found on spock at ~/tpa41j/newYMR-TC/ETRuns/dosFiles.

April 17, 2002 Found error in Fig 3-21 of Sensitivity Analysis Report

There was an error in Fig 3-21, infiltration average, minimum, and maximum.
The problem arose in my multiVectorMakeplot.f program. In my algorithm to determine average, minimum and maximum, I used erronous initial values. I previously used the section of code shown below to initialize the values.

```
do k = 1,ntim
   avginfil=0.D0
   amininfil=0.D0
   amaxinfil=0.D0
   do i = 1,nvectors
       .
       .
       .
```

I should have used the following.

```
do k = 1,ntim
   avginfil=0.D0
   amininfil=9999999.D0
   amaxinfil=0.D0
   do i = 1,nvectors
       .
       .
       .
```

May 28, 2002 Getting Average WP Failure from corrosion time.

To get the average WP failure time (from corrosion), do the following steps

1. Read in wpsfail.res into an excel spreadsheet. Use fixed width instead of delimited mode to read in the data.

2. Assuming the vector column is column A, in the first blank column to the right in the 10th line type the following formula
   =IF(A10=A9,(B9+B10)/2,"")
   and copy it in the remainder of the column for the length of the data.

3. In the next blank column to the right in the 10th line type the following formula
   =IF(AND(A10<>A9,A10<>A11),B10,"")
   and copy it in the remainder of the column for the length of the data.

4. Assuming that the column in step 2 is G and the column in step 3 is H, in the next blank column to the right in the 10th line type the following formula
   =IF(G10="",H10,G10)
   and copy it in the remainder of the column for the length of the data.

5. Assuming that the column of step 4 type is column I, type in the following formula at the next available blank space below the formulas of step 4
   =AVERAGE(Inn:Imm)
   Where nn is the first line containing the formula in step 4 and mm is the last line containing the formula in step 4.

The answer arrived at in Step 5 is the average WP failure time from corrosion.

The results of tpa41j are stored in a file on softbd:\jmench\tpa41j that is labeled "wpsfail.res to get Average corrosion Failure time.xls".

May 31, 2002 Solubility limit runs.

Tried to use high solubility limits for testing purposes. Started at 1×10^6 kg/m^3 and reduced it by decades (i.e. powers of 10) until I was able to get a complete run which occured at 100kg/m^3. High solubilities always completed to the flowghrough models by always stuck at realization 123 of 350.

June 10, 2002 New Cladding Credit Alternative model

Instead of reducing each of the SFWettedFraction_*failuretype* from a range of 0.0, 1.0 to a range of 0.0049, 0.0051 as specified in Chapter 2 of the sensitivity analysis report, the CladdingCorrectionFactor is reduced from 1.0 to 0.01.

June 12, 2002 Conversion from gal/day to m^3/day to acre-ft/yr

Here is the conversion from gal/day to acre-ft/yr.

2.68×10^6 gal/day * 3.7854×10^{-3} m^3/gal * 8.107×10^{-4} Acre-ft/m^3 * 365 days/yr = 3,000 acre-ft/yr.

June 13, 2002 Conversion from sieverts to rems

One sievert is equivalent to 100 rem; one millisievert (0.001 Sv = 0.1 rem).

One rem *0.01 = 1 mSeivert

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e
July 18, 2002 No Matrix Diffusion Alternative model

The previous version of tpa had no matrix diffusion as its basecase and had some matrix diffusion as its alternative model case. In the tpa 4.1 code, some matrix diffusion is assumed ($1\times 10^{-3}yr^{-1}$) for the basecase and therefore the alternative model is to assume no matrix diffusion.

August 20, 2002 Finding the min and max of Wind Speed.

Using the readsp.e program written by Rob Rice and modified by me, I got a list of all the values used in the basecase run. I then read it into an excel file and did a min and max function (results 1.140, 8353.746). These are the values I used in minsAndMaxes.txt that was later imported to spFirstHalf.txt and spSecondHalf.txt. This information was used in SampledParametersFromVector000To175.xls which was an attempt to see what position relative to the minimum and maximum each sampled parameter held for any particular vector. This is part of the analysis of why a narrowing of DSFailTi has an increase in variance as opposed to a reduction.

Printed: September 30, 2002

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e INITIALS: JMM
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Entries into Scientific Notebook No. 170-5e for pages 5-9 have been made by Jose M. Menchaca. Jose M. Menchaca September 30, 2002

No original text entered into this Scientific Notebook has been removed.
Jose M. Menchaca September 30, 2002

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e

October 4, 2002 Picking 3 peak doses for the Risk Analysis Report

First point 1.15E+00 mrem/yr at 5563.8 years is realization 297

Second point 8.39E-01 mrem/yr at 7913.7 years is realization 114

Third Point 6.45E-01 mrem/yr at 7551.3 years is realization 27

October 7, 2002 Pick 3 new peak doses for the Risk Analysis Report

The three points selected on Friday Oct 4th did not work out. The second and third points were too close together. I am going to select three others.

First point 1.15E+00 mrem/yr at 5563.8 years is realization 297

Second point 8.39E-01 mrem/yr at 7913.7 years is realization 114

Third Point 7.99E-01 mrem/yr at 9322.7 years is realization 262

Those didn't work either so I am picking 3 more that have a more spread out dose curve and are mid-range in their peaks.

First point 4.60E-01 mrem/yr at 9107.2 years is realization 118

Second point 3.92E-01 mrem/yr at 9543.3 years is realization 151

Third Point 3.55E-01 mrem/yr at 7730.4 years is realization 134

This set seems to display what Sitakanta was looking for.

October 10, 2002 New points for Sitakanta's Risk Analysis Paper.

The previous point that I've chosen always have a an expected dose peak at the same time step as one of the three contributing peak dose curves. Sitakanta wants a separate

expected dose peak any of the individual peak doses.

Sorting the peak doses as found in the gwpkds_c.res file, I choose three curves that were close in peak dose level but spread out in time. The three chosen were

Realization 75 at 7,205.3 years with a peak dose of 3.01×10^{-5}

Realization 269 at 9,543.3 years with a peak dose of 3.09×10^{-5}

Realization 311 at 8,896.6 years with a peak dose of 3.08×10^{-5}

With these realizations, no one peak dose dominated the average calculation which allowed the peak of the expected dose curve to occur at a different time step than any of the 3 peak dose time steps used. The Peak Expected Dose from these three realizations is 0.015 mrem/yr occuring at 9323 years.

October 28, 2002 Getting nuclide dose contributions for volcanic runs.

The data containing airborne radionuclide contributions to dose is located in airpkdos.res for 100kyrs and in arpkds_c.res for 10kyrs. These files are only written after all realizations for a particular run have completed. Consequently, as of October 28, 2002, we have no completed data for the basecase with the VolcanismDisruptiveScenarioFlag because the original basecase run was interrupted at vector 87.

A new basecase run with the VolcanismDisruptiveScenarioFlag set to 1 was started on October 28, 2002 and the results are located in the following subfolder: /net/spock/home/jmench/newYMR-TC/basecaseRuns/bcrVolcanicComplete

October 29, 2002 Results of basecase volcanic run

I tested the output of the gwpkds_c.res file and totdos_c.res file with the files that I

had generated in combinedVolcanic. Except for the header info the two files are identical. Below is a portion of the screen capture showing usage of the diff command on these files:

```
/net/spock/home/jmench/tpa41j/newYMR-TC/basecaseRuns/bcrVolcanicComplete{71}>!dif
diff gwpkds_c.res ../combinedVolcanic
2,3c2,3
<  Base case with volcanic flag turned on.
<  TPA 4.1j, Job started: Mon Oct 28 16:37:02 2002
---
>  Base case.
>  TPA 4.1j, Job started: Thu Jun  7 16:45:52 2001
/net/spock/home/jmench/tpa41j/newYMR-TC/basecaseRuns/bcrVolcanicComplete{72}>^gwpkds^totdos^
diff totdos_c.res ../combinedVolcanic
2,3c2,3
<  Base case with volcanic flag turned on.
<  TPA 4.1j, Job started: Mon Oct 28 16:37:02 2002
---
>  Base case.
>  TPA 4.1j, Job started: Thu Jun  7 16:45:52 2001
/net/spock/home/jmench/tpa41j/newYMR-TC/basecaseRuns/bcrVolcanicComplete{73}>
```

October 30, 2002 Calculating radionuclide contribution to total airborne dose.

To arrive at the percent contribution of each radionuclide to airborne dose from a basecase with volcanism the following steps were done.

1. Read in arpkds_c.res into an excel spreadsheet.

2. Sum the dose output from the 350 realization for each column that represents dose, this will include the pktede column and each of the radionuclide columns. For the particular case being discussed, these sums are on line 359 of the spreadsheet with the sum of the pktede column occurring at cell C359.

