

# **SCIENTIFIC NOTEBOOK**

**170-17E**

Printed: March 23, 2005

B. Winfrey

SCIENTIFIC NOTEBOOK No. 170-17e

## **SCIENTIFIC NOTEBOOK**

by

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## INITIAL ENTRIES

Scientific Notebook: #170

Issued to: S. Mohanty

Issue Date: Apr. 3, 1996

Account Number: 20-5708-762

Title: EXEC

Participants: Brandi Winfrey

Unless otherwise specified, the following environment is used for all source code compiled for this notebook:

**Host Machine:** SUN Ultra-4 Server: spock   **Host OS:** Solaris 5.8

**Computer Language:**      Fortran      **Compiler:** Sun F77

June 12, 2002

Obtained TPA 5.0 source code from */nfs/scratchy1/janetzke/tpa/dev* and the SRD, SDP, and SCR PA-SCR-373 from *g:\pa\tpa50*. I am to test the code in SCR-373.

Notes:

Logical ltemp defined in "Description of changes..." block of SCR, but not used. It is redefined on page 5 of the Functional level tests, where it is used.

TPA.INP – code from */nfs/scratchy1/janetzke/tpa/dev* has some mismatched values for CHnv... variables (i.e., the "Description

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of changes...” attachment assumes values in the range 0.01-0.04 while the actual file has the same values at 0.0.

- The “Description of changes...” block mentions changes to the files uzft.f, szft.f, and tpa.inp. The Test Plan also mentions changes to these same files. The changes are exactly the same for tpa.inp but are different for uzft.f and szft.f. There doesn’t seem to be a need to repeat the same changes for tpa.inp. Also, the mismatched values mentioned earlier for tpa.inp do not exist in the Test Plan (i.e., the values are shown as 0.0 as they should be).
- The variables UFZ\_Thickness\_10... are listed to be modified in tpa.inp (Test Plan page 4), but no changes are suggested. These lines should be removed from the Test Plan.
- Under Functional Level Tests it should describe that the Environmental variables will most likely point to the same path as the run directory (because it contains the /data and /codes directories).
- On page 6 of the Test Plan why use the phrase “Program modes to be used”? It doesn’t seem to relate to the directions immediately following it.
- On page 7 of the Test Plan what is the purpose of step 5? If it is simply to save a copy of the just created tpa.e then mention something about moving it to the archive directory.
- The archive directory is not mentioned in the Functional Level Tests after its initial definition. Maybe the step-by-step procedure should mention archiving results.

June 13, 2002 -

Starting from TPA version 5.0, I made changes to the code as indicated in the “Description of Changes...” block of the SCR as well as the changes indicated by the Test Plan. The following things were observed:

- The output file tpa\_flt1.out had an entirely different format than the one shown in the Test Plan. This leads me to believe that I have started with the wrong initial version.

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- I spent the rest of the day trying to locate the correct input files and redo the changes indicated by the Test Plan. After accomplishing this, I ran the test and got the correct file format, but the numbers were incorrect:  
spname = CHnvThickness\_2SubArea[m]  
          0.71576900000000  
spname = CH\_Total\_Thickness\_2SubArea[m]  
- CHnv = CHnz = 107.28423100000

June 19, 2002 - I have run all of the tests in the Test Plan and they have all passed with the exception of the System Level Tests for Subareas 4 and 7. These two tests both use the exact same tpa\_base.inp, tpa\_sl6.inp, tpa\_base.e. After all indicated changes are made, the only differences are in tpa\_bsa4.inp and tpa\_tsa4.inp which have each had only the subarea number modified. This was verified by running diff on the required files. After running the following commands:

```
tpa.e > tpa_bsa1.out  
tpa.e > tpa_tsa1.out  
tpa.e > tpa_bsa4.out  
tpa.e > tpa_tsa4.out
```

the first two commands above each produced nefiuz.inp files (copied to sa1/nefiuz\_bsa1.inp and sa1/nefiuz\_tsa1.inp). The second two commands DID NOT produce nefiuz.inp files and therefore sa4/nefiuz\_bsa4.inp and sa4/nefiuz\_tsa4.inp cannot be compared to see if the test passed. I do not know why because the only differences between the files used are shown below.

```
spock:bwinfrey:/net/spock/home/bwinfrey/rjanetzke/SCR373_TPA {192}  
diff tpa_bsa1.inp tpa_bsa4.inp  
267c267  
< 1  
---  
> 4  
271c271  
< 1  
---  
> 4  
spock:bwinfrey:/net/spock/home/bwinfrey/rjanetzke/SCR373_TPA {193}  
diff tpa_tsa1.inp tpa_tsa4.inp
```

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267c267  
< 1  
---  
> 4  
271c271  
< 1  
---

I have two other notes/changes which I have not added to the revised Test Plan because I am not sure why they are so or if they are correct even though they will produce the desired output as described in the Test Plan. On page 17, test 5, the input `tpa_base.inp` has to have the `CHnzThickness_#SubArea[m]` variables set to uniform in order for the output to be correct but it does not say to make this change in the directions (and even if it did, then you will be comparing a modified code with a modified code, not with the base code. Is this right?). Then on page 20, test 6, the input `tpa_base.inp` has to have the `CHnzThickness_#SubArea[m]` variables all set to constant in order to obtain the desired output. These values for `tpa_base.inp` remain the same (constant) for every test after test 6.

June 28, 2002 - Obtained TPA 4.2d source from `rlt/spock/home/cscherer/tpatest/scr375` and SCR PA-SCR-375 from Ron Janetzke I am to validate the Test Plan for SCR-375.

Notes:

- This test plan went much smoother than the last one. I started with the correct files and made minimal changes to the Test Plan (consisting mainly of typos) and no changes to the code.
- The Test plan was completed on 7/3/02 and the archive directories were copied to a CD.

July 19, 2002 - Begin work on testing the Test Plan for SCR 395 (DSFAIL/DSFAILT).

July 30, 2002 -

SCR 395 (Task ID EX5) Test Plan testing complete. I've finished going through the test plan and everything has passed successfully. I burned a copy of the directories in which I ran the tests and made the following changes to the test plan:

added to `tpa.inp` table in SL-1, SL-2, SL-3:

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	OutputMode(0=None,1=All,2=UserDefined)		2	
--	--	--	---	--

changed typo "sl-1" to "sl-3" in SL-3 test.

changed tester name to Brandi L. Winfrey

changed date to July 30, 2002.

All of this has been given to Ron Janetzke.

July 30, 2002 - Begin development of Test Plan for SCR 327 Groundwater Protection Calculations.

Coding was done by James Weldy (JRW) and Rob Rice (RWR).

Aug 02, 2002

SCR 327. I see where `exec.f` writes the headers to `epa_ave.out` and `epapktim.out` and have been able to remove the uranium header column, change radon to radium, and remove all of the "scaled" labels. Now with the easy stuff out of the way, I'm trying to get rid of the actual uranium data. `dcagw.f` performs the calculation of uranium concentration (around lines 1179 and 1248) and fills arrays with the data in the other columns in `epa_ave.out` and `epapktim.out`, but I don't see where the columns actually get written to these files. The `.out` filenames are not mentioned in `dcagw.f` unless the variables `iwriteepapktim` and `iwriteepa_ave` (around lines 1363-1394) are used to write to the files? but I don't know where they get initialized.

Aug 08, 2002

SCR 327. References to `epa_dose.out` should be removed from Part I. The groundwater protection info should be written to `epa_ave.out` and `epapktim.out`.

Aug 09, 2002

SCR 327 is not closed and can be modified.

Aug 13, 2002

SCR 327: Send a note to Pat Laplante about the units to use:

Do you know what units I should use in the column labels in the `epa_ave.out` and `epapktim.out` files? `mrem/yr` or `pCi/L`? These values are for concentration and dose. We would like the concentration units to be in `pCi/L` and the dose units to

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be in mrem/yr. To determine what units the current calculations produce would take more checking of the source code. If the last version determined the "scaled" results by dividing the concentration results by 5 for radium, and 15 for gross alpha activity then the calculated concentrations are in pCi/L. If the scaled dose results are produced by dividing by 4, then the calculated doses are in mrem/yr.

Aug 26, 2002

I met with Osvaldo Pensado to discuss SCR 398. He emailed me the results of our discussion. email from Osvaldo Pensado:

In the attached document is a summary of our discussion. Let me know if something is not clear.

The linear interpolation subroutine is

linintrp.f (it uses srchpos.f; thus make sure that you have both of them). These library routines are available for TPA 4.2j

I checked the code, and it seems that the only file that you need to manipulate is **nfenv.f**

-attachment:-----

Strategy to select ion concentrations (chloride, fluoride, pH, carbonate) and DeltaECrit

Temperature (C)	Relative Humidity (%)	Time (year)	Chemistry Data Source	Sampled/Constant parameter name from <i>tpa.inp</i>
T < 97	all values	all values	<b>multifbe.dat</b> if before dry-out period and <b>multifaf.dat</b> if after dry-out period	N/A
97 < T	<b>RH &lt; Critical</b> Relative Humidity Aqueous Corrosion	all values	<i>tpa.inp</i> constant values for dry period (dummy values)	Cl_conc_Dry = 0 Fl_conc_Dry = 0 pH_Dry = 7 CO3_Dry = 0 DeltaECrit_Dry=0



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	CriticalRelativeHumidityAqueousCorrosion < RH	t < TimeOfPeakTemperature	tpa.inp sampled parameters for epoch 1.	Cl_epoch_1 FI_epoch_1 pH_epoch_1 CO3_epoch_1 DeltaECrit_epoch_1
		TimeOfPeakTemperature < t	tpa.inp sampled parameters for epoch 2.	Cl_epoch_2 FI_epoch_2 pH_epoch_2 CO3_epoch_2 DeltaECrit_epoch_2

**Parameters currently available in tpa.inp**

BoilingPointOfWater[C] : Constant = 97 C

CriticalRelativeHumidityAqueousCorrosion : Uniform[0.242, 0.56]

**Need to introduce to tpa.inp**

Cl\_epoch\_1 : loguniform[2.0E-4,10.0]

FI\_epoch\_1 : loguniform[1.15E-4,0.52]

pH\_epoch\_1 : uniform[5.78, 11.0]

CO3\_epoch\_1 : uniform[0.0,0.8324]

DeltaECrit\_epoch\_1 : constant=0.0

Cl\_epoch\_2 : loguniform[2.0E-4,10.0]

FI\_epoch\_2 : loguniform[1.15E-4,0.52]

pH\_epoch\_2 : uniform[5.78, 11.0]

CO3\_epoch\_2 : uniform[0.0,0.8324]

DeltaECrit\_epoch\_2 : constant=0

**Local variables**

The following are just local variables and should not have any influence on the results. They are just dummy constants, and there is no need to specify them in tpa.inp

Cl\_conc\_Dry = 0

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Fl\_conc\_Dry = 0

pH\_Dry = 7

CO3\_Dry = 0

DeltaECrit\_Dry=0

The following variable changes from subarea to subarea and from realization to realization:

**TimeOfPeakTemperature**

This variable must be computed for every realization and subarea

---

Aug 30, 2002

SCR 398. multiflo.dat will be replaced by multibe.dat and multiaf.dat. Both of them are look-up tables that will be constructed manually and available in a directory (same directory where we have placed multiflo.dat).

The only code to manipulate is nfenv.f. exec.f does not need to be touched at all. No need to worry about the creation of the input files ebstrh.inp and all of the \*.inp files. Those will be created automatically if the changes in nfenv.f are well done.

The fluoride and chloride subroutines presume certain format for multiflo.dat. We have changed that format in multibe.dat and multiaf.dat. We assume now that the temperature is the independent variable (before, with multiflo.dat, we assumed that the temperature was the independent variable).

Sept 05, 2002

SCR 398: email from Osvaldo to me:

I gave what you gave us to George Adams ...

He pretty much cleaned your code and has it running.

I would appreciate if you develop the test plan and perform it.

The test plan should be quite simple. It is just matter of inspecting the output file nfenv.rlt and making sure that the entries there coincide with our expectations.

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It is my understanding that you have developed already a test plan. You can follow that example.