3. On the next line divide the sum of each radionuclide dose by the pktede dose sum. For example, the column next to the pktede column, column D, represents U238. Below the sum of the U238 doses is the formula D359/$C359, i.e., the sum of all the U238 dose contributions divided by the sum of all total dose for all 350 realizations. As this formula is copied to each successive column, the '$' anchor symbol before the C359 will assure that each radionuclide dose sum is divided by the pktede dose sum.

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e
December 10, 2002 Making KaleidaGraph plots for tpa 5.0 betaB

Below is a portion of the differences between the tpa4.1j version and tpa5.0betaB versions of multiVectorMakePlot.f, the post processing program used to produce many of the chapter 3 figures of the Sensitivity Analysis Document. For the basecase tpa 5.0 betaB run the following conditions are true.

1. The colloidal nuclides (Jc246, Jc245, Ja241, Ja243, Jp239, Jp240, and Jt230) have been commented out of the tpa.inp file. This to have a true comparison with the tpa4.1j results.

2. There are 400 realizations.

3. The maximum time is 100,000 years.

4. The output mode is 1 meaning that the append files are saved.

5. The MeanAnnualPrecipitationMultiplierAtGlacialMaximum has been changed from their minimum, maximum of 1.5, 2.5 to 1.0, 1.5 to prevent the code from halting prematurely.

```
diff multiVectorMakePlot.f ~/tpa41j >> tpa41jVStpa5.0BDiffs.
6c6
<       parameter (nvectors=400)
---
>       parameter (nvectors=350)
198c198
<       parameter (nvectorsp=400)
---
>       parameter (nvectorsp=350)
257c257
<       parameter (nvectorsp=400)
---
>       parameter (nvectorsp=350)
830,833c830,831
< cjmm    do i = 1,42 for tpa 3.2
< cjmm    do i = 1,52 for tpa 4.1j
< cjmm    For tpa 5.0 betaB
<         do i = 1,53
---
> cjmm    do i = 1,42
>         do i = 1,52
992c990
<       parameter(nvectorsp = 400)
---
>       parameter(nvectorsp = 350)
1014c1012
```

```
<       do i = 1,4
---
>       do i = 1,3
1924,1926c1917
< cjmm    do i = 1,47  tpa 4.1j
< cjmm    For tpa 5.0 betaB with No Colloidal Nuclides
<         do i = 1,48
---
>         do i = 1,47
2976,2978c2967
< cjmm    do i = 1,3 for tpa4.1j
< cjmm    Skip 4 lines for tpa 5.0 betaB
<         do i = 1,4
---
>         do i = 1,3
3568c3557
<       parameter (nvectorsp=400)
---
>       parameter (nvectorsp=350)
```

Printed: March 12, 2003

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```
< cjmm    For tpa 5.0 betaB
<         do i = 1,53
---
> cjmm    do i = 1,42
>         do i = 1,52
992c990
<       parameter(nvectorsp = 400)
---
>       parameter(nvectorsp = 350)
1014c1012
<       do i = 1,4
---
>       do i = 1,3
1924,1926c1917
< cjmm    do i = 1,47  tpa 4.1j
< cjmm    For tpa 5.0 betaB with No Colloidal Nuclides
<         do i = 1,48
---
>         do i = 1,47
2976,2978c2967
< cjmm    do i = 1,3 for tpa4.1j
< cjmm    Skip 4 lines for tpa 5.0 betaB
<         do i = 1,4
---
>         do i = 1,3
3568c3557
<       parameter (nvectorsp=400)
---
>       parameter (nvectorsp=350)
```

Entries into Scientific Notebook No. 170-5e for pages 5-9 have been made by Jose M. Menchaca. Jose M. Menchaca March 12, 2003

No original text entered into this Scientific Notebook has been removed.
Jose M. Menchaca March 12, 2003

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e
May 6, 2003 Numerical Results for Morris Method.

Below are the numerical values used to rank the top ten parameters for the 10,000 year Morris run used for the Sensitivity Analysis report shown in Table 4-3. The ymd values are the square root of the sum of the mean squared plus the standard deviation squared.

```
Morris method results.
ymean: mean of dy/dx
ydev: standard deviation of dy/dx

Job started: Fri May 31 10:37:21 2002

  i          ymean          var abb   Variable Name
   1       0.1054743E-02   AAMAI@S   ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
   2       0.1029117E-02   MAPM@GM   MeanAveragePrecipitationMultiplierAtGlacialMaximum
  12       0.4749824E-03   DSFailTi  DripShieldFailureTime[yr]
  60       0.3851846E-03   WPFlowMF  WastePackageFlowMultiplicationFactor
 292       0.2383734E-03   gen_PUSF  PlantUptakeScaleFactor
 239       0.1341222E-03   WPRRG@20  WellPumpingRateAtReceptorGroup20km[gal/day]
 223       0.1090367E-03   IPPFSTFF  ImmobilePorosityPenetrationFraction_STFF
  63       0.1072371E-03   PSFDM1    Preexponential_SFDissolutionModel2
 225       0.9787750E-04   ARDSAVNp  AlluviumMatrixRD_SAV_Np
  61       0.8549087E-04   SbArWt%   SubAreaWetFraction

  i          ydev           var abb   Variable Name
   1       0.2790586E-02   AAMAI@S   ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
   2       0.2722787E-02   MAPM@GM   MeanAveragePrecipitationMultiplierAtGlacialMaximum
  12       0.7311665E-03   DSFailTi  DripShieldFailureTime[yr]
  60       0.6547752E-03   WPFlowMF  WastePackageFlowMultiplicationFactor
 292       0.5935826E-03   gen_PUSF  PlantUptakeScaleFactor
 239       0.2716469E-03   WPRRG@20  WellPumpingRateAtReceptorGroup20km[gal/day]
 225       0.2589595E-03   ARDSAVNp  AlluviumMatrixRD_SAV_Np
 223       0.2407189E-03   IPPFSTFF  ImmobilePorosityPenetrationFraction_STFF
  61       0.1554054E-03   SbArWt%   SubAreaWetFraction
  63       0.1523626E-03   PSFDM1    Preexponential_SFDissolutionModel2