Sept 06, 2002

SCR 398. Email from me to G. Adams:

Oswaldo said that he sent you the code that I was working on (nfenv.f) for cl/fl/pH/C03/deltaECrit concentrations and that you got it working. Would you be able to send me the working code so that I can run the Test Plan for it? Also, I just noticed that I forgot to add C03 to the arguments passed from nfenv.f to exec.f. I don't think it is used anywhere yet, but it should be in the args list.

Sept 09, 2002

SCR 398: Email from George Adams:

Please find the attached files: nfenv.f, exec.f, and tpa.inp, multifaf.dat, and multifbe.dat. I integrated these into version 4.2k which I had on my PC. I built the code and ran it on spock as well as on my pc. The build and run directories on spock are under the following directory: /home/gadams/PA-SCR-398/code42k. I made the change that you mentioned to exec so that carbonate would appear in the nfenv.rlt file for testing. I also followed your logic in the nfenv code.

Sept 10, 2002

SCR 398: email from G. Adams:

I updated the nfenv module and the test plan that you generated. I think the code is ready to run the test plan on. I'm including the source code that I generated along with the updated test plan. I'm also including the modified data files that I mention in the test plan. All of my work on this SCR is in the directory /home/gadams/PA-SCR-398. The testing is under the test subdirectory and the source code is in the code directory (integrated into 4.2k). I did a quick check of the output for nfenv and it looks like it is producing the correct values.

Sept 11, 2002

SCR 398. I am now running the revised test plan sent to me by G. Adams.

The output files *nfenv.rlt* and *nfenv.ech* were generated per 8.5 step 2. To verify the correct vales in accordance with 8.5 step 3, bullets 1 through 5, the following lines from *nfenv.rlt* were used:  
bullet 1 -----

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3	4.6744E+00	7.4653E+01	8.5908E+01	6.3416E-01	7.4373E+00	2.2733E-04
	5.9553E+00	9.8453E-02	1.1773E-04	2.1373E-03		5.7327E-01
17	4.4219E+01	8.0102E+01	8.6082E+01	7.8851E-01	7.4401E+00	2.3005E-04
	5.9729E+00	8.0894E-02	1.1801E-04	2.1401E-03		6.0051E-01

bullet 2 -----

130	1.8543E+03	8.8932E+01	8.9685E+01	9.7166E-01	7.4945E+00	2.8447E-04
	6.2875E+00	7.2970E-02	1.2345E-04	2.1945E-03		1.1447E+00
195	8.6908E+03	5.3887E+01	5.4279E+01	9.8126E-01	7.4769E+00	2.6694E-04
	1.1625E+01	1.4950E-01	1.2169E-04	2.1769E-03		9.6944E-01

bullet 3 -----

23	6.5503E+01	1.5193E+02	1.5846E+02	1.5276E-01	7.0000E+00	0.0000E+00
	5.9768E+00	7.6937E-02	0.0000E+00	0.0000E+00		0.0000E+00
71	3.9990E+02	1.2590E+02	1.2823E+02	3.5465E-01	7.0000E+00	0.0000E+00
	6.0537E+00	0.0000E+00	0.0000E+00	0.0000E+00		0.0000E+00

bullet 4 -----

19	5.0988E+01	1.1272E+02	1.2143E+02	4.3756E-01	8.3900E+00	4.4700E-02
	5.9730E+00	8.0792E-02	7.7300E-03	4.1620E-01		1.0000E-01

bullet 5 -----

81	5.2972E+02	1.2112E+02	1.2309E+02	4.1540E-01	8.4000E+00	4.4800E-02
	6.0489E+00	4.8643E-03	7.7400E-03	4.1630E-01		2.0000E-01
113	1.2191E+03	1.0144E+02	1.0251E+02	8.2115E-01	8.4000E+00	4.4800E-02
	6.0853E+00	7.0095E-02	7.7400E-03	4.1630E-01		2.0000E-01

The Test Plan passed and has been burned to a CD and handed in to Ron Janetzke.

Sept 12, 2002

SCR 398. Email from Osvaldo.

I modified SCR\_398. I just reorganized it and added a description of why we did what we did.

By the way, I noted that Brandi refers to the boiling point of water, 97 C, as a hard-wired parameter. It should not be hard wired, it should be read from tpa.inp: BoilingPointOfWater[C].

George and Brandi, is it hard-wired?

If it is, no big deal, it is just necessary to do a little change. This will not affect the test already done.

Thanks ... Osvaldo

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SCR 398. Email from G. Adams.

Osvaldo,

Thanks for the updates on the SCR. The Boiling Point of Water was already defined in the TPA.INP file and was already retrieved by nfenv into variable tboil. I pass this parameter to the new module that I created (assignConcentrations) within nfenv.

George

Sept 16, 2002

SCR 398. Email from Ron Janetzke.

All,

I think the parameter names could be more descriptive in the tpa.inp file for the new chemistry, but the code is being integrated anyway to keep things moving. Maybe Brandi can address this under a new SCR400.

thanks for your help,

ron j

Sept 18, 2002

SCR 400. Email from Ron Jantezke.

Brandi,

Please continue to make the CD for 398. Attached is SCR400. See me about the new names discussed in the SCR.

thanks,

ron j

Sept 20, 2002

I used the template SCR emailed to me from Ron to create SCR400.

Changed the following names in *tpa.inp* and *nfenv.f* per SCR400 as follows:

<u>old:</u>	<u>new:</u>
Cl_Epoch_1	Indrift_CL_Epoch_1

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FI_Epoch_1	Indrift_FI_Epoch_1
pH_Epoch_1	Indrift_pH_Epoch_1
CO3_Epoch_1	Indrift_CO3_Epoch_1
DeltaECrit_Epoch_1	Wastepackage_DeltaECrit_Epoch_1
CI_Epoch_2	Indrift_CI_Epoch_2
FI_Epoch_2	Indrift_FI_Epoch_2
pH_Epoch_2	Indrift_pH_Epoch_2
CO3_Epoch_2	Indrift_CO3_Epoch_2
DeltaECrit_Epoch_2	Wastepackage_DeltaECrit_Epoch_2

After the changes were implemented, I recompiled the source code and ran the Test Plan for SCR 398 (since the only difference between this SCR and SCR 398 is the parameter names). The results were the same and the Test Passed.

SCR 327. Email from Pat LaPlante.

We can talk on Monday. We are still working at isolating a problem with the summing of doses. This will probably be easy to trace and the documentation for the testing will probably be completed next week.

Have a nice weekend.

Pat

-----Original Message-----

From: Brandi L. Winfrey [mailto:[bwinfrey@swri.edu](mailto:bwinfrey@swri.edu)]  
Sent: Friday, September 20, 2002 5:38 PM  
To: [plaplante@swri.edu](mailto:plaplante@swri.edu)  
Subject: SCR 327

Pat,

Ron said that I should check with you on SCR 327. Are the two tests you were working on ready for inclusion in the Test Plan? Is there anything that you need me

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to do?

Brandi

Sept 30, 2002

email from R. Janetzke:

The new charge number for TPA code development, effective today is  
20.06002.01.113.

Nov 11, 2002

email from R. Janetzke:

Effective immediately we can no longer use the default **f77** compiler on **SPOCK** for TPA work. Please use the following compiler for all development and testing, and use it as soon as possible to check all of your work to date on **5.0beta**.

/solapps/SUNWspro.4.2/bin/f77 myprog.f

A sample *make* file is in

/home/janetzke/Makefile

Nov 11, 2002

email from P. LaPlante:

I have completed the hand calculation/verification test of the revised groundwater protection calculations covered by SCR 327 that can be added to your tests. My test plan w/ results is a word perfect file on S:\PLaplane\SCR327\ with the same content as your entries (maybe it could be copied into your test plan). I had some problems with the auto formatting so my file below is "minimally formatted". Please take a look and if there are parts that are unclear let me know and I will fix them. Same goes for

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Ron if you are interested and have the time etc. The referenced/supporting files have been place on S:\PLaplante\SCR327\TPA50BETA directory. I will ask C. Weaver to burn it onto a disk for you for archiving. Sorry it took so long...many interruptions.

All hand calculations were successful so no problems were identified other than the need to update the groundater pumping rate (already discussed with Ron).

Thanks  
Pat

Dec 3, 2002

Began testing the Test Plan for SCR 415, given to me by G. Adams.

Dec 10, 2002

Working on SCR 416.

Email to C. Scherer:

I just re-ran tpa50charlie and came up with the following errors.  
Do you have any suggestions as to why?

```
tpa.e > PA-SCR-416_SL1-A.out  
STOP: RDPAR
```

output file PA-SCR-416\_SL-A.out (last two lines):

```
***>>> Error in Sampler:checklhsout <<<***  
Hit end of File reading lhs.out file.
```

The only changes I made to tpa.inp are:

```
OutputMode = 1  
NumberOfRealizations = 10
```

and I set two volcanism flags to 1

C. Scherer response email:



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I don't know why you're getting those messages. The only thing I can suggest off the top of my head is to make sure that you recompile all the executables with the same compiler. I've had some weird things happen when tpa was compiled with the solapps 4.2 compiler and the standalones in codes were compiled with the default compiler.

Her suggestion worked. When I removed all of the \*.o files and recompiled, everything worked fine. Apparently, if you do not remove the \*.o files, when it recompiles it does not create them if they are already there and have no changes to them, even if they were compiled with another version of compiler.

Dec 17, 2002

Working on SCR377.

Dec 23, 2002

The numbers in neffisz.vel for 10,000 years don't look linear. R. Janetzke wanted to know if they have to be exactly linear or if it is ok for them to just be close.

Jan 03, 2003

email from R. Janetzke:

Here is the SCR and files from Bob Rogers for SCR386. Please prepare a test plan and results. We can discuss this after you have read through it once.

Jan 07, 2003

email from me to R. Janetzke:

I have access to Techplot (on spock), however I have never used it. Is it command line based or is there a GUI? Is there a tutorial? or could you give me some basic commands just to get it started? This is for SCR386.

Response from R. Janetzke:

It used to be a two step process. Run **preplot** on your ASCII text numbers to create a TECPLOT binary \*.plt file. Then use **tecplot** GUI to display it. The GUI has changed quite a bit since I used it years ago, so I may not be much help. If you just want a binary file to play with, try

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*~janetzke/ss\_bcr/gwttuz.plt*. It does not seem to be backward compatible to all previous files generated under V5 or V6. If it takes too much time jump over to excel.

I do not know if there is a new manual floating around.

Email from me to R. Fedors:

Randy,

George Adams said that you might be familiar with Tecplot. I have an ASCII file that I need to read in and plot but I am spinning my wheels right now. I am not familiar with Tecplot at all. If it wouldn't take too much time, could you give me some advice on how to read in and plot my file?

The file format is:

<X1> <Y1> <X2> <Y2> <numWP>

where numWP is the number of waste packages. It should be simple, there are two points in each line, each line is divided into a specified number of waste packages, and there are approx 40 lines.

thank you for any help,  
Brandi

response from R. Fedors:

Brandi,

Looks like drift coordinates and number of WPs in each drift.

You'll likely have to reformat the data. If you want to plot the drifts as lines, you'll just have to add keyword lines between each drift record. Though, maybe you want to plot something other than what I am envisioning; e.g., separate lines for each WP.

Check with me early tomorrow and we can talk about what you want the plot to show.

--Randy  
x6818

Jan 17, 2003

email to R. Fedors:

Randy,

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I've finally gotten back to TPA and using Tecplot to plot the new vs old drifts.dat. I used your example file to create the proper Tecplot input file but I am having a few difficulties. All of my files are located in:

spock:/home/bwinfrey/rjanetzke/SCR386/test/sltest/sl-1/code42u/junk

Basically, the difficulties are this:

1) The file tec42\_u.dat shows the drifts exactly as I want them to be shown but I can't figure out how to overlay them on the repository outline repository.dat.

2) The file tec42\_v.dat has too many lines to have a separate zone for each line. It causes errors, so I did not list them as separate zones. You can tell that the drifts are separated into wastepackages only if you select scatter plot because all of the points are treated as one zone and therefore connected by one line. The symbols for each point on a scatter plot are so large that the plot looks completely shaded in.