  i          ymd            var abb   Variable Name
   1       0.2983262E-02   AAMAI@S   ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
   2       0.2910782E-02   MAPM@GM   MeanAveragePrecipitationMultiplierAtGlacialMaximum
  12       0.8719018E-03   DSFailTi  DripShieldFailureTime[yr]
  60       0.7596695E-03   WPFlowMF  WastePackageFlowMultiplicationFactor
 292       0.6396579E-03   gen_PUSF  PlantUptakeScaleFactor
 239       0.3029534E-03   WPRRG@20  WellPumpingRateAtReceptorGroup20km[gal/day]
 225       0.2768394E-03   ARDSAVNp  AlluviumMatrixRD_SAV_Np
 223       0.2642623E-03   IPPFSTFF  ImmobilePorosityPenetrationFraction_STFF
  63       0.1863173E-03   PSFDM1    Preexponential_SFDissolutionModel2
  61       0.1773684E-03   SbArWt%   SubAreaWetFraction
```

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e
May 6, 2003

~~The data used for Table 3-13 of the Sensitivity Analysis Report comes from four different files. The 10,000 year data comes from the gwpkds_c.res file in both the single realization mean value file and the multiple realization probabilistic run. The 100,000 year data comes from the gwpkdos.res file in the same two runs as previously discussed. The gwpkd[o]s files are the Ground Water Peak Dose files generated by the TPA 4.1j code.~~ JMM - May 7, 2003. The corrected information appears on the following pages starting at date May 7, 2003.

Spreadsheet converted version of gwpkds_c.res (10,000 years) with selected columns as shown in Table 3-13.

Input file tpa.inp as supplied with TPA Version4.1j Code.
Base case.
TPA 4.1j, Job started: Fri Jun1 11:10:07 2001
Groundwater Total Peak Dose and Peak Time with Doses for Compliance Period
for Each Nuclide at Peak Time -Values for Each Vector

vector	pktime	pktede	Np237de	U234de	I129de	Tc99de	Se79de	Cl36de
unitless	yr	rem/yr	rem/yr	rem/yr	rem/yr	rem/yr	rem/yr	rem/yr
1	1.00E+04	3.46E-05	0.00E+00	0.00E+00	1.30E-05	2.15E-05	0.00E+00	7.11E-08

Spreadsheet converted version of gwpkdos.res (100,000 years) with selected columns as shown in Table 3-13.

Input file tpa.inp as supplied with TPA Version4.1j Code.
Base case.
TPA 4.1j, Job started: Fri Jun1 11:10:07 2001
Groundwater Total Peak Dose and Peak Time withDoses
for Each Nuclide at Peak Time -Values for Each Vector

vector	pktime	pktede	Np237de	U234de	I129de	Tc99de	Se79de	Cl36de
unitless	yr	rem/yr	rem/yr	rem/yr	rem/yr	rem/yr	rem/yr	rem/yr
1	1.00E+05	3.79E-03	3.69E-03	4.62E-08	3.90E-05	6.17E-05	9.31E-07	1.35E-07

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e
May 7, 2003

As noted in the entry dated March 5, 2002, the data for Table 3-13 is from the nucdose100k_allnuc.plt file. The nucdose100k_allnuc.plt file is generated from the rgwna.tpa file produced by the TPA 4.1j code. Sections of the nucdose100k_allnuc.plt file, as read in by Excel are shown below with a discussion for each following.

Single-realization mean value results:

max_time	total	Np-237	U-234	I-129	Tc-99	Se-79	Cl-36
2	2.00E-11	1.00E-12	1.00E-12	1.00E-12	1.00E-12	1.00E-12	1.00E-12
5	2.00E-11	1.00E-12	1.00E-12	1.00E-12	1.00E-12	1.00E-12	1.00E-12
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
9320	1.66E-02	1.00E-12	1.00E-12	6.21E-03	1.04E-02	1.00E-12	3.39E-05
9540	2.67E-02	1.00E-12	1.00E-12	1.00E-02	1.66E-02	1.00E-12	5.47E-05
9770	3.29E-02	1.00E-12	1.00E-12	1.23E-02	2.05E-02	1.00E-12	6.75E-05
10000	3.46E-02	1.00E-12	1.00E-12	1.30E-02	2.15E-02	1.00E-12	7.11E-05
10900	2.42E-02	1.00E-12	1.00E-12	9.08E-03	1.51E-02	1.00E-12	4.92E-05
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
98200	3.10E+00	3.00E+00	4.36E-05	3.86E-02	6.14E-02	9.32E-04	1.34E-04
99100	3.50E+00	3.40E+00	4.49E-05	3.89E-02	6.16E-02	9.32E-04	1.35E-04
100000	3.79E+00	3.69E+00	4.62E-05	3.90E-02	6.17E-02	9.31E-04	1.35E-04

For the single-realization mean value case, the peak expected dose for the 10,000 year case occurred at 10,000 years. The values corresponding to 10,000 years appear in the second column of table 3-13 of the Sensitivity Analysis report. The peak expected dose for the 100,000 year case occurred at 100,000 years. The values corresponding to 100,000 years appear in the fourth column of 3-13 of the Sensitivity Analysis report. Only the pertinent nuclide columns are in this excerpt, all other columns had no contribution to the peak expected dose. The data in Table 3-13 are presented in mSv/yr whereas the data in the spreadsheet excerpts are in mrem/yr so there is a factor of 100 difference with the spread sheet values in mrem/yr being 100 times as large as the mSv/yr values of Table 3-13.

Multiple-realization, probabilistic run results:

max_time	total	Np-237	U-234	I-129	Tc-99	Se-79	Cl-136
2	2.00E-11	1.00E-12	1.00E-12	1.00E-12	1.00E-12	1.00E-12	1.00E-12
5	2.00E-11	1.00E-12	1.00E-12	1.00E-12	1.00E-12	1.00E-12	1.00E-12
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
9320	1.90E-02	2.77E-03	1.15E-07	5.44E-03	1.08E-02	3.47E-06	2.71E-05
9540	2.03E-02	3.47E-03	1.43E-07	5.55E-03	1.12E-02	3.63E-06	2.74E-05
9770	2.06E-02	4.29E-03	1.77E-07	5.34E-03	1.09E-02	3.74E-06	2.64E-05
10000	2.01E-02	5.07E-03	2.23E-07	4.94E-03	1.01E-02	3.85E-06	2.48E-05
10900	2.37E-02	7.97E-03	5.25E-07	5.25E-03	1.04E-02	4.64E-06	2.73E-05
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
98200	9.79E+00	9.43E+00	7.02E-03	1.34E-01	2.10E-01	1.12E-03	5.15E-04
99100	9.81E+00	9.46E+00	6.90E-03	1.33E-01	2.08E-01	1.13E-03	5.08E-04
100000	9.89E+00	9.54E+00	6.80E-03	1.33E-01	2.09E-01	1.14E-03	5.10E-04