So, if you have time and could tell me how to make the symbols smaller and how to overlay two .dat files, it would be a great help.

I will be out of my office until after 2:00.

thank you,  
Brandi

Jan 20, 2003

response from R. Fedors:

Brandi,

I was out Friday.

See my file /iscr0/rfedors/tec42.dat. I created this file by combining tec42\_v.dat and repository.dat.

First, switch to "2D", turn off the "Boundary."

Then, from the main menu bar, chose Field->Mesh Attributes. For the 9th zone (Zone Name=WP), deactivate the "Mesh Show."

Switch to Scatter Attributes and make sure that Zones 1-8 have "scatter show" deactivated and the 9th zone (called WP) has scatter attributes activated. Change the symbol and symbol size for the WP zone (I just set symbol size to 0.001%).

If this doesn't help, or I didn't do what you wanted, check with me again.

--Randy

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working on SCR 400.

**Jan 21, 2003**

email from me to R. Fedors:  
Randy,

I can't find the file tec42.dat. Is t.dat the file you mean?  
If so, when I am looking at the Field->Mesh Attributes window,  
there are only 8 zones. The screen plot also looks like the  
only thing there is the repository outline, not the x,y points.

Brandi

**Jan 22, 2003**

email to R. Janetzke:  
Ron,

The overlayed plots are located here:

[bwinfrey@spock]/home/bwinfrey/rjanetzke/SCR386/test/sltest/sl-1/tec\_drifts.  
lay

the data file is tec\_drifts.dat

The green points are from the tpa4.2u drifts.dat file and the  
red points are from the tpa4.2v drifts.dat file. Let me know  
if this is ok.

Brandi

response from R. Janetzke:  
Brandi,

On the scale of a waste package it seems the canister is placed at an angle to  
the drift. Can you determine what the error is (in meters) at the can end  
points?

thanks,

ron j

email from me to R. Janetzke:

After looking at a number of waste packages, it seems that  
the endpoints are not at consistant distances from the  
drift. Some of the endpoints are right on the drift while

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others are varrying distances from it. Would these variations in the location/angle from the drift be the cause for the differences in temperatures? I noticed that comparing 4.2u nfenv.rlt and 4.2v nfenv.rlt (with the oneTemperatureCellperWP flag set to 0), there are still differences in the temperatures.

Maybe the angle of the waste package is an artifact of the method of interpolation of waste packages between the two endpoints of the drift. The angles are not all the same, but when averaged together, form a (somewhat) straight line.

Are the x,y coordinates in kilometers?

Response from R. Janetzke:  
x,y should be in meters.

Email from me to B. Rogers:  
Robert,

I am writing the Test Plan for SCR 386 which has you listed as an implementor. I am trying to answer a question from Ron Janetzke about the angle of the canisters with respect to the drift. Attached is a Tecplot8 layout file which, if you zoom in very close, shows what he is talking about. This file does not open correctly in Tecplot7. I'm using Tecplot8 on spock.

The red points are for each waste package. The green points and lines are for each drift and the black lines are the repository outline. The plot only has start/stop endpoints for each waste package. There are no lines connecting them. If you zoom close it seems that each canister is not on the same angle as the drift.

I looked in reader.f at the subroutine outputWPendpoints and it looks like the canisters should be on the same angle as the drifts. The x values all have deltaX of ~5.8577 and the y values all have deltaY of ~-1.839. I'm not sure why they look like they have different angles from the drift data. Can you explain this to me? After looking at the Tecplot8 layout, do you think that the apparent difference could be caused by Tecplot? If not, I'm not sure what it is.

thank you,  
Brandi

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Jan 24, 2003

Email to R. Janetzke:

Ron,

I Can't figure out why they look like they're at angles.  
In the file reader.f in the subroutine outputWPendpoints  
is the formula for calculating the endpoints for each  
waste package:

```
-----  
angle = -.304d0 per repdes.dat (same angle used for drifts)  
WPSpacingAlongEmplacementDrift[m] = 6.1392
```

```
deltaX = WPSpacingAlongEmplacementDrift * cos(angle)  
        = 6.1392 * cos(-.304)  
        = 5.8577
```

```
deltaY = WPSpacingAlongEmplacementDrift * sin(angle)  
        = 6.1392 * sin(-.304)  
        = -1.839
```

```
newX1 = oldX1 - deltaX  
newY1 = oldY1 - deltaY  
newX2 = oldX2 - deltaX  
newY2 = oldY2 - deltaY  
-----
```

After checking numerous endpoints I noticed that some of the  
deltaX values were 5.858 and some were 5.857 while some  
of the deltaY values were -1.83 and some were -1.84. Could  
this be the cause of the apparent angle differences? If  
not, I'm not sure what it is. I emailed R. L. Rogers to see  
if he could explain it. I'm waiting on his reply.

Brandi

response from R. Janetzke:

Write a small test program for the trig section that uses the same input and  
algorithm but uses the double precision trig functions instead of the single  
precision.

response from B. Rogers:

I don't have access to Tecplot since I'm outside of the CNWRA firewall.  
If you have time, I can stop by your office and look at the file.

Jan 27, 2003

B. Winfrey

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email from me to R. Janetzke:

Ron,

I changed to double precision sin/cos in a seperate script. You can find the fortran code, data file, and a tecplot layout file showing the waste packages plotted against the drift in the following directory:

```
/net/spock/home/bwinfrey/rjanetzke/SCR386/test/sltest/sl-1/junk
```

If my code is correct, double precision doesn't seem to change things. I'm going to make the changes in the reader.f file and run tpa.e to see if this changes things.

Brandi

Jan 28, 2003

email from R. Janetzke:

Could you run this program and prepare the two data sets for plotting, one for "singlep()" and one for "doublep()"?

Email to R. Janetzke:

Ron,

I ran your wpangle.f code and obtained the attached data plotted with tecplot. The single precision line is acting like I expected from a problem with the angle. The double precision line still looks like each WP has random looking angles, however, it does start and stop at the correct locations.

Brandi

Jan 29, 2003

response from R. Janetzke:

The red lines appear way off the mark. Please explain.

email to R. Janetzke:

Ron,

I plotted the nfenv.rlt files for comparison and they are pretty different. Each file is the same length. I thought that maybe the one broken down to waste packages per drift

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would longer, but no. I plotted temprep vs the first column  
(I think it is drift) and tempwp vs the first column for  
each run. The attached Excel file shows the differences.  
Is this how you want to see them plotted? or what would you  
suggest for the x-axis?

Brandi

Jan 30, 2003

email from me to B. Rogers:

Bob,

After running the same algorithm in single precision and  
comparing it to the double precision version, we have  
decided that the problem lies not with the precision of  
the angles, rather with the precision of the endpoints.  
Attached are two jpg pictures of the results. the single  
precision (endpoints and angle) causes the waste packages  
to be straight, however not on the drift. The cumulative  
error from using single precision causes the line to angle  
away from the drift. Using double precision corrects this  
but leaves the "wiggle" in the waste packages. Rather  
than change the number of digits in the endpoints in the  
drifts.dat file (since it is also used by nfenv.f), Ron  
said that it would be sufficient to state in the Test  
Plan that it is the number of digits after the decimal  
place (in the endpoints) that is causing the wiggle, we  
are aware of it, and it is not a problem.

Brandi

Jan 31, 2003



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response from R. Janetzke:

Try setting the number of time steps to 2, and put a write statement in *nfenv.f* for **tbump** right after the call to *cond3dxyzt*. Then plot some or all of the **tbumps**.

Email from me to S. Mohanty:  
Sitakanta,

I am working on the Test plan for SCR386 and I was hoping you could explain something to me. I graphed temprep and tempwp (from *nfenv.rlt*) in Excel to see what the differences would look like before and after the drifts were separated into individual waste packages. Can you explain why the graphs look as they do and if I should plot them differently. I am not sure what to use for the x-axis. Currently I am using column one from *nfenv.rlt*. I would like to plot the temperature changes for one drift with the x-axis representing the waste packages, but it doesn't look like *nfenv.rlt* contains that info. If it did, wouldn't the *nfenv.rlt* file with drifts broken into waste packages be much larger than the *nfenv.rlt* with the drifts not broken up?

Attached is the Excel file with the charts I am talking about.

Brandi

Feb 4, 2003

email from me to R. Janetzke:

Attached is the Excel file with all of the **tbumps** plotted. **tbump8** looks a little different from the others, but otherwise, they all look consistent.

Feb 7, 2003

email from me to R. Janetzke:

Attached are the 2D and 3D **tbump** plots. Let me know if you think this is good and should be added to the Test Plan. The files are also located at [bwinfrey@spock]/net/spock/home/bwinfrey/rjanetzke/SCR386/test/sltest/sl-1/50m\_drifftest

Feb 10, 2003

Email from B. Rogers:  
Brandi,

I looked at the *fillsubareas()* subroutine, and that is where the

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difference is being generated for the number of WP's per subarea between a run with the 'OneTemperatureCellPerWP(yes=1,no=0)' flag set and with it not set.

The inaccuracy is in the computation of the variable

$\text{driftfra} = \text{alengthinsa} / \text{driftlength}$ .

For a regular run with the flag not set, the driftlength includes the whole drift and the spacing between WP's. With the flag set, the driftlength is approximately the length of a WP. The variable alengthinsa also contains inaccuracies based on the computations that cut off the drift at the boundaries of the repository and then again at the boundaries of the subarea.

After all this computation, fillsubareas() then rounds the number off using a call to idnint(). So per drift computation in a subarea, the number of WP's for that drift in that subarea could be off by one.

To add to this, there are many drifts per subarea. So as Ron said, the slight inaccuracy per drift builds into the noticable difference that you see in the number of WP's in each subarea.

Hope this helps. If not let me know.

Bob

email from me to R. Janetzke:

Ron,

Attached is the Tecplot layout for the two runs I just completed (with and without OneTemperatureCellPerWP flag set). You can see that the drifts and waste packages clearly fit within the repdes (green) repository outline and that the repository outlines for repdes and tpa.inp do not match for subareas 9 and 10.

Brandi

response from R. Janetzke:

I think I will need the location of the tec\_drifts.dat file also.

Email from me to R. Janetzke:

Ron,

Bob sent me an explanation as to why the number of waste packages do not match. Does this need to be explained in the Test Plan? Does this need to be corrected (new SCR?) or will an explanation as to why the differences exist suffice?

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Brandi

response from R. Janetzke:

Yes, we need to explain the planned test and the expected results and why the results should be different.

Email from me to R. Janetzke:

Ron,

all of the tests have been run (I'm not going to delete any more files). They are located in the following directory:

```
[bwinfrey@spock]/net/spock/home/bwinfrey/rjanetzke/SCR386/test/sltest/sl-1
```

You should also see the file tec\_temps.lay. I've superimposed both runs (with the OneTemperatureCellPerWP flag set and unset) in a 3D plot. The peak temperatures do not match exactly, but they look well behaved. This can also be seen on the 2D Excel plots tbumps.xls.

Brandi

(Note: the reason the temperature contributions do not match exactly is explained in the Test Plan. Here, a short description: the center of the drift that passes through the centroid of the subarea is used when OneTemperatureCellPerWP flag is NOT set. When it is set, the center of the waste package located closest to the centroid of the subarea is used. Naturally, these are not the exact same locations.)

Feb 11, 2003

email from me to R. Janetzke:

Ron,

Attached are the Test Plan and SCR for SCR386. Please look over them and let me know what needs to be done to complete them. I believe that they are close to being complete. I am not sure that my description of the tests in the SCR is completely accurate. Also, I still have nfenv\*.rlt files listed in the Test Plan as output files, however I do not use them in any tests (since they each only have 2 points in them, they are not useful for testing - Is the tbumps test sufficient to explain temperature differences?)

Please let me know what you think. If this is good for you, I can begin on my next SCR.

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Brandi

Email from me to R. Janetzke:

Ron,

All of your suggestions have been incorporated into the SCR and Test Plan for SCR 386. Please find them attached and let me know if you have any further suggestions. If not, then I will burn this and the test results to a CD.

Brandi

email from me to R. Janetzke:

Ron,

I made one more change to the Test Plan for SCR 386, including an explanation for the differences in subarea/repository outlines in the Tecplot layout file `tec_drifts.lay` and how they relate to the drifts.

Brandi

response from R. Janetzke:

It looks good, but do not put the SCR on the CD.

Email from R. Janetzke:

Here are the values to compress into *tpa.inp* **usersuppliedpwisecdf** format. The same program should be able to average (compress) either file.

Feb 12, 2003

email from me to R. Janetzke:

Ron,

I have a basic fortran script that will read in the data from either file and print it in *tpa.inp* **usersuppliedpwisecdf** format, but the data are not compressed yet. I noticed that the number of points per parameter changes from 50 to 51 about halfway through both files. Will this always be the case? Also, for the averaging part, could you explain exactly what is supposed to be averaged? The parameter

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names seemed to all be different. Do I average the 50/51 points for all parameters?

thanks,

Brandi

email from me to R. Janetzke:

Ron,

Attached is the fortran code that compresses the values into tpa.inp usersuppliedpwiseCDF format.

This code works for both files you sent me. Just rename them to points.dat or change the input

filename in the code. Please let me know what to do next. My working directory for this is:

/net/spock/home/bwinfrey/rjanetzke/reversible\_colloids

Brandi

Feb 13, 2003

February 13, 2003  
SCR 424

Modified tpa.inp to include the following usersuppliedpwiseCDF parameters:

MatrixKD\_TSw\_\*, MatrixKD\_CHnv\*, MatrixKD\_CHnz\*, MatrixKD\_PPw\_\*, MatrixKD\_UCF\_\*,  
MatrixKD\_BFw\_\*, MatrixKD\_UFZ\_\*, and AlluviumMatrixRD\_SAV\_\*

where \* is Se, Ni, Cs, Pb, Ra, Th, Pu, U, Np, and Am

Wrote a fortran script to read in a file and compress (average) into tpa.inp usersuppliedpwiseCDF format.

The script follows:

```
-----  
      program inpdatt  
c  
c      This program will read in a file and compress (average) into tpa.inp
```

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```

c      usersuppliedpwisecdf format
c
c      Note:  code assumes there is a return carriage at the end of file
c
c      Input looks like:
c      Rd,eff, cumul prob
c
c      AlluviumMatrixRD_SAV_Am
c      2.03E+04,0.0013
c      2.15E+04,0.0019
c
c      OR ...
c
c      Kd,eff (m3/kg),cumul prob
c
c      MatrixKD_TSw_Am
c      1.6933,0.0013
c      1.6934,0.0019
c
c      Output looks like:
c      **
c      usersuppliedpwisecdf
c      FractureRDLog10_STFF_Ja
c      6
c      0.025308,    0.0
c      0.04139,    0.039
c      0.77815,    0.08125
c      2.0,        0.2605
c      2.4472,    0.7605
c      2.9031,    1.0
c      **
c
c      new create by Brandi L. Winfrey
c      February 12, 2003
c
c      Usage:  a.out > filename
c
c      integer nmax, u, n
c      double precision temp_x, temp_y
c      character*30 param_name
c      character*30 junk
c      parameter (nmax=1000, u=5)
c      double precision x(nmax), y(nmax)
c
c      Open the data file
c      open (u, FILE='points.dat', STATUS='OLD')
c
c      Read the first two lines, discard them
c      read(u,100) junk
c      read(u,100) junk
c      write (*,'(A2)') '***'
10 continue

```

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```

c          Read the parameter name
          read(u,100,END=9999) param_name
100 format (a30)

          n=2
          read(u,200,END=9999) x(1), y(1)
20         read(u,200,END=9999) temp_x, temp_y
          if ( temp_x .ne. 0. ) then
            if ( temp_x .eq. x(n-1) ) then
              x(n-1) = temp_x
              y(n-1) = temp_y
c          y(n-1) = ( ( temp_y + y(n-1) ) / 2 )
              n = n-1
            else
              x(n) = temp_x
              y(n) = temp_y
            endif
            n = n+1
            goto 20
          else if ( temp_x .eq. 0. ) then
            n = n-1
            y(n) = 1.00
          endif
200        format (2(F10.6))

c          Write the data to a file
          write (*,'(A20)') 'usersuppliedpwisecdf'
          write (*,'(A30)') param_name
          write (*,'(I2)') n
          do i= 1, n
            write (*,*) x(i), y(i)
          enddo
          write (*,'(A2)') '***'

          goto 10

c          Close the file
9999 stop
end

```

-----

I ran into a few problems when I ran the new tpa.inp file with tpa50betaP:

I changed the value of maxudist in the file samplerx.i from 20 to 52 and then to 100 to get rid of the following error:

```

=====
          exec: Welcome to TPA Version 5.0betaP
          Job started: Thu Feb 13 10:41:17 2003
=====
***>>> Error in addusersuppliedpwisecdf <<<***

```

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```
kntudist .gt. maxudist
kntudist = 21
maxudist = 20
name = AlluviumMatrixRD_SAV_Cs
```

I then ran the code again and got the following errors:  
The file PA-SCR-424\_test.out (screen dump) had this error:

```
**To modify global parameters or the path, stop code execution using control-
C**
***>>> Error in Sampler:checklhsout <<<***
Hit end of File reading lhs.out file.
```

The above error is generated in sampler.f. It is caused because the lhs.out file is empty. I looked in the lhse.out file:

The contents of *lhse.out*:

```
SNLLHS started: Thu Feb 13 12:20:14 2003
xval( 1)= 0.203E+05 cdf( 1)= 0.001300
FOR THE USER SUPPLIED PIECE-WISE CDF THE FIRST CUMULATIVE PROBABILITY MUST
EQUAL 0
```

the error comes because usrfreq(1) is not equal to 0 in subroutine CHKUSRPWISE in file code *snllhs.f*. To correct this, I changed the first y value to zero for all of the new usersuppliedpwiscdf parameters. This corrected the above problem. The next error was:

exec: calling uzft

```
***>>> Error in ispquery <<<***
can not find name of parameter
dump of first 15 PDFs defined
ipdf, description
1 GenerateRestartFiles(yes=1,no=0)
2 ImportanceAnalysisFlag(yes=1,no=0)
3 SubsystemNaturalStudy
4 BarrierBiosphereStudy
5 ComponentPrecipitationStudy
6 BarrierUpperUnsaturatedZoneStudy
7 ComponentTivaCanyonStudy
8 BarrierLowerUnsaturatedZoneStudy
9 ComponentTSwStudy
10 ComponentCHnvStudy
11 ComponentCHnzStudy
12 ComponentPPwStudy
13 ComponentUCFStudy
```



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14 ComponentBFwStudy  
15 BarrierSaturatedZoneStudy

```
***>>> Error in ispquery <<<***  
can not find name of parameter  
in above list of all PDF names  
name =MatrixKD_TSw_Ra[m3/kg]
```

In the file *sampler.f*, the following line makes a comparison between the parameter and  
some description ( from "consequence modules") where `namin = MatrixKD_TSw_Ra[m3/kg]`      from  
*tpa.inp*. The names do not match.?

The above error was corrected by adding "[m3/kg]" to the end of all new parameters (in *tpa.inp*) with  
`MatrixKD_*` as the beginning part of their name. *Tpa.e* successfully completed execution after this change  
was made.

email from me to R. Janetzke:

Ron,

I've commented out all of the appropriate parameters and now am getting  
errors. The error  
below was generated from the following *tpa.inp* lines and the file *samplerx.i*  
which has  
`maxudist = 20`. I changed this to `maxudist = 52`. Then got the error that  
another parameter  
had `kntudist=53 .gt. 52`, so I changed `maxudist=100`.

```
**  
usersuppliedpwisecdf  
AlluviumMatrixRD_SAV_Cs  
6  
21200.000000000 4.00000000000000D-02  
21300.000000000 0.220000000000000  
21400.000000000 0.420000000000000  
21500.000000000 0.620000000000000  
21600.000000000 0.820000000000000  
21700.000000000 1.00000000000000  
**
```

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```
=====
=====
exec: Welcome to TPA Version 5.0betaP
Job started: Thu Feb 13 10:41:17 2003
=====
```

```
=====
***>>> Error in addusersuppliedpwiseCDF <<<***
kntudist .gt. maxudist
kntudist = 21
maxudist = 20
name = AlluviumMatrixRD_SAV_Cs
```

After changing maxudist=100, I got the following error:

```
tpa.e > PA-SCR-424_test.out
STOP: CHKUSRPWISE
```

The file PA-SCR-424\_test.out (screen dump) had this error:

```
**To modify global parameters or the path, stop code execution using
control-C**
```

```
***>>> Error in Sampler:checklhsout <<<***
Hit end of File reading lhs.out file.
```

The above error is generated in sampler.f. It is caused because the lhs.out file is empty. I can't find where this file is generated and why it is empty. Is there a flag in tpa.inp that I should have set? I already have the OutputMode flag set to 1.

I'll be back from lunch ~1:30.

Brandi

response from R. Janetzke:

We need to look at the file *lhse.out*.

Email from me to R. Janetzke:

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The contents of *lhse.out*:

```
SNLLHS started: Thu Feb 13 12:20:14 2003
xval( 1)= 0.203E+05 cdf( 1)= 0.001300
FOR THE USER SUPPLIED PIECE-WISE CDF THE FIRST CUMULATIVE PROBABILITY MUST EQUAL
0
```

the error comes because `usrfreq(1)` is not equal to 0 in subroutine `CHKUSRPWISE` in file *code/snllhs.f*

Does this mean that the first y value in each `usersuppliedpwiscdf` parameter must be zero?

Email from me to R. Janetzke:

I replaced all of the first y values for the `usersuppliedpwiscdf` parameters with a zero and got

the code to run further before it had errors. The next error is:

```
exec: calling uzft

***>>> Error in ispquery <<<***
can not find name of parameter
dump of first 15 PDFs defined
ipdf, description
1 GenerateRestartFiles(yes=1,no=0)
2 ImportanceAnalysisFlag(yes=1,no=0)
3 SubsystemNaturalStudy
4 BarrierBiosphereStudy
5 ComponentPrecipitationStudy
6 BarrierUpperUnsaturatedZoneStudy
7 ComponentTivaCanyonStudy
8 BarrierLowerUnsaturatedZoneStudy
9 ComponentTSwStudy
10 ComponentCHnvStudy
11 ComponentCHnzStudy
12 ComponentPPwStudy
13 ComponentUCFStudy
14 ComponentBFwStudy
15 BarrierSaturatedZoneStudy

***>>> Error in ispquery <<<***
can not find name of parameter
in above list of all PDF names
name =MatrixKD_TSw_Ra[m3/kg]
```

In the file *sampler.f*, the following line makes a comparison between the parameter and

some description ( from "consequence modules") where `namin = MatrixKD_TSw_Ra[m3/kg]`

from *tpa.inp*. The names do not match. What are the consequence modules?