For the multiple-realization case the peak expected dose for the 10,000 year case occurred at 9,770 years. The values corresponding to 9,770 years appear in the third column of table 3-13 of the Sensitivity Analysis report. The peak expected dose for the 100,000 year case occurred at 100,000 years. The values corresponding to 100,000 years appear in the fifth column of 3-13 of the Sensitivity Analysis report. Only the pertinent nuclide columns are in this excerpt, all other columns had no contribution to the peak expected dose. The data in Table 3-13 are presented in mSv/yr whereas the data in the spreadsheet excerpts are in mrem/yr so there is a factor of 100 difference with the spread sheet values in mrem/yr being 100 times as large as the mSv/yr values of Table 3-13.

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e
May 8, 2003 Answering comments on Sensitivity Analysis Report, CNWRA 2002-05

Comments concerning the Sensitivity Analysis report were raised stating that certain sections from the fourth paragraph of page 3-37 were "a bit confused". The section in question, with the called out phrases is presented:

"The gap fraction inventory has a longer impact on dose in the 100,000-year simulation period (a 300 percent increase in dose at the time of corrosion failure of waste package) compared with the 10,000-year simulation period (a 12 percent increase in the peak expected dose. This is primarily the result of a proportionately larger gap inventory being available after the corrosion failure than the initially defective failure. The gap fraction inventory, however, influences the 10,000-year simulation period peak while it does not affect the 100,000-year simulation period peak."

The justification for these comments (300 percent increase at time of the corrosion failure and 12 percent increase in the peak expected dose) is shown on the following page as a portion of an excel file.

Towards the end of section 8.3.4 of the TPA Version 4.0, Module Description and User's Guide is a small discussion on the gap fraction inventories. The text discussing gap fraction inventories is presented below:

For all four release rate models, a portion of the radionuclide inventory is assumed to be held loosely on the grain boundaries, cladding/fuel gap, and cladding, referred to collectively as gap inventories. These inventories are available for instantaneous release, which could be a major contributor to peak dose. The gap and grain boundary inventories for each radionuclide are specified by the user as an input parameter in the *tpa.inp* file.

max_time	no gap total	basecase total	% diff
year	mrem/yr	mrem/yr	
2.31	0.00000	0.00000	
4.67	0.00000	0.00000	
.	.	.	.
.	.	.	.
.	.	.	.
8100.00	0.00000	0.00000	
8290.00	0.00000	0.00000	
8490.00	0.00000	0.00000	11.66%
8690.00	0.00013	0.00014	11.39%
8900.00	0.00138	0.00153	11.00%
9110.00	0.00627	0.00696	11.08%
9320.00	0.01494	0.01664	11.39%
9540.00	0.02400	0.02665	11.08%
9770.00	0.02944	0.03287	11.63%
10000.00	0.03095	0.03457	11.71%
10900.00	0.02181	0.02423	11.08%
11800.00	0.01439	0.01581	9.86%
12700.00	0.00727	0.00780	7.34%
13600.00	0.00355	0.00363	2.27%
.	.	.	.
.	.	.	.
.	.	.	.
69400.00	0.27173	0.27171	-0.01%
70300.00	0.27904	0.32743	17.34%
71200.00	0.30957	0.84029	171.44%
72100.00	0.37566	1.49495	297.95%
73000.00	0.41362	0.84181	103.52%
73900.00	0.41963	0.47718	13.71%
74800.00	0.41443	0.41544	0.24%
75700.00	0.40563	0.40201	-0.89%

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e
May 12, 2003 Revising Figure 3-37 Fuel Wetting Assumptions

On June 10, 2002 the cladding with dissolution model 1 was changed but figure 3-37 of the Sensitivity Analysis report was never changed to reflect this. To change this figure I called in the new 7b_claddingdissmod1 expected dose curves and substituted the old Clad-M1 with the new Clad-M1. An adjustment was made so that the resulting new trace of Clad-M1 would be in milliSeiverts/yr instead of millrems/yr. The following Kaleidagraph formula was used:

C2 = C2/100.

May 16, 2003 Source data for confirming Morris ranking

Source data is being collected to verify the ranking of the Morris method ranking as it appears in Table 4-3 of the Sensitivity Analysis Report, CNWRA 2002-05, Revision 1. Each spreadsheet is for a single parameter. The parameter name is in the upper left hand corner of the spreadsheet. The start and stop values for the distribution of the parameter are next to the parameter name. This range is used to multiply the average and standard deviation values to normalize the values for ranking purposes. The first five columns of the spreadsheet represent the input values as extracted from the samplpar.res file which is the input Morris matrix. Only the column with different parameters for the initial and subsequent line apply for this calculation. The sixth column is the dx (difference) for that parameter. Columns 7 through 9 are extracted from the output file, gwpkds_c.res. Column 7 is the realization number, column 8 is the time (in years) that the peak occurred and column 9 is the peak value. Column 10 is the dy (difference) for the output values and column 11 is the quotient or dy/dx. Columns 12 and 13 are the average and standard deviation respectively of the dy/dx column values, with the normalized values appearing in the 6th row of the same columns.

AAMAI@S		Start,Stop 4		13	dx				dy dy/dx		Average	Std Dev
						vector	pktime	pktede			dy/dx	dy/dx
1	330					unitless	yr	rem/yr				
7.86E+00	2.21E+00	-5.71E+00	3.57E-02	4.57E-01	-5.14E+00	1	1.00E+04	0.00E+00	0.00E+00	0.00E+00	1.17E-04	3.10E-04
2	330					2	1.00E+04	0.00E+00				
1.30E+01	2.21E+00	-5.71E+00	3.57E-02	4.57E-01						normalized	-1.05E-03	-2.79E-03
1	330											
5.29E+00	1.93E+00	-1.00E+01	1.43E-01	3.21E-01	-5.14E+00	332	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
2	330					333	1.00E+04	0.00E+00				
1.04E+01	1.93E+00	-1.00E+01	1.43E-01	3.21E-01								
1	330											
7.86E+00	2.07E+00	-8.57E+00	0.00E+00	3.21E-01	-5.14E+00	663	5.56E+03	5.67E-04	-4.22E-03	8.20E-04		
2	330					664	1.00E+04	4.79E-03				
1.30E+01	2.07E+00	-8.57E+00	0.00E+00	3.21E-01								
1	330											
6.57E+00	2.07E+00	-5.00E+00	2.14E-01	3.21E-01	-5.14E+00	994	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
2	330					995	1.00E+04	0.00E+00				
1.17E+01	2.07E+00	-5.00E+00	2.14E-01	3.21E-01								
1	330											
1.17E+01	2.50E+00	-1.00E+01	2.14E-01	5.93E-01	5.14E+00	1325	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
2	330					1326	1.00E+04	0.00E+00				
6.57E+00	2.50E+00	-1.00E+01	2.14E-01	5.93E-01								
1	330											
5.29E+00	2.07E+00	-6.43E+00	1.43E-01	1.86E-01	-5.14E+00	1656	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
2	330					1657	1.00E+04	0.00E+00				
1.04E+01	2.07E+00	-6.43E+00	1.43E-01	1.86E-01								
1	330											
1.17E+01	2.21E+00	-7.86E+00	2.14E-01	7.29E-01	5.14E+00	1987	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
2	330					1988	1.00E+04	0.00E+00				
6.57E+00	2.21E+00	-7.86E+00	2.14E-01	7.29E-01								

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e

MAPM@GM		Start,Stop 1.5		2.5	dx	vector	pktime	pktede	dy dy/dx		Average	Std Dev
						unitless	yr	rem/yr			dy/dx	dy/dx
2	330											
1.30E+01	2.21E+00	-5.71E+00	3.57E-02	4.57E-01	5.71E-01	2	1.00E+04	0.00E+00	0.00E+00	0.00E+00	1.03E-03	2.72E-03
3	330					3	1.00E+04	0.00E+00				
1.30E+01	1.64E+00	-5.71E+00	3.57E-02	4.57E-01						normalized	-1.03E-03	-2.72E-03
2	330											
1.04E+01	1.93E+00	-1.00E+01	1.43E-01	3.21E-01	-5.71E-01	333	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
3	330					334	1.00E+04	0.00E+00				
1.04E+01	2.50E+00	-1.00E+01	1.43E-01	3.21E-01								
2	330											
1.30E+01	2.07E+00	-8.57E+00	0.00E+00	3.21E-01	5.71E-01	664	1.00E+04	4.79E-03	4.12E-03	7.20E-03		
3	330					665	5.56E+03	6.69E-04				
1.30E+01	1.50E+00	-8.57E+00	0.00E+00	3.21E-01								
2	330											
1.17E+01	2.07E+00	-5.00E+00	2.14E-01	3.21E-01	5.71E-01	995	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
3	330					996	1.00E+04	0.00E+00				
1.17E+01	1.50E+00	-5.00E+00	2.14E-01	3.21E-01								
2	330											
6.57E+00	2.50E+00	-1.00E+01	2.14E-01	5.93E-01	5.71E-01	1326	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
3	330					1327	1.00E+04	0.00E+00				
6.57E+00	1.93E+00	-1.00E+01	2.14E-01	5.93E-01								
2	330											
1.04E+01	2.07E+00	-6.43E+00	1.43E-01	1.86E-01	5.71E-01	1657	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
3	330					1658	1.00E+04	0.00E+00				
1.04E+01	1.50E+00	-6.43E+00	1.43E-01	1.86E-01								
2	330											
6.57E+00	2.21E+00	-7.86E+00	2.14E-01	7.29E-01	5.71E-01	1988	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
3	330					1989	1.00E+04	0.00E+00				
6.57E+00	1.64E+00	-7.86E+00	2.14E-01	7.29E-01								

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e

DSFailTi		Start,Stop 2700		20400	dx	vector	pktime	pktede	dy dy/dx		Average	Std Dev
						unitless	yr	rem/yr			dy/dx	dy/dx
12	330					12	1.00E+04	0.00E+00	-1.05E-03	-1.04E-07	-2.68E-08	4.13E-08
2.86E+00	1.49E+04	4.14E+10	2.36E-01	6.00E-01	1.01E+04	13	5.31E+03	1.05E-03				
13	330									normalized	4.75E-04	-7.31E-04
2.86E+00	4.81E+03	4.14E+10	2.36E-01	6.00E-01								
12	330											
1.00E+00	1.28E+04	3.55E+10	1.50E-01	5.62E-01	1.01E+04	343	1.00E+04	0.00E+00	-1.39E-04	-1.37E-08		
13	330					344	3.90E+03	1.39E-04				
1.00E+00	2.70E+03	3.55E+10	1.50E-01	5.62E-01								
12	330											
3.23E+00	4.81E+03	3.94E+10	2.50E-01	4.66E-01	-1.01E+04	674	5.56E+03	6.63E-04	6.63E-04	-6.56E-08		
13	330					675	1.00E+04	0.00E+00				
3.23E+00	1.49E+04	3.94E+10	2.50E-01	4.66E-01								
12	330											
3.23E+00	1.65E+04	4.14E+10	2.07E-01	5.43E-01	1.01E+04	1005	1.00E+04	0.00E+00	-4.82E-05	-4.77E-09		
13	330					1006	7.73E+03	4.82E-05				
3.23E+00	6.42E+03	4.14E+10	2.07E-01	5.43E-01								
12	330											
3.60E+00	4.81E+03	2.96E+10	2.21E-01	5.04E-01	-1.01E+04	1336	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
13	330					1337	1.00E+04	0.00E+00				
3.60E+00	1.49E+04	2.96E+10	2.21E-01	5.04E-01								
12	330											
1.74E+00	2.70E+03	2.76E+10	2.50E-01	5.23E-01	-1.01E+04	1667	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
13	330					1668	1.00E+04	0.00E+00				
1.74E+00	1.28E+04	2.76E+10	2.50E-01	5.23E-01								
12	330											
3.23E+00	1.28E+04	3.55E+10	1.93E-01	5.04E-01	1.01E+04	1998	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
13	330					1999	1.00E+04	0.00E+00				
3.23E+00	2.70E+03	3.55E+10	1.93E-01	5.04E-01								

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e

WPFlowMF		Start,Stop 0.0315		1050	dx	vector	pktime	pktede		dy dy/dx	Average	Std Dev
											dy/dx	dy/dx
60	330					unitless	yr	rem/yr				
7.07E+00	1.27E+01	1.15E+01	2.43E+00	6.01E+02	6.00E+02	60	5.31E+03	1.05E-03	1.01E-03	1.69E-06	3.67E-07	6.24E-07
61	330					61	8.90E+03	3.46E-05				
7.07E+00	1.27E+01	1.15E+01	2.43E+00	6.17E-01						normalized	-3.85E-04	-6.55E-04
60	330											
5.43E+00	9.19E+00	5.99E+00	1.40E+01	6.00E+02	6.00E+02	391	3.90E+03	1.39E-04	1.38E-04	2.30E-07		
61	330					392	7.91E+03	1.11E-06				
5.43E+00	9.19E+00	5.99E+00	1.40E+01	1.39E-01								
60	330											
5.00E-01	9.19E+00	9.64E+00	1.21E+01	6.00E+02	6.00E+02	722	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
61	330					723	1.00E+04	0.00E+00				