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```
if( namin .eq. description(i) ) then
```

Brandi

Email from me to R. Janetzke:

Ron, I corrected the last error by adding [m3/kg] to the end of some of the parameter names. The last run completed successfully. It is located in the following directory: /net/spock/home/bwinfrey/rjanetzke/reversible\_colloids/code50P/compiled\_50betaP The screen output can be found in file PA-SCR-424\_test.out What do I do next? Brandi

response from R. Janetzke:

Here are some parameters that also need adjustment for this case. These should be made constants with the values shown in the file.

Feb 14, 2003

Email from me to R. Janetzke:

Ron, All of the constants you sent yesterday have been added to tpa.inp and the run successfully executed. Attached is the new tpa.inp file. Everything else can be found here: /net/spock/home/bwinfrey/rjanetzke/reversible\_colloids/code50P/compiled\_50betaP Brandi

response from R. Janetzke:

Thanks for the files.

Here is the next SCR to check. I hope you can work with Mike Smith on this, but he is not here today, so maybe I can get you started.

Take a look at the exec.f, and look for entries associated with SCR389, and see if you can understand what the changes are and let me know how we should test them.

Email from R. Janetzke:

Did you make any changes to the TPA code to make this work?

Response from me to R. Janetzke:

I changed the value of *maxudist* in the file *samplerx.i* from 20 to 52 because of the following error, then got the error for *kntdist*=53 .gt. 52, so I changed it to 100 to get rid of the error. This number may be lower, but 100 worked for me.

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=====

exec: Welcome to TPA Version 5.0betaP

Job started: Thu Feb 13 10:41:17 2003

=====

\*\*\*>>> Error in addusersuppliedpwisecdf <<<\*\*\*

kntudist .gt. maxudist

kntudist = 21

maxudist = 20

name = AlluviumMatrixRD\_SAV\_Cs

email from R. Janetzke:

Complete the first two sections of this SCR, describing the change to samplerx.i, and the utility program that you wrote for the conversions.

Also make a CD of the original files from Pickett, your converted files, the tpa.inp, and the conversion utility.

Email from M. Smith:

Brandi,

This and following email are what I could find related to SCR-389. I'll stop by in a few minutes to chat.

--Mike

-----Original Message-----

From: Michael A. Smith [mailto:masmith@cnwra.swri.edu]

Sent: Monday, August 05, 2002 5:46 PM

To: 'Bob Rogers'

Subject: RE: DCAGW/DCAGS array

From the name, that sounds like what we need. We'll have to see what's inside.

-----Original Message-----

From: Bob Rogers [mailto:robert.rogers@swri.org]

Printed: March 23, 2005

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Sent: Monday, August 05, 2002 5:21 PM  
To: Michael A. Smith  
Subject: DCAGW/DCAGS array

Mike,

Here are the array names -- I'm not sure that they have the data you were looking for:

```
in dcags.f
remperyrpernuclgs[mxntime,nnucldr] = output, double precision, array of
    annual EDE (effective dose equivalent) per nuclide

in dcagw.f
remperyrpernuclgw[mxntime,nnucldr] = output, double precision, array of
    annual EDE (effective dose equivalent) per nuclide
```

Bob

Email from M. Smith:  
Another SCR-389 email.

-----Original Message-----

From: Michael A. Smith [mailto:masmith@cnwra.swri.edu]  
Sent: Thursday, August 29, 2002 12:32 PM  
To: Patrick Laplante  
Subject: FW: New rgw\* files

Pat,

Here are examples of new dose output files from Bob. I think you'll like the formatting that is directly importable to Excel. Attached are original rgwna.tpa and rgwsa.tpa files along with 7 new files. The change to 6 pathway-specific rgwna files (instead of one super file) came a few days ago after discussion that Bob and I had with Ron. This change allowed us to use the existing file creators in exec.f that are used to create rgwna and rgwsa.  
--Mike

p.s. I found that the extra rows (2 additional time steps) at the bottom of some output files are required by Kaleidagraph. Kaleidagraph is also the reason that values of zero are changed to 1e-14. The change to 1e-14 is the last step before the files are written, so you'll notice that the sum of the 6 pathways (6e-14) is greater than the total dose (1e-14).

Printed: March 23, 2005

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-----Original Message-----

From: Bob Rogers [mailto:robert.rogers@swri.org]  
Sent: Thursday, August 29, 2002 11:47 AM  
To: Michael A. Smith  
Subject: New rgw\* files

Mike,

Here's the 6 new rgwnap\*.tpa files and the new rgwsap.tpa file. I have also included the rgwna.tpa and rgwsa.tpa files.

I ran the numbers through Excel and found a error, which I have finally fixed. So all of the new files correspond to the data in the rgwna.tpa and rgwsa.tpa files.

I adjusted the column headings in rgwsap.tpa so that they end up above the numbers. Unfortunately, the column headings in the rgwna\*.tpa files can't be fixed so easily. Currently the column headings for the rgwna\*.tpa files must fit into a 320-character array. Since the column width is 11 characters and there are 44 columns, the headings just will not fit into the array with the correct spacing.

But if you set up Excel to import the rgwna\*.tpa files using space delimiters instead of fixed width, it works fine (except that the first column in the spreadsheet is blank).

Let me know if need anything else done.  
Bob

**email from R. Janetzke:**

Do you have an electronic file of the SCR? Also, are the files on the CD Unix format? Also, you started to indicate which parameters were involved in this SCR, but omitted their names (see description of changes).

**Email from R. Janetzke:**

Here are the correct SCRs.

**Feb 17, 2003**

**email from me to R. Janetzke:**

Ron,

Attached is the SCR. I've added the parameter names. The files on the CD are in Unix format. Although, I copied the original files unmodified, so they may have DOS return carriages in them. I just noticed that the file with the

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new constants was not unix when I opened it.

Brandi

Email from B. Rogers:

Brandi,

Here is the spreadsheet that I used to compare the data for the different pathways. It probably isn't that useful, and it took me a few minutes to understand what I had done (it's rather cryptic).

Basically I pulled the data from the individual pathway files and compared them to the data for files we had generated before (were they rgwna and rgwsa?). It's been a while since I did this, but I could walk you through it.

Let me know if you want some help with this.

Bob  
4971

Feb 18, 2003

Email from me to B. Rogers:

Here are some questions I have on your spreadsheet. I took your format and inserted the files from a tpa run with tpabetaR.

-----  
Why are we only interested in calculations for lines 184 thru 201 in rgwna for InSu-Mlk and Sum-InSu?

Why subtract 2.00E-15 from the sum of dose per element in rgwna?

which values should be equal? within what tolerance (+/-)? on the rgwna sheet cols V-AB

why do we need to know the difference of the sums of rgwna and rgwsa? Is there a specific tolerance?

-----  
---  
With my input files, columns V (Sum), Y (Sum-InSu), and AA (rgwsa) are all equal +/- .01. I don't see a correlation between col AB (Sum-rgwsa) and any



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other column. I also don't see a correlation between col W (IndSum)  
and any  
other column.

I understand the rgwsa calculations.

thanks,  
Brandi

response from B. Rogers:  
Brandi,

These are in the order of the questions below:

I only did calculations for lines 184 through 201 because the others  
were zero at the time.

In the Sum column, I subtract  $20 * 1.00E-15$ . The DCAGW module has to  
use a very small number ( $1.00E-15$ ) instead of zero, to avoid some  
divide-by-zero problems. So the values of  $1.00E-15$  in columns B through  
U are actually "zeros", which meant I had to do the subtraction in the  
Sum column. The number  $1.00E-15$  had to be subtracted on the individual  
pathways' sheets also, which became rather annoying, but otherwise the  
numbers couldn't be compared.

As far as what numbers should be equal:

- The value for each nuclide per time step on rgwna should equal the sum  
of the individual pathways for that nuclide and that time step.
- The value for each time step on rgwsa should equal the sum for the  
individual pathways on rgwsap for that time step. (rgwsa is the final  
total sum of all GW numbers for the time step, so everything should be  
comparable to rgwsa.)

I did not check the first item above, which would have meant a lot of  
summing and comparing ( $20 \text{ nuclides} * 6 \text{ pathways} * 202 \text{ time steps}$ ), so I  
just did a quick comparison.

My trail of logic for the quick comparison that I did was: I summed up  
the pathways on rgwsap (column D on rgwsa) and compared those to rgwsa  
column C on rgwsa). Then I summed up the nuclides per time step on rgwna  
(column V on rgwna) and compared those to rgwsa (column AB on rgwna).  
Then I summed up the pathways from the rgwna\* sheets (column V on the  
individual rgwna\* sheets and their sum in column W on rgwna) and  
compared their sum to the sum from rgwna (see columns W, X, and Y for  
the rambling comparison -- description below).

Comparing rgwsa (column C on rgwsa) and the sum from rgwsap (column D on  
rgwsa) shows a close match. Comparing the sum on nuclides from rgwna

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(column V on rgwna) and rgwsa (column AA on rgwna) showed a close match (column AB on rgwna).

The rambling comparison: In comparing the sums of the pathways ([IndSum: Individual Sum] column V on the rgwna\* sheets with their sum in column W on rgwna) with the sum on rgwna (column V on rgwna), the numbers were off. I noticed that if I removed the milk pathway from the sum in column W ([InSu-Mlk: Individual Sum - Milk] column X on rgwna) that the numbers matched the rgwna sum better (column Y on rgwna), in most cases. Since I was doing SCR-381 at about the same time (where the milk pathway was added to the calculation of DCF for ground water), I don't remember why this made sense at the time.

As written in the code, the DCF per nuclide should equal the sum of the DCF's for its six individual pathways, meaning column W on rgwna should be approximately equal to column V on rgwna. Let me know if they match any better with your data.

Mike Smith may know what the tolerance is for comparing all of these numbers.

I hope this makes some sense.  
Bob

response to B. Rogers from me:  
Bob,

Thanks, that helped a bunch. Turns out, I wrote one of the functions incorrectly in Excel (I used colU instead of colV=Sum for IndSum). Here is a sample of my numbers. They match a lot better than the ones from your spreadsheet. Also, not as many zeros (cols 52-201 contained non-zero data).

V Sum	W IndSum	X InSu-Mlk	Y Sum-InSu	AA rgwsa	AB Sum-rgwsa
1.71E-06	1.71E-06	4.92E-09	-1.70E-06	1.71E-06	-1.81E-09
1.83E-06	1.83E-06	5.32E-09	-1.82E-06	1.83E-06	-2.52E-09
1.95E-06	1.95E-06	5.72E-09	-1.94E-06	1.95E-06	-1.93E-11
2.08E-06	2.08E-06	6.13E-09	-2.07E-06	2.08E-06	-4.50E-09
2.21E-06	2.20E-06	6.55E-09	-2.20E-06	2.20E-06	5.03E-09
2.34E-06	2.34E-06	6.97E-09	-2.33E-06	2.34E-06	-4.44E-09

Brandi

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Feb 19, 2003

email from me to B. Rogers:

Bob,

Ron said I should do a system level test for the Test Plan  
with two flags set:

```
DirectReleaseOnlyFlag(yes=1,no=0)
VolcanismDisruptiveScenarioFlag(yes=1,no=0)
```

when I set them both I get the following error:

```
exec: calling dcags
***>>> Error in Gentpags <<<***
trouble running envin.e,  istatus= 256
```

This error is generated in dcags.f line 2144:

```
      if( istatus .ne. 0 ) then
cc rlr 12/13/02 SCR417 Modified error message to output Gentpags
cc      print *, ' ***>>> Error in Gentpa <<<*** '
      print *, ' ***>>> Error in Gentpags <<<*** '
      print *, ' trouble running envin.e,  istatus=',istatus
      stop
    endif
```

Ron said that you may have been working with this area of the code  
recently and might recognize the error. Do you have any suggestions?

Brandi

email from B. Rogers to R. Janetzke:

Ron,

The system level test that Brandi is attempting to run below will not  
run due to the logic error that is in dcags -- the one on copying the  
needed executables and data files into the working directory. The fix  
to this is the one George has in SCR-425, which I am currently testing.

Do you want Brandi to skip her test, since I will be running that test  
for SCR-425?

Bob

email from G. Adams:

Please find attached the updated dcags module.

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email from me to G. Adams:  
George,

I replaced my dcags module with the one you sent, recompiled  
and ran. I still have the same error. The screen output ends  
with:

```
exec: calling dcags
***>>> Error in Gentpags <<<***
trouble running envin.e,  istatus= 256
```

This warning comes from dcags.f line 2144:

```
if( istatus .ne. 0 ) then
  print *, ' ***>>> Error in Gentpags <<<*** '
  print *, ' trouble running envin.e,  istatus=',istatus
  stop
endif
```

I think this is different from the error you were getting.

Brandi

(NOTE: It turns out, when I saved the file, it saved as dcags.f.txt so it was  
compiling with the old dcags.f file. Once I renamed it to the correct name,  
all was well.)

email from R. Janetzke:  
I gave the wrong SCR#. It should be 428, see attachment.

email from me to R. Janetzke:  
Ron,

I've plotted the tbumps up for SCR 428. It looks like everything  
is working correctly. I am still working on the Test Plan, but  
here is a Tecplot layout file that shows where I am at.

Included in the layout are:

the repository outline (black)  
the subarea outlines (subarea 1 is blue, others, not activated)

4 tpa runs:

- 1) (custom8) OneTempCellPerWP = 0 and TemperatureReferencePoint = 1
- 2) (cyan) OneTempCellPerWP = 0 and TemperatureReferencePoint = 2
- 3) (green) OneTempCellPerWP = 1 and TemperatureReferencePoint = 1
- 4) (red) OneTempCellPerWP = 1 and TemperatureReferencePoint = 2

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runs 1) and 2) are not activated. To see them, go to Field -> Mesh  
Attributes -> Mesh Show

I'm not certain, but I may have confused runs 1 and 2. they're a little  
difficult to see on the scale shown.

I'm thinking of some process level tests to add to this.

Brandi

Feb 20, 2003

response from R. Janetzke:

Your plots look great. We should include a color hard copy, and explanation of  
axes and curves, in the Test Results .

Email from B. Rogers:

Brandi,

Here's what I received from Andy on SCR-422.

Bob

----- Original Message -----  
Subject: PA-SCR-422  
Date: Wed, 19 Feb 2003 10:44:54 -0600  
From: Andrew C Jank <andrew.jank@swri.org>  
To: brogers@swri.org

Bob,

Attached is a Winzip file that contains the SCR, the Test Plan, and the  
modified code files. It is ready to be tested against version  
tpa50betaP. Also, included is a modification to the codes\Makefile4.2  
where I added "..\array.o" to the Makefile to access the Zero utility in  
releaset.f. Please let me know if you have any problems with the test  
plan or extracting the files. Thanks.

Andy Jank

Feb 21, 2003

email from B. Rogers:

Brandi,

Here's what I received from Andy on SCR-422.

Bob

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----- Original Message -----  
Subject: PA-SCR-422  
Date: Wed, 19 Feb 2003 10:44:54 -0600  
From: Andrew C Jank <andrew.jank@swri.org>  
To: brogers@swri.org

Bob,

Attached is a Winzip file that contains the SCR, the Test Plan, and the modified code files. It is ready to be tested against version tpa50betaP. Also, included is a modification to the codes\Makefile4.2 where I added "..\array.o" to the Makefile to access the Zero utility in releaset.f. Please let me know if you have any problems with the test plan or extracting the files. Thanks.

Andy Jank

email from me to B. Rogers:  
Bob,

When I copy the modified files to my tpabeta50P directory, re-make tpa (with Makefile4.2), modify tpa.inp iaw the test plan for pl-1, and run tpa.e, I get the following error:

cp: ebsnef.dat: No such file or directory

In my output file PA-SCR-422\_PL-1-B.out the following message:

```
***>>> Error in ebsrel <<<***  
istatus .ne. 0  
istatus = sh(  
cp ebsnef.dat ebssf.dat  
  
)  
istatus = 256
```

Am I forgetting to do something?

Brandi

email from me to R. Janetzke:  
Here are the modified files for SCR 422 as well as the SCR and Test Plan. I am currently going through the Test Plan, so this is not a done deal yet, just forwarding you the info.

email from me to R. Janetzke:  
Ron,

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I finised with the testing of SCR422. Everything passed and is located at:

/net/spock/home/bwinfrey/rjanetzke/SCR422

I still need to make a CD, but otherwise it is finished.

Brandi

email from R. Janetzke:

Where can I find the electronic copy of your text for SCR428?

Feb 24, 2003

My response to R. Janetzke:

The SCR is located at:

/net/spock/home/bwinfrey/rjanetzke/SCR422/docs/scr\_422.wpd

Also, attached to this email.

email from me to R. Janetzke:

Attached is the modified Description of Change(s) for SCR 424.

Mar 11, 2003

In relation to TPA validation:

email from me to R. Janetzke:

Ron,

Is there a seperate .h and .t file for each .f file or for each  
subroutine/function? If for each .f, then

do you include that .f's .h and .t files for each subroutine?

Brandi

response from R. Janetzke:

There is a separate .h and .t file for each subroutine/function.

Mar 11 - Mar 12, 2003

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modified .f files to reflect new format and created .h and .t files for subroutines. I will add the actual tests to the .t files in the coming weeks. The .f files I am responsible for are:

ashplumo.f  
ashrmovo.f  
condxyzt.f  
dcagw.f  
dsfail.f  
faulto.f  
fileunit.f  
findelev.f  
iareader.f  
mv.f  
peakfind.f  
volcano.f  
zportunx.f

The new format modifies the comments in addition to including the two new file types (\*.h and \*.t). The new format includes the following:

```
c  CONTENTS:
c      function
c      subroutine
c  HISTORY:

c  NAME: -
c
c  PURPOSE:
c
c  METHOD:
c
c  INPUT:
c
c  OUTPUT:
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c  --- TEST DRIVER ---
c      include 'fileunit.t'

c  --- HEADER ---
c      include 'fileunit.h'
c
```



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```
cccccc
c
c  GLOSSARY:
c
c
cccccc
c----- declaration of all variables
    character*
    integer
    double precision

c----- disposition of variables
    save
    common
    data

c----- declaration of externals
c
c  Declare subroutines and functions that do not reside in this file.
c
    external

c----- declaration of external function types
c
c  Declare external function types.
c
    character*
    integer
    double precision

c
c  Start here.
c
```

The header file (\*.h) includes an “implicit none” declaration and declares all of the input and output parameters to its subroutine.

The test file (\*.t) contains the tests to be performed on the subroutine for validation. An example would look like:

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```
c  Test driver for filename.f
include 'filename.h'
integer iEntryCount
save iEntryCount
data iEntryCount /0/

c
c  Start here.
c

iEntryCount = iEntryCount + 1
if (iEntryCount .eq. 1) then
    call filename_tc1( val1,val2,val3)
else if (iEntryCount .eq.2) then
c    call filename_tc2(val1,val2,val3)
else
    call filename_t(val1,val2,val3)
end if
return
end
```

```

=====
subroutine filename_tc1(val1,val2,val3)

```

C

```
c  NAME:
c  filename_tc1 -
```

c PURPOSE:  
c  
c  
c METHOD:

```

c
c      INPUT:
c
c      OUTPUT:
c

```

[illegible]

```
print *, val1, val2, val3
```

call filename\_t(val1, val2, val3)