5.00E-01	9.19E+00	9.64E+00	1.21E+01	3.15E-02								
60	330											
1.20E+01	5.00E-01	5.99E+00	4.36E+00	6.03E+02	6.00E+02	1053	7.73E+03	4.82E-05	2.86E-05	4.77E-08		
61	330					1054	9.77E+03	1.96E-05				
1.20E+01	5.00E-01	5.99E+00	4.36E+00	2.73E+00								
60	330											
1.04E+01	3.97E+00	9.64E+00	1.01E+01	3.15E-02	-6.00E+02	1384	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
61	330					1385	1.00E+04	0.00E+00				
1.04E+01	3.97E+00	9.64E+00	1.01E+01	6.00E+02								
60	330											
3.79E+00	5.71E+00	9.64E+00	5.00E-01	2.73E+00	-6.00E+02	1715	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
61	330					1716	1.00E+04	0.00E+00				
3.79E+00	5.71E+00	9.64E+00	5.00E-01	6.03E+02								
60	330											
5.00E-01	1.09E+01	5.99E+00	1.21E+01	3.15E-02	-6.00E+02	2046	1.00E+04	0.00E+00	-3.59E-04	5.99E-07		
61	330					2047	9.54E+03	3.59E-04				
5.00E-01	1.09E+01	5.99E+00	1.21E+01	6.00E+02								

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e

gen_PUSF		Start,Stop 0.1		9.8	dx	vector	pktime	pktede	dy dy/dx		Average	Std Dev
						unitless	yr	rem/yr			dy/dx	dy/dx
292	330											
1.46E+03	5.74E+00	5.91E+00	6.29E+06	8.57E+04	5.54E+00	292	7.55E+03	4.25E-05	3.73E-05	6.73E-06	2.46E-05	6.12E-05
293	330					293	7.55E+03	5.23E-06				
1.46E+03	1.93E-01	5.91E+00	6.29E+06	8.57E+04						normalized	-2.38E-04	-5.94E-04
292	330											
1.40E+03	7.13E-01	5.64E+00	6.29E+06	9.94E+00	-5.54E+00	623	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
293	330					624	1.00E+04	0.00E+00				
1.40E+03	6.26E+00	5.64E+00	6.29E+06	9.94E+00								
292	330											
9.50E+01	1.00E-01	1.00E-01	6.29E+06	2.00E+00	-5.54E+00	954	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
293	330					955	1.00E+04	0.00E+00				
9.50E+01	5.64E+00	1.00E-01	6.29E+06	2.00E+00								
292	330											
3.78E+02	5.64E+00	6.26E+00	1.43E+01	8.58E+04	5.54E+00	1285	9.77E+03	4.89E-05	1.14E-05	2.06E-06		
293	330					1286	9.77E+03	3.75E-05				
3.78E+02	1.00E-01	6.26E+00	1.43E+01	8.58E+04								
292	330											
1.40E+03	7.13E-01	6.26E+00	6.29E+06	2.46E+02	-5.54E+00	1616	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
293	330					1617	1.00E+04	0.00E+00				
1.40E+03	6.26E+00	6.26E+00	6.29E+06	2.46E+02								
292	330											
1.51E+02	1.93E-01	5.74E+00	1.31E+03	8.60E+04	-5.54E+00	1947	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
293	330					1948	1.00E+04	0.00E+00				
1.51E+02	5.74E+00	5.74E+00	1.31E+03	8.60E+04								
292	330											
3.78E+02	5.64E+00	5.91E+00	1.50E+00	2.00E+00	5.54E+00	2278	8.10E+03	9.47E-04	9.05E-04	1.63E-04		
293	330					2279	8.10E+03	4.24E-05				
3.78E+02	1.00E-01	5.91E+00	1.50E+00	2.00E+00								

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e

WPRRG@2 Start,Stop 4.50E+06 1.30E+07 dx dy dy/dx Average Std Dev

0

						vector	pktime	pktede			dy/dx	dy/dx
						unitless	yr	rem/yr				
239	330											
1.29E-01	1.28E+01	2.28E+05	8.14E+06	4.86E+01	-4.86E+06	239	7.55E+03	7.43E-05	2.77E-05	-5.71E-12	-1.58E-11	3.20E-11
240	330					240	7.55E+03	4.65E-05				
1.29E-01	1.28E+01	2.28E+05	1.30E+07	4.86E+01						normalized	1.34E-04	-2.72E-04
239	330											
1.36E-01	1.28E+01	2.64E+05	6.93E+06	8.71E+01	-4.86E+06	570	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
240	330					571	1.00E+04	0.00E+00				
1.36E-01	1.28E+01	2.64E+05	1.18E+07	8.71E+01								
239	330											
1.00E-01	1.00E+01	1.93E+05	8.14E+06	1.00E+02	-4.86E+06	901	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
240	330					902	1.00E+04	0.00E+00				
1.00E-01	1.00E+01	1.93E+05	1.30E+07	1.00E+02								
239	330											
1.07E-01	1.28E+01	2.28E+05	5.71E+06	6.14E+01	-4.86E+06	1232	9.77E+03	1.91E-04	8.78E-05	-1.81E-11		
240	330					1233	9.77E+03	1.03E-04				
1.07E-01	1.28E+01	2.28E+05	1.06E+07	6.14E+01								
239	330											
1.50E-01	1.85E+01	1.57E+05	6.93E+06	1.00E+01	-4.86E+06	1563	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
240	330					1564	1.00E+04	0.00E+00				
1.50E-01	1.85E+01	1.57E+05	1.18E+07	1.00E+01								
239	330											
1.14E-01	1.99E+01	8.61E+04	1.30E+07	1.00E+01	4.86E+06	1894	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
240	330					1895	1.00E+04	0.00E+00				
1.14E-01	1.99E+01	8.61E+04	8.14E+06	1.00E+01								
239	330											
1.07E-01	1.71E+01	1.22E+05	9.36E+06	7.43E+01	4.86E+06	2225	8.10E+03	3.90E-04	-4.21E-04	-8.67E-11		
240	330					2226	8.10E+03	8.11E-04				
1.07E-01	1.71E+01	1.22E+05	4.50E+06	7.43E+01								

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ARDSAVNp		Start,Stop 1		3900	dx	vector	pktime	pktede	dy dy/dx		Average	Std Dev
						unitless	yr	rem/yr			dy/dx	dy/dx
225	330											
6.14E-04	1.00E-03	1.00E-02	3.89E+10	2.26E+03	2.23E+03	225	6.56E+03	9.64E-05	0.00E+00	0.00E+00	-2.51E-08	6.64E-08
226	330					226	6.56E+03	9.64E-05				
6.14E-04	1.00E-03	1.00E-02	3.89E+10	3.46E+01						normalized	9.79E-05	-2.59E-04
225	330											
7.07E-04	1.93E-03	1.00E-02	3.89E+10	2.23E+03	2.23E+03	556	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
226	330					557	1.00E+04	0.00E+00				
7.07E-04	1.93E-03	1.00E-02	3.89E+10	1.00E+00								
225	330											
6.53E-04	6.53E-03	7.83E-02	3.89E+10	1.06E+01	-2.23E+03	887	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
226	330					888	1.00E+04	0.00E+00				
6.53E-04	6.53E-03	7.83E-02	3.89E+10	2.24E+03								
225	330											
7.07E-04	2.68E-03	1.93E-02	3.89E+10	2.26E+03	2.23E+03	1218	9.77E+03	2.06E-04	0.00E+00	0.00E+00		
226	330					1219	9.77E+03	2.06E-04				
7.07E-04	2.68E-03	1.93E-02	3.89E+10	3.46E+01								
225	330											
6.14E-04	1.93E-03	1.39E-02	7.50E+04	3.46E+01	-2.23E+03	1549	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
226	330					1550	1.00E+04	0.00E+00				
6.14E-04	1.93E-03	1.39E-02	7.50E+04	2.26E+03								
225	330											
7.07E-04	1.39E-03	6.53E-02	2.68E+07	2.23E+03	2.23E+03	1880	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
226	330					1881	1.00E+04	0.00E+00				
7.07E-04	1.39E-03	6.53E-02	2.68E+07	3.26E+00								
225	330											
6.14E-04	6.14E-03	1.39E-02	3.89E+10	1.00E+00	-2.23E+03	2211	8.49E+03	7.71E-04	3.92E-04	-1.76E-07		
226	330					2212	4.09E+03	3.80E-04				
6.14E-04	6.14E-03	1.39E-02	3.89E+10	2.23E+03								

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IPPFSTFF		Start,Stop 0.01		0.1	dx	vector	pktime	pktede	dy dy/dx	Average	Std Dev
						unitless	yr	rem/yr			dy/dx dy/dx
223	330										
6.14E-04	1.00E-03	6.14E-02	5.32E+05	2.26E+03	5.14E-02	223	7.04E+03	6.65E-05	-2.99E-05	-5.82E-04	-1.21E-03 2.67E-03
224	330					224	6.56E+03	9.64E-05			
6.14E-04	1.00E-03	1.00E-02	5.32E+05	2.26E+03						normalized	1.09E-04 -2.41E-04
223	330										
7.07E-04	1.93E-03	6.14E-02	3.78E+06	2.23E+03	5.14E-02	554	1.00E+04	0.00E+00	0.00E+00	0.00E+00	
224	330					555	1.00E+04	0.00E+00			
7.07E-04	1.93E-03	1.00E-02	3.78E+06	2.23E+03							
223	330										
6.53E-04	6.53E-03	2.68E-02	3.78E+06	1.06E+01	-5.14E-02	885	1.00E+04	0.00E+00	0.00E+00	0.00E+00	
224	330					886	1.00E+04	0.00E+00			
6.53E-04	6.53E-03	7.83E-02	3.78E+06	1.06E+01							
223	330										
7.07E-04	2.68E-03	7.07E-02	2.68E+07	2.26E+03	5.14E-02	1216	1.00E+04	1.73E-04	-3.39E-05	-6.58E-04	
224	330					1217	9.77E+03	2.06E-04			
7.07E-04	2.68E-03	1.93E-02	2.68E+07	2.26E+03							
223	330										
6.14E-04	1.93E-03	6.53E-02	3.89E+10	3.46E+01	5.14E-02	1547	1.00E+04	0.00E+00	0.00E+00	0.00E+00	
224	330					1548	1.00E+04	0.00E+00			
6.14E-04	1.93E-03	1.39E-02	3.89E+10	3.46E+01							
223	330										
7.07E-04	1.39E-03	1.39E-02	3.89E+10	2.23E+03	-5.14E-02	1878	1.00E+04	0.00E+00	0.00E+00	0.00E+00	
224	330					1879	1.00E+04	0.00E+00			
7.07E-04	1.39E-03	6.53E-02	3.89E+10	2.23E+03							
223	330										
6.14E-04	6.14E-03	6.53E-02	5.32E+05	1.00E+00	5.14E-02	2209	8.69E+03	3.99E-04	-3.72E-04	-7.24E-03	
224	330					2210	8.49E+03	7.71E-04			
6.14E-04	6.14E-03	1.39E-02	5.32E+05	1.00E+00							

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PSFDM1		Start,Stop 1200		1200000	dx					dy dy/dx	Average	Std Dev
						vector	pktime	pktede			dy/dx	dy/dx
						unitless	yr	rem/yr				
63	330											
2.86E-01	2.93E-03	8.64E+03	2.67E-03	9.29E-07	-6.85E+05	63	8.90E+03	3.30E-06	-7.08E-05	1.03E-10	8.95E-11	1.27E-10
64	330					64	8.90E+03	7.41E-05				
2.86E-01	2.93E-03	6.94E+05	2.67E-03	9.29E-07						normalized	-1.07E-04	-1.52E-04
63	330											
0.00E+00	1.51E-03	3.22E+03	7.00E-04	1.36E-06	-6.85E+05	394	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
64	330					395	1.00E+04	0.00E+00				
0.00E+00	1.51E-03	6.88E+05	7.00E-04	1.36E-06								
63	330											
8.57E-01	4.34E-03	6.94E+05	7.00E-04	1.36E-06	6.85E+05	725	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
64	330					726	1.00E+04	0.00E+00				
8.57E-01	4.34E-03	8.64E+03	7.00E-04	1.36E-06								
63	330											
7.14E-01	1.51E-03	2.32E+04	2.34E-03	7.14E-07	-6.85E+05	1056	9.77E+03	1.72E-05	-1.43E-04	2.09E-10		
64	330					1057	9.54E+03	1.60E-04				
7.14E-01	1.51E-03	7.08E+05	2.34E-03	7.14E-07								
63	330											
2.86E-01	5.76E-03	6.86E+05	3.00E-03	1.14E-06	6.85E+05	1387	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
64	330					1388	1.00E+04	0.00E+00				
2.86E-01	5.76E-03	1.20E+03	3.00E-03	1.14E-06								
63	330											
5.71E-01	4.34E-03	3.22E+03	3.00E-03	1.57E-06	-6.85E+05	1718	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
64	330					1719	1.00E+04	0.00E+00				
5.71E-01	4.34E-03	6.88E+05	3.00E-03	1.57E-06								
63	330											
2.86E-01	1.51E-03	8.64E+03	1.03E-03	2.00E-06	-6.85E+05	2049	9.54E+03	1.94E-05	-2.15E-04	3.14E-10		
64	330					2050	9.54E+03	2.35E-04				
2.86E-01	1.51E-03	6.94E+05	1.03E-03	2.00E-06								

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SbArWt%		Start,Stop 0		1	dx	vector	pktime	pktede	dy dy/dx		Average	Std Dev
						unitless	yr	rem/yr			dy/dx	dy/dx
61	330											
8.57E-01	8.59E-03	8.64E+03	2.67E-03	9.29E-07	5.71E-01	61	8.90E+03	3.46E-05	2.31E-05	4.04E-05	8.55E-05	1.55E-04
62	330					62	8.90E+03	1.15E-05				
2.86E-01	8.59E-03	8.64E+03	2.67E-03	9.29E-07						normalized	-8.55E-05	-1.55E-04
61	330											
5.71E-01	7.17E-03	3.22E+03	7.00E-04	1.36E-06	5.71E-01	392	7.91E+03	1.11E-06	1.11E-06	1.94E-06		
62	330					393	1.00E+04	0.00E+00				
0.00E+00	7.17E-03	3.22E+03	7.00E-04	1.36E-06								
61	330											
2.86E-01	1.00E-02	6.94E+05	7.00E-04	1.36E-06	-5.71E-01	723	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
62	330					724	1.00E+04	0.00E+00				
8.57E-01	1.00E-02	6.94E+05	7.00E-04	1.36E-06								
61	330											
1.43E-01	7.17E-03	2.32E+04	2.34E-03	7.14E-07	-5.71E-01	1054	9.77E+03	1.96E-05	-7.83E-05	1.37E-04		
62	330					1055	9.77E+03	9.78E-05				
7.14E-01	7.17E-03	2.32E+04	2.34E-03	7.14E-07								
61	330											
8.57E-01	1.00E-04	6.86E+05	3.00E-03	1.14E-06	5.71E-01	1385	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
62	330					1386	1.00E+04	0.00E+00				
2.86E-01	1.00E-04	6.86E+05	3.00E-03	1.14E-06								
61	330											
0.00E+00	1.00E-02	3.22E+03	3.00E-03	1.57E-06	-5.71E-01	1716	1.00E+04	0.00E+00	0.00E+00	0.00E+00		
62	330					1717	1.00E+04	0.00E+00				
5.71E-01	1.00E-02	3.22E+03	3.00E-03	1.57E-06								
61	330											
8.57E-01	7.17E-03	8.64E+03	1.03E-03	2.00E-06	5.71E-01	2047	9.54E+03	3.59E-04	2.40E-04	4.19E-04		
62	330					2048	9.54E+03	1.20E-04				
2.86E-01	7.17E-03	8.64E+03	1.03E-03	2.00E-06								

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June 10, 2003 Orders of magnitude in Peak Groundwater Dose

In the comments in response to the Sensitivity Analysis report (CNWRA 2002-05 Revision 1) an objection is raised to using "6 orders of magnitude" in describig the variability of peak groundwater dose. ~~In the basecase gwpkdos.res, ignoring no-release cases, th peak groundwater dose (labeled pktede) varies from 2.94E-4 rem/yr to 4.1e+2 rem/yr or 0.294 mrem/yr to 410,000 mrem/yr. This is not a result of calculating the dose to very small values "(i.e. 0.001 mrem)" as the comments suggest.~~

This information was gathered by importing the gwpkdos.res file found in jmench/tpa41j/newYMR-TC/basecaseRuns/bcrWithAppendFiles2 into Microsoft Excel 2000 and using the min and max features. The no-release occurences were blanked so as not to skew the data downward.

June 17, 2003 Calculating Mass Of Neptunium For 3 Halflives

These calculations were done to verify the statements made in Section 3.2.2 of the Sensitivity Analysis report concerning the solubility limited control verses the dissolution limited control of Np-237.

Calculated mass of neptunium (Np-237) necessary to make up 0.434 Ci at three different half lives. The 0.434 Ci is the amount of Np-237 for each megaton of uranium at 10 years as specified in nuclides.dat

HalfLife (yrs)	lambda (sec^{-1})	Disintegrations/sec for 1kg of Np-237	mass of 0.434 Ci of Np-237 (kg)
2.14E+05	1.03E-13	2.61E+11	0.0615
2.14E+06	1.03E-14	2.61E+10	0.6152
2.14E+07	1.03E-15	2.61E+09	6.1521

lambda = ln(2)/(halflife × 365 days/year × 86400 seconds/day)

disintegrations/sec for 1 kg of Np-237 = (6.023×10^{23} nuclei / 0.237 kg) × lambda

mass of 0.434 Ci of Np-237 = ($0.434 \times 3.7 \times 10^{10}$) / (disintegrations/sec for 1 kg of Np-237)

With ten times higher mass required to produce the same amount of Ci per megaton of uranium for the long halflife case, the solubility limit is hit much sooner. The same amount of Np-237 being carried out means less activity in the mass that is being carried away.

June 23, 2003 Correction to notebook entries made on June 10, 2003

The data that was bing viewed was already in mrems/yr so the values cited are actually vary from 0.000294 rem/yr to 410 mrem/yr, in keeping with the original objection. The comment should stand and the line will be struck from the text of the Sensitivity Analysis report (CNWRA 2002-05 Revision 1).

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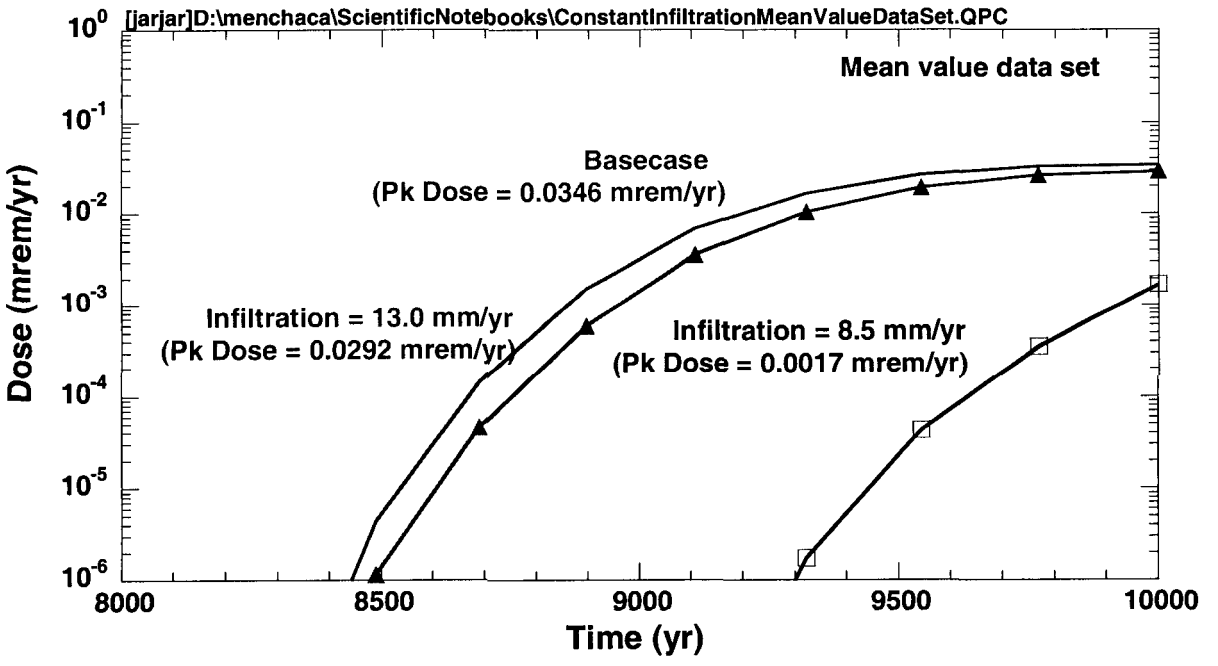
August 12, 2003 Running Constant Infiltration Runs for S. Mohanty.

Base case runs (both mean value and multi-vector) with constant infiltration were required by S. Mohanty. From previous work (from June 12, 2003) demonstrating the depletion of ^{237}Np by water contacting the waste package, I using the following method to hold the infiltration constant:

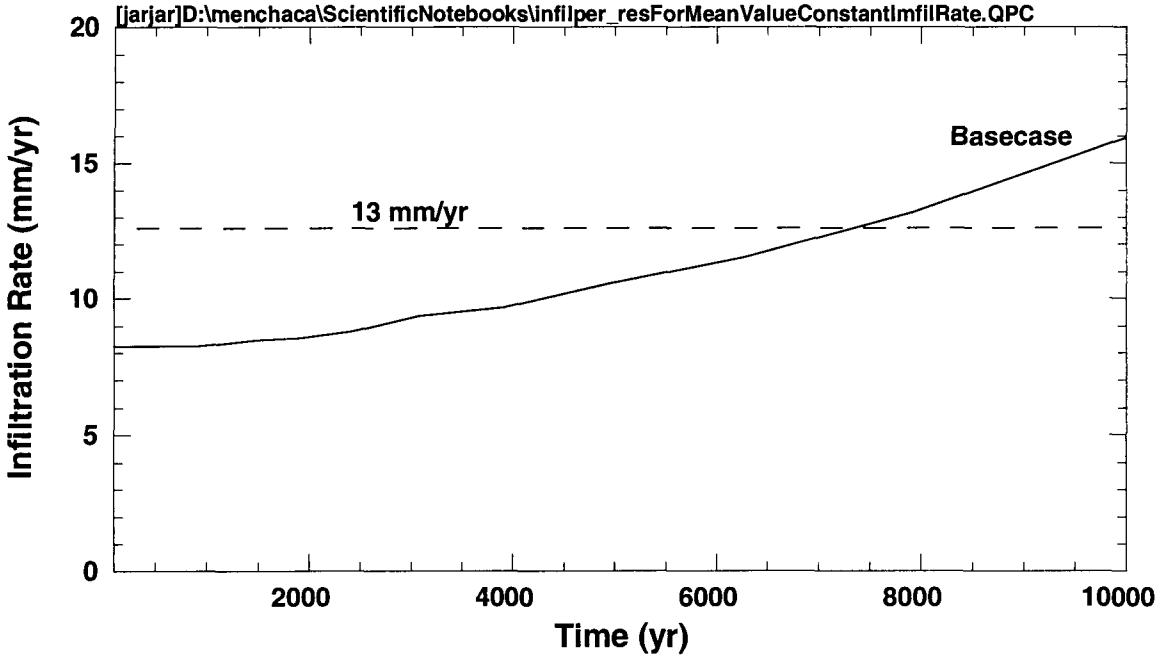
1. Changed the value of the parameter "Mean Average Precipitation Multiplier At Glacial Maximum" (MAPM@GM) from 2.0 to 1.0.

2. Changed the value of the parameter "Mean Average Temperature Increase At Glacial Maximum" (MATI@GM) from -7.5 to 0.0.

The results of this run, which was executed on August 7, 2003, are saved on
`[jarjar]D:\menchaca\ScientificNotebooks\ConstantInfiltrationMeanValueDataSet.QPC`

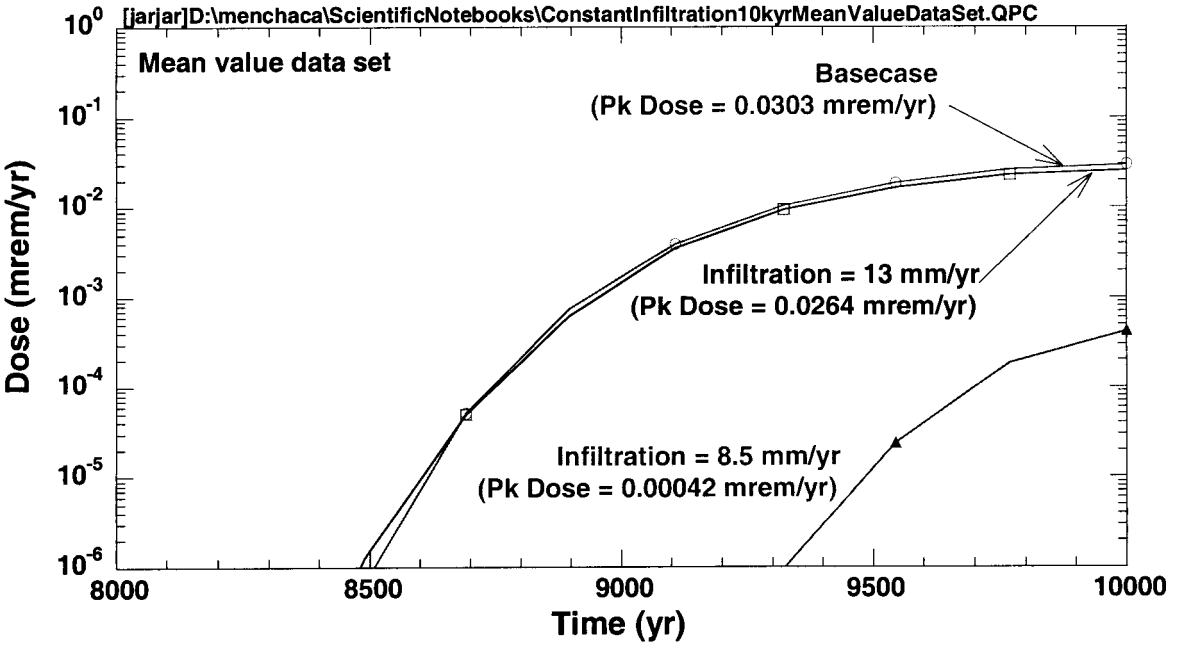


From this run it is seen that the basecase run has higher dose than the constant high infiltration run using a constant infiltration of 13.0 mm/yr. This was an unexpected result. The actual infiltration rates from infilper.res for the basecase and the constant high infiltration rate run are plotted on
[jarjar]D:\menchaca\ScientificNotebooks\infilper_resForMeanValueConstantInfilRate.QPC

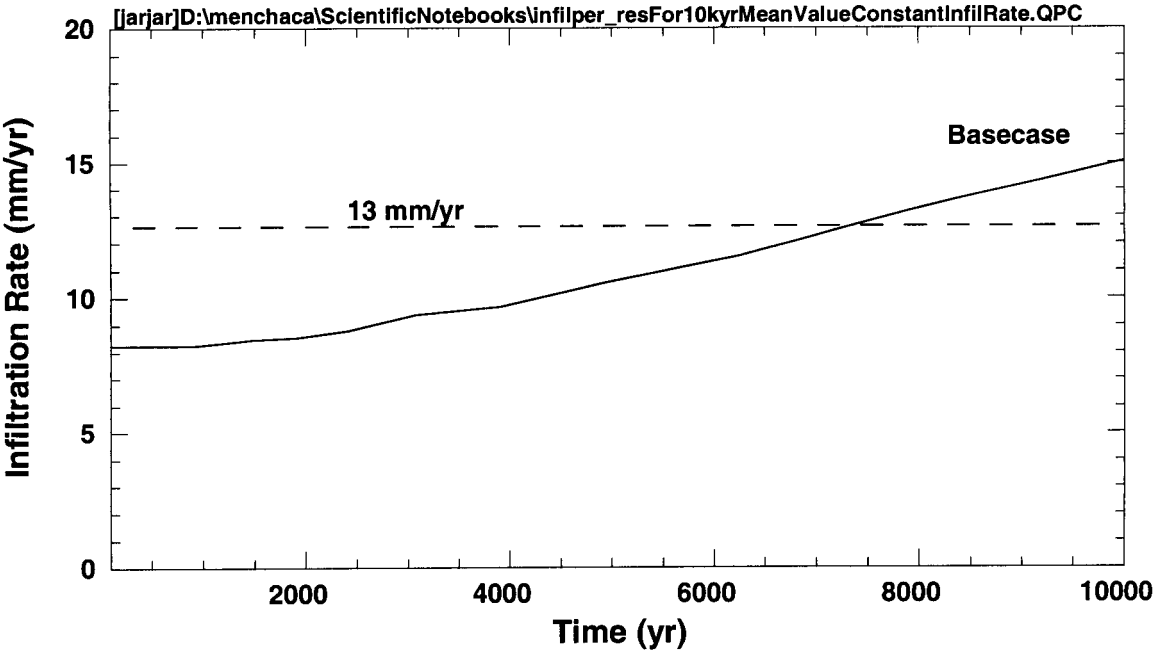


From this figure it is seen that by the time that dose is appearing in the totdose.res file, the basecase infiltration has exceeded the constant high infiltration of 13.0 mm/yr. This causes the basecase dose to exceed the high infiltration dose.

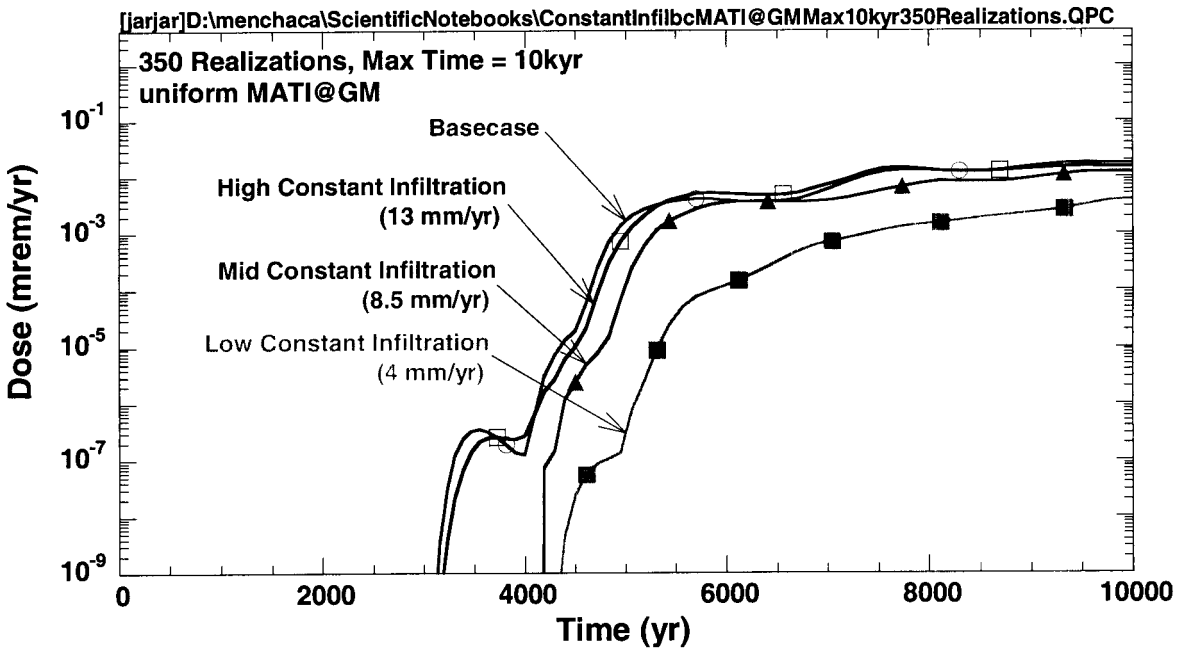
It was suggested by S. Mohanty that the reason that this appears this way is because the max time in the tpa.inp file is set for 100,000 years. Setting the max time for 10,000 years should fix it. The two files that correspond to these conditions (from runs executed on August 8, 2003) are
[jarjar]D:\menchaca\ScientificNotebooks\ConstantInfiltration10kyrMeanValueDataSet.QPC



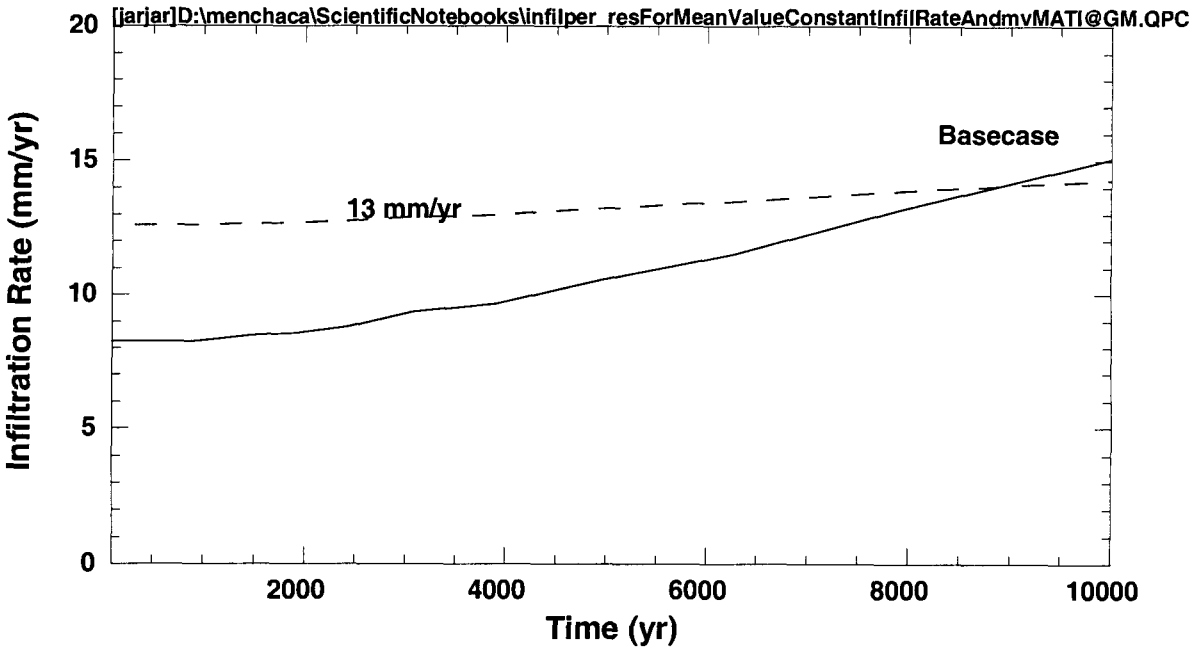
and
[jarjar]D:\menchaca\ScientificNotebooks\infilper_resFor10kyrMeanValueConstantInfilRate.QPC



Finally in an attempt to have the constant high infiltration rate dose exceed the basecase dose I returned the value of the parameter "Mean Average Temperature Increase At Glacial Maximum" (MATI@GM) from 0.0 back to -7.5. The results of these conditions (from runs executed on August 11, 2003) are saved on
[jarjar]D:\menchaca\ScientificNotebooks\ConstantInfilbcMATI@GMMax10kyr350Realizations.QPC



[jarjar]D:\menchaca\ScientificNotebooks\infilper_resForMeanValueConstantInfilRateAndmvMATI@GM.QPC



Printed: March 23, 2005

J. Menchaca SCIENTIFIC NOTEBOOK No. 170-5e

Entries into Scientific Notebook No. 170-5e for pages 5-9 have been made by Jose M. Menchaca. ~~March 23, 2005~~ JMM 09/15/05

No original text entered into this Scientific Notebook has been removed.
Jose M. Menchaca ~~March 23, 2005~~ JMM 09/15/05
09/15/05

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

11-07-05