```
print *
```

return

end

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subroutine filename\_t (val1, val2, val3)

Mar 18, 2003

TPA meeting 9:00 am Tues. Mar. 18th in rm A237.

Mar 21, 2003

TPA meeting scheduled for 9:00 am Tues. Mar. 25th in rm A237.

Email from R. Janetzke:

If you have not already submitted your scientific notebook #170e to me for this period, please do so by close of business Tuesday, March 25, 2003. I will need a hard copy of entries made since Sept. 30, 2002, and an electronic copy of the entire notebook. Entries should be complete as of March 21, 2003.

Apr 01, 2003

TPA meeting at 0900 in rm A237.

Continued making changes to the formatting for the .f files. I should have this complete by the end of the day and begin creating the tests. I'll begin with dsfail.f.

Created file tpatestcase.wpd in my home directory. It contains a table with the names of the subroutines/functions, names of the tests, and descriptions of the tests.

Apr 07, 2003

Sent tpatestcase.wpd file to R. Janetzke. All module names listed, but not all test cases defined.

Apr 10, 2003

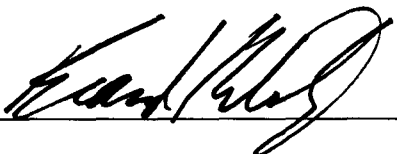
Email from A. Jank:

I'm currently working on nfenv::getLastTimeOfDryout test subroutine. My question is that only values above the peak time are considered. If the boiling point is less than the peak time, then even though dryout is occurring, a -1 is returned. Maybe I'm misinterpreting what this subroutine is supposed to do. I would expect that the largest time should be returned is the dryout period has begun (the boiling point is exceeded). Shed some light? :)

Printed: April 1, 2003

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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.

 04/01/03

.

B. Winfrey

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Apr 15, 2003

Email from C. Scherer:

I put the file [vt\_print\_utilities.f] in /net/spock/home/cscherer/checkin.  
I'll let you know if  
there are any updates. George, the one I emailed you has changed slightly.  
If anyone knows Eric's email address, please let him know, too.

Apr 22, 2003

Email from R. Janetzke:

All,

After a visit from the QA staff they suggested that we enhance our test reports to include information on all tests that are run, whether that are successful or fail. Over the last few days a standard format has evolved among the team. So to the extent as is reasonable, consider applying this format to your output of test activity. Carol and George have put together some utilities that you may like to use for this purpose (talk to Carol for a description and access to these routines). One of the main features of the standard format is the character string "VT:" that appears in the first 3 columns of EVERY line of the test report. See attachment for a sample outline of the format.

thanks,

ron j

May 01, 2003

Email from A. Jank:

Brandi,

I've completed the work on IAREADER, and now I'm going to work on DCAGW. You should be back next week, so we can talk more about it then. Thanks.

Andy

May 06, 2003

Email from R. Janetzke:

Brandi,

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See the attached agenda. You have no presentation, but we would value your critique of the presentations.

thanks,

ron j

Email from R. Janetzke:

Brandi,

·I couldn't find it either. Let's remove it from the '*makefile*'.

thanks,

ron j

May 08, 2003

Email from R. Janetzke:

All,

Just a reminder that for each module assigned there is a corresponding section in the Software Validation Test Plan. It lists a minimum set of tests to be done. Please look these over and include them in your tests.

thanks,

ron j

May 14, 2003

Email from R. Janetzke:

Presenters,

·As mentioned in one of the PA staff meetings, each presenter at the TPA code review on Monday will take the lead for performing the validation tests for the module assigned. Some NRC staff have also been assigned to collaborate in preparing the details of the tests (see attached *vtr-matrix.wpd* or *vtr-matrix.doc* file). Please review the validation test plan, and the tests listed therein for the corresponding module, to see if there are any tests that are unclear. If there are some common themes of concern, Monday would be a good time to discuss them.

Printed: March 23, 2005

B. Winfrey

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Every one should be able to demonstrate by June 13th that they can perform and evaluate all of their tests within a 24 hour period (wall clock time). This is necessary since we may have to perform validation more than once before we deliver the code, due to continuing bug fixes throughout the summer. To this end a "software validation test report" form (*vtp\_template.\**), and sample completed copy of the form (*vtp\_sample.\**), are attached which can be used to speed up the reporting process. The SVTR number will be assigned by the code custodian.

Thanks,

ron j

May 14, 2003

Email to R. Janetzke:

Ron,

I finally got zportunx to compile and run successfully with the new format. I discovered that the following subroutines and functions are not called from anywhere. Can you double check for me? Should I comment them out?

subroutines:  
zportparseunixcmdtodos  
zportfddate

functions:  
sigfpe\_abort  
zportieee\_handler

thanks,  
Brandi

Email from R. Janetzke:

BW,

Yes, comment them out.

thanks,

ron j

May 29, 2003

Email from R. Janetzke:

All,

B. Winfrey      SCIENTIFIC NOTEBOOK No. 170-17e

It has been suggested that the validation schedule be clarified.

All teams should demonstrate that they can perform all of their validation tests, within a 24 hour period, by June 13.

All Software Validation Test Report (SVTR) forms should be completed by July 3.

The teams may be requested to perform a re-test and prepare the associated SVTRs at anytime between June 13 and July 27 to accommodate bug fixes. So all 'on site' members of the team should be able to perform the tests in case one of the members is on travel for more than a day.

The final Software Validation Report will be prepared in the next fiscal year.

thanks for your help,

ron j

Email from M. Smith:

Greetings TPA5.0 Verification Team,

We have been assigned to work together to complete verification testing for VOLCANO, ASHPLUMO, and ASHRMOVO modules that was outlined in CNWRA report "Software Validation Test Plan for the Total-System Performance Assessment Version 5.0 Code." I am a little behind schedule in contacting you due to work I was completing for the INEEL ISFSI SER. That is behind me now and I am ready to get started on this work.

I have begun reviewing the test requirements for these modules and it looks fairly straight forward.

I am writing to gauge your level of interest and availability in assisting with developing, designing, and/or implementing the required tests.

At a minimum I would like to get your input for designing the tests. The basic requirements are that the tests need to be designed such that they all can be run and results determined in less than 24 hours (1 work day). This is so that if (when) last minute changes are made to TPA5.0, we can rerun the verification tests in short order.

I will be on travel next Tuesday-Thursday (June 3-5), so would like to set up a short meeting for Monday so that we can discuss the test requirements for these modules and make sure that I understand those requirements. Before that meeting, I will provide a summary of my understanding of the required tests. Our first deadline is June 13th to provide software verification test plans (brief formatted reports) and to have a good sense that the tests can be completed in less than 24 hours.



Printed: March 23, 2005

B. Winfrey

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Are you available to meet on Monday and when?

Thanks,

--Mike

May 30, 2003

Email from J. Trapp:

I am still not sure what I am expected to do, even after reading the test plan. I will be glad to help out, once it becomes clearer what is expected, but will say that during this next month my main focus will be on anything I need to do for the TE on the first of July, however, I don't expect that the TE will really take that much effort because of the way it is structured. I am free most of Monday except I have a dental appointment which means I will be out of the office from about 2:30 onward.

For reference, put James Rubenstone on distribution also. He is our new guy and want to keep him aware of what is going on with the program, and knowing the code will help.

Have a real question about the 3dr bullet under 5.2.13.1. How can the number of waste packages not differ if you change the width of the dike or its length? Same thing with cone diameter.

Under ASHREMOVO, I wasn't aware that the code now accounts for deposition of material after the main eruption. Need to check that out.

Email from M. Smith:

How about 11:00 a.m. Eastern (10:00 a.m. Central). We can meet in CNWRA A239 (NRC folks will need to call in on one line to 210-522-6838 or provide a number that I could call you on).

·This should be a short meeting to discuss the tests and provide insights for trouble areas that I may not be aware of...I'm depending on you guys to be the experts because I have not been heavily involved in the volcanism/TPA effort in the past.

I will send a summary of my understanding of the tests on Monday morning.

Thanks,

--Mike

June 02, 2003

Printed: March 23, 2005

B. Winfrey

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Email from M. Smith:

TPA5.0 Test Team,

Attached are my notes for each of the TPA5.0 validation tests for VOLCANO/ASHPLUMO/ASHRMOVO. Most seem straight forward, but there are a few that will take a team effort (see yellow highlights in the attachment).

Of special note (and need) is Test C15-2 that calls for a comparison of ASHRMOVO models with leaching/erosion models in the published literature. Following the initial event, ASHRMOVO considers subsequent radionuclide removal by leaching, erosion, and decay and radionuclide addition by erosion from other locations to yield time-dependent areal concentrations at the compliance point. This feature was added to TPA5.0 to increase future flexibility, but I don't believe the parameter values related to this change are well justified. What published leaching/erosion models might be used? Is anyone interested/available to use this opportunity to pursue some justified parameter values? These new features could be "turned off" by parameter value selection to mimic the TPA4.0 model, if those values are better justified.

Thanks,

--Mike

p.s. Dick, sorry I just noticed that you are on the ASHPLUMO test team. We are meeting today at 11:00 a.m. Eastern to discuss TPA5.0 validation tests (including ASHPLUMO). I've asked the NRC folks to call into 210-522-6838 (only one line), so please coordinate with Tim McCartin, John Trapp, or James Rubenstone if you would like to participate. Otherwise, I can take your comments by email/phone. For this meeting I would like to review the test requirements, discuss test designs, and make any assignments, if necessary.

June 03, 2003

Email from T. McCartin:

All:

Regarding the ash thickness from TPA runs (based on an ash deposit density of 1.2 g/cc and assuming the ash is evenly spread over a 20 km by 5 km rectangle):

0 - 5 cm thick	:	21% of the realizations
5-10 cm	:	12 %
10-25 cm	:	20 %
25-50 cm	:	12 %
50-100 cm	:	13 %
> 100cm	:	22%

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Generally the smaller events give much larger doses - in the above example (assuming an event at 100 years and 10 waste packages entrained) the largest dose was 11,000 rem and the average thickness (as calculated above) for this vector was 1.6 cm - this vector was 20% of the mean dose. Also, one important fact is that the lowest dose is 10 rem and the 2nd lowest is 20 rem - there are no low doses EVER with the current approach - consideration of the wind rose will take some of the initial doses to ZERO - yes doses will be affected at later times due to remobilization but it will take very large doses to come close to the many REMs we are now estimating. I will provide more as my calculations become more refined. I am certainly welcome to comments and suggestions on further calculations.

Tim

**Email from B. Hill:**

Tim - Thanks for the follow-up on the discussion in yesterday's telecon. Using TPA 4.1j, I've approached things somewhat differently (and long-windedly).

Last week, I ran a 400 realization run with the "distribution" option, and all other parameters at default values. Input file attached. From ASHOUT and AIRPKDOS.RES, I get the expected 1-150 WP entrained with an average of 51. But for deposit thickness, I get this distribution at 20 km (which should be time independent):

0 - 5 cm thick	:	64% of the realizations
5-10 cm	:	12 %
10-25 cm	:	12.5 %
25-50 cm	:	6 %
50-100 cm	:	3.5 %
> 100cm	:	0.2%

I think you're taking the total volume of the eruption (ashmass) and distributing it uniformly over 5x20km to determine your distribution? Such an approach would definitely overestimate deposit thickness at 20km, as it doesn't account for the general exponential decrease in deposit thickness away from the vent.

This exponential function also is important as much of the tephra volume is deposited within about 5 km of the vent. From my last TPA run, I'm getting tephra volumes ranging from 5e5 to 3e8 m3, with an average of 3e7. That is what I'd expect from the input parameters. So, for an average eruption with winds blowing in a roughly 180 degree sector from N-E-S, roughly 50% of the tephra will be deposited in sloping terrane within the Fortymile catchment basin. That gives on order of 1e7 m3 tephra for remobilization, versus stabilization on fairly flat surfaces(?).

Using our GIS, the depositional basin for Fortymile Wash is on order of 1e8 m2. Even using a uniform thickness, net influx of 1e7 m3 gives 10 cm of

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remobilized tephra deposited throughout the basin, which exceeds initial depositional thickness for at least 75% of eruptions. However, fluvial deposition is not uniform and probably follows an exponential decrease as well for this type of setting. So net influx of tephra is likely >10 cm at RMEI area. Although on a simple mass-basis there's more net tephra than many initial deposits, the risk significance depends on the rate and concentration of the remobilized tephra.

Bulking or deposit dilution is a poorly constrained process. Based on the Extreme Erosion legacy, data show the YM slopes and secondary drainages are sediment starved and Fortymile Wash is still incising in response. During infrequent high-velocity floods, the active sediment moves predominantly as bed load as it is relatively coarse and dense. The sediments also are fines depleted, as these fines have been winnowed from the system. If tephra is dumped on the surrounding terrane, this will dramatically change the character of the sedimentary system. Equilibrated low-load drainages will be essentially choked with easily mobilized tephra. Rough, light tephra particles will be entrained at lower channel velocities than current sediments, and likely flow as suspended loads rather than bed loads during peak flow only. Peak-flow events, which mobilized bedload, will likely dilute the tephra load. However, more frequent lower-velocity events will necessarily contain much less diluted tephra, as only local reworking of bed-load sediment occurs in these events. These processes likely operate on decade-century scale.

While the variable windfield will give many realizations with no initial deposit and thus dose, there will be very few simulations (i.e., wind blowing due west at pretty high velocity) without some tephra deposited in the Fortymile catchment basin. I can't yet guess what the magnitude of that remobilized mass will be, nor how long it will take to reach the RMEI area. This is something that we'll work on once Don Hooper starts work at the Center.

Naturally, initial doses will be highest for the youngest HLW inventory. But that trade-off between [high dose x  $1e-7$  x 1yr] versus [lower dose x  $1e-7$  x multiple years] is not intuitive to me. Using the runs we did for IRSR rev 2 (page 14), the average conditional dose of 120 rem at t+100 is down to 12 rem at t+1000. That gives a crude inventory half-life around 200 yr. That is on the rough order of "deposit half-lives" I'd guess for tephra on the slopes of YM. Given these relationships, will the net influx of remobilized tephra offset the in-situ inventory decay function? Given the uncertainties, either "yes" or "no" can be supported.

Based on all this, I don't think the current approach is off by an order of magnitude, as many processes seem to be offsetting orders-of-magnitude. But we still could be in that 2x-5x under- or over-estimating range by neglecting remobilization through time. If peak dose corresponded to peak risk, then I'd agree that the [t+100 doses x  $1e-7$ /yr probability] were the maximum risk. Unfortunately, the accumulation of risk from prior events offsets the timing

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of peak risk to some later date. DOE (and we) need to develop a technical basis to support the risk convolution necessary for 10CFR63. With our new staff on board, I think this basis is achievable within the next year.

Britt

Email from T. McCartin:

We can follow up with a phone call later - it's too complex for email - I was not trying to calculate the thickness at 20 km but rather give a sense of how little material is being ejected for the large doses (a few centimeters over a 20x5 km strip is not a lot of material) - when wind rose is accounted for doses will drop to zero for many relaxations and remobilization will come in later but to offset some large doses will be very difficult to do - the persistence of the deposit has very little effect. I need to do some further calculations to put this into more readily explained terms. In a nut-shell the small eruptions, which currently give the largest doses, will be reduced the most due to incorporating the wind rose and will be the least significant from a remobilization stand point - thus I believe doses will be reduced.

Email to M. Smith:

Mike,

Attached is the SVTR for c13-2. I have some questions about the results:

Run1: minimum values:

diameter = 24.6

that means that ~ 5 wp can fit

MTU per wp is ~ 7.8

so, shouldn't mass ejected be  $\sim 5 * 7.8 = 39$  ??

the result for amtuejected is 7.4928081461320 using the following values:

<<<<<<<<<<<<< area = 784763.04659987

<<<<<<<<<<<<< diameter = 24.600000000000

<<<<<<<<<<<<< amtupersa = 12371.5200000000

<<<<<<<<<<<<< average loading per subarea = 1.5764656673886D-02

<<<<<<<<<<<<< conduitarea = 475.29155256160

<<<<<<<<<<<<< amtuejected = 7.4928081461320

and the formula

$\text{amtuejected} = \text{amtupersa} * \text{conduitarea} / \text{area}$

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Run2: maximum values:

diameter = 77.9

that means that ~ 15 wp can fit

MTU per wp is ~ 7.8

so, mass ejected should be  $\sim 15 * 7.8 = 117$

the result for amtuejected is 75.136215020935 using the following values:

<<<<<<<<<<<<<<< area = 784763.04659987

<<<<<<<<<<<<<<< diameter = 77.900000000000

<<<<<<<<<<<<<<< amtupersa = 12371.5200000000

<<<<<<<<<<<<<<< average loading per subarea = 1.5764656673886D-02

<<<<<<<<<<<<<<< conduitarea = 4766.1180687427

<<<<<<<<<<<<<<< amtuejected\_1 = 75.136215020935

Does this difference have anything to do with geometric vs distribution volcano model?

Do the values look correct?

Also, the average loading per subarea ranges from 1.2 to 1.6. Is this difference within an acceptable range?

Brandi

Email from R. Janetzke:

Brandi,

·The volcano parameters in *tpa.inp* are divided into two sections.

Geometric: from "Xlocation..." to "DiameterOf..." and

Distribution: from "SubareaOf..." to "NumberOfMag...".

The geometric model will be affected by the geometric parameters. So the test should be reconfigured to vary only the distribution model parameters while keeping the geometric ones constant. The criterion mentioned in the SVTP will then be valid.

thanks,

ron j

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**/solapps/cnwra/A\_tpa5.0f**

This version has a more realistic way to handle the colloids. The colloid chains were extended to include long half life solute nuclides as a sink for the colloid decay products. Also the *szft.rlt* file was modified to include colloid information. New data is available in *strmtube.dat* with Winterle's latest numbers and in *tpa.inp* with Picket's numbers for colloid release factors and colloid filter factors.

A note to the coders:

The basic philosophy for handling chains had to be changed to accommodate this version. In the past the rule was enforced that prohibited duplicate nuclide names. This no longer can be enforced due to the requirement to have solute nuclide names in the colloid chains. However, having duplicate names in the nuclide list fouls up all the logic in the modules that search for a name that matches a nuclide name. Before, the modules could just search for a name and when they found it, they had a match. This technique is no longer valid. Instead, a strict order for nuclides is now imposed such that the order in *tpa.inp* is maintained in all of the internal arrays and data transfers. If you know of any logic that will be affected by this change, let me know ASAP.

The following files were modified:

invent.f  
uzft.f  
szft.f  
reader.f  
exec.f  
ebsrel.f

If you have any automated test using the \*.t files check these files and merge them to your \*.f files. Any files still in *checkin* should be updated as needed.

thanks,

ron j

June 14, 2003

Email from R. Janetzke:

All,



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The latest version of TPA is 5.0g. It contains several data file fixes (including the one T. McCartin discussed last week) and the releaset bug fix for zero flow. The executable only is in **/solapps/cnwra/A\_tpa5.0g** and the source code is in **/home/janetzke/tpa50g**.

Use this version for all test that do not require comparison with old version. The new results vary slightly in the 3rd or 4th digit.

ron j

June 23, 2003

Email from R. Janetzke:  
Brandi,

A couple of notes on your test files. Where planning on implementing the IMPLICIT NONE construct? Do you have some \*.f files to go with your test modules?

thanks,

ron j

Note: Answer to above email: Yes, implemented implicit none construct. Put .f files in home directory under the "checkin" directory.

Email from R. Janetzke:

All,

This is a cautionary note to all coders.

If you change an \*.i file you are responsible for reconciling its use everywhere, including \*.f files in the *codes* subdirectory!

Also, although the SUN compiler does not object, the PC compiler gives FATAL errors if you use an integer as part of an array declaration before the integer itself is declared.

thanks,

ron j

B. Winfrey

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Email to T. McCartin:

Tim,

Mike sent me your write up for c14-1 and I am trying to run the tests but am having difficulty understanding how you want tpa.inp set up. Under the Assumptions, constraints section of the SVTR you mention the user specified option for number of waste packages. What do you want the user specified option for number of waste packages to be and where do I set it (what tpa.inp parameter)?

I have the following parameters set in tpa.inp:

```
DirectReleaseOnlyFlag(yes=1,no=0) = 1
VolcanismDisruptiveScenarioFlag(yes=1,no=0) = 1
VolcanoModel(1=Geometric,2=Distribution) = 1
NumberOfRealizations = 400
```

Is this all I need to set before I start the run? Also, can I get a copy of your Excel spreadsheets for this test?

thank you,  
Brandi Winfrey

Email from T. McCartin:

You have the set-up right - just set the VolcanoModel to 1 to test the geometric model and you will need to do a separate run to test the user specified distribution (setting the VolcanoModel to 2). The spreadsheet is attached - it may be a little hard to follow call if you have questions (301-415-7285).

Tim

Email from R. Janetzke:

All,

The latest TPA version is 5.0h and it is on

/solapps/cnwra/A\_tpa5.0h

It contains a new algorithm for calculating UZ fracture flow, updated SZ parameters in *tpa.inp*, and new SZ flow rates in *strmtube.dat*.

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It also includes reformatted source code for atomated testing in modules: *exec.f*, *uzflow.f*, *ran1.f*, and *uzft.f*.

ron j

June 29, 2003

Email from R. Janetzke:  
Brandi,

Nefmks.f has a surprise for us, it uses subroutine zportfdate that was commented out. Check this out and see if it is right.

thanks,

ron j

June 29, 2003

Email from R. Janetzke:

All,

A new version of TPA is now available as TPA5.0i in

/solapps/cnwra/A\_tpa5.0i

It has an update to the relative humidity model for **nfenv**.

The next version will have the drip shield model update discussed with Firth at last Thursday's meeting.

ron j

July 01, 2003

Email from R. Janetzke:

All,

B. Winfrey

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Some of you may have been visited recently by QA surveillance personnel (Randy Folck). On Tuesday he gave me a heads up on his findings. In general the SVTRs are looking good, but he also identified the following area that could use improvement.

-- When describing the test procedure (8th vertical cell in the form) or the changes required to be made to the input files for a given test ( 6th vertical cell in the form), a justification should be provided for the particular values chosen for parameters that are critical to the performance of the tests.

other hints:

-- Try to complete the form electronically. It may be helpful to know that the check boxes in the Test Method section can be filled by replacing them with the

Insert -> Symbols -> Iconic Symbols -> 5,25

menu sequence.

-- Leave the SVTR number cell blank.

-- Be accurate when specifying the Version of TPA under test.

-- Try to keep the main form to one page and include longer sections as attachments referenced in the main form.

-- The due date for testing is July 3 you may submit completed forms to me via e-mail up to July 6.

-- A tally will be prepared on July 7, to see which tests have passed. If any tests fail, it will mean that another round of tests will need to be conducted in the very near future.

thanks,

ron j

July 02, 2003

Email from C. Scherer:

Michael, I've run out of time to finish these tests (C11-1, last line, and C16-1, last line). Brandi has taken over.

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Note: these tests involve checking output files for dcagw and dcags to ensure they are correct. Used an excel spreadsheet to verify.

July 03, 2003

Email from R. Janetzke:

All,

·The latest version of TPA is 5.0j and is on

/solapps/cnwra/A\_tpa5.0j

ron j

July 05, 2003

Email from R. Janetzke:

Brandi,

There was a bug in the volcano model 2. So the next version 5.0k should have the fix for test C13-3.

good catch,

ron j

July 05, 2003

Email to R. Janetzke:

Ron,

Attached is the SVTR for c11-1 and the Excel spreadsheet (and supporting files). I am going to model c16-1 after this to test dcags. I expect that c16-1 will be finished tomorrow.

I have tested and passed all of my tests on version 5.0i except e4-2, e12-1, and c13-3. SCR458 corrected e4-2 and e12-1. I will test these three on version k when it is ready.

Email from R. Janetzke:

Brandi,

Are you preparing the SCR458 or am I? Please refresh my memory.

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thanks,

ron j

Email to R. Janetzke:

I have already prepared SCR458 as well as the Test Plan and emailed them both to you.

Brandi

Email from R. Janetzke:

Thanks, I have it. The attachments were not visible below the end of the page of the original message.

July 10, 2003

Email to M. Smith:

Mike,

Carol gave me these two SVTRs to complete. Attached are the SVTRs [dcagw and dcags]. I've tested and passed them.

Email from M. Smith:

Thanks Brandi...great work. These will be in addition to what Pat and I turned in for C11-1 and C16-1. The other sections for these tests have also passed.

--Mike

July 11, 2003

Email from R. Janetzke:

Brandi,

Although these have no test plan yet, a couple are trivial file inspections, so I think they will go rather quickly.

See me, if needed, for clarification on any of these.

thanks,

ron j

The SCR's referred to in the above email are 452, 455, 447, and 449.

July 12, 2003

B. Winfrey      SCIENTIFIC NOTEBOOK No. 170-17e

Email from R. Janetzke:

Brandi,

I did not merge these changes in, because the code is compiling OK as is.  
Were these cosmetic changes or where they needed for compilation?

thanks,

ron j

Note: the changes mentioned in the email above were, indeed, cosmetic and only suggested to have the files follow the suggested new format style (i.e., declaring externals).

July 14, 2003

All,

·The latest version of TPA is 5.0k. It is in

**/solapps/cnwra/A\_tpa5.0k**

It contains mostly cosmetic changes and should not effect most of the previous tests. However, if your tests are critically sensitive to "in-can" pH or extrusive volcanic release you should rerun the tests.

thanks,

ron j

July 15, 2003

Email from J. Winterly to R. Janetzke (forwarded to me):

Ron,

the distribution of StreamTubeWidthMultiplier[] should have been "uniform" in the last email I sent you. Corrected version is below.

--Jim

```
=====
uniform
DistanceToTuffAlluviumInterface[km]
12., 18.
```

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Basis: The mid-range value of 15 km is consistent with the modeling results obtained by Winterle (2003), which were based on an underlying hydrogeologic framework model by Sims et al. (1999). Lower bound value of 12 is based on location of Nye County well NC-EWDP-10S, which penetrates saturated alluvium at a distance of 12 km from the boundary of the EDA-II repository design. Upper bound of 18 km is based on a possible conceptual model in which a confining tuff-alluvium interface keeps flow paths within volcanic units beyond the 18-km compliance boundary.

=====

```
constant
SZFluxMultiplierAtGlacialMaximum[]
1.0
```

Basis: Modeling by Winterle (2003) suggests that groundwater fluxes and travel times in the saturated zone would not change significantly in the event of a regional water table rise and increased recharge. Additionally, the base case strmtube.dat file for TPA 5.0 is already based on a potential wetter future climate scenario.

=====

```
uniform
StreamTubeWidthMultiplier[]
0.8, 1.2
```

Basis: Evaluation of several alternative conceptual models (Winterle et al., 2002; Winterle, 2003) suggests that the widths of flow paths originating beneath the repository vary significantly only slightly between differing alternative model scenarios. Twenty percent above and below the mean value of 1.0 should bound this uncertainty.

Email from R. Janetzke:

All,

·The latest version of TPA is 5.0l. It is in

*/solapps/cnwra/A\_tpa5.0l*

It contains an adjustment of how the colloid filter factors are used in the UZ. So, if your tests are critically sensitive to colloid transport in the UZ you should rerun the tests.

thanks,



B. Winfrey

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ron j

July 16, 2003

Email to R. Janetzke:

Ron,

Attached is the SVTR for c13-3. Also, I left the SVTRs for e4-2 and e12-1 along with CDs for SCRs 447, 449, 452, and 455 on your chair. Please let me know if there is anything else you need.

Email from M. Smith to R. Janetzke:

Ron,

·Attached is SVTR for TPA test C16-1 that I received from Brandi. I added a line to the notes section of the SVTR indicating that the remaining tests for C16-1 are described in SVTRs for C11-1b and C11-1c. With Brandi's latest testing and the links to C11-1b and C11-1c, the testing for C16-1 is complete and passed.

--Mike

Email from M. Smith:

Hi Brandi. I need your help to finish up paper work for C13-3. Ron has the C13-3 test files on CD, but is missing the SVTR. I know you sent this to Ron and I June 4th...I would resend to him, but I was concerned that it may have been updated since then. Please send SVTR to Ron when you get a chance.

·Thanks,

--Mike

July 19, 2003

Email from R. Janetzke:

All,

·The latest version of TPA is 5.0m. It is in :

/solapps/cnwra/A\_tpa5.0m

It contains a new *dsfail.f*, updated weld corrosion parameters in *tpa.inp*, a bug fix for glass waste form, updated coordinates in *repdes.dat*, and an updated *mechfail.f*.

thanks,

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ron j

Email from R. Janetzke:

Brandi,

Here is a new set of SCRs. They need to be finished by Thursday. So look them over and see if it is possible or whether we need to split the load.

thanks,

ron j

The SCR's mentioned in the email above are 467, 455, 456, 461, 462, and 452.

July 21, 2003

Email to R. Janetzke:

Ron,

I've already given you SCR 452. I will be finished with SCR455 probably this morning. I'll look at the rest you sent me and let you know if I can finish them by thursday.

Brandi

Email to R. Janetzke:

Ron,

I will be able to finish these SCRs by thursday.

Brandi

July 22, 2003

Email to R. Rice:

Rob,

I'm testing SCR 456 which adds the subroutine querystop to reader.f. Can you send me a copy of your querystop.t file. I've tried to compile tpa using a querystop.t file that contains only the line "iset = 1"

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and I get the following error. Rather than guess at what should be in there,  
it would be helpful to just see your original file.

"querystop.t", line 1: Error: illegal continuation card ignored  
make: \*\*\* [reader.o] Error 1

thanks,

Brandi

Email from R. Rice:

Brandi,

"iset = 1" is all that  
I had in querystop.t, basically (there  
was also the implicit none statement and  
then the usual comment stuff).

Possibly I should have done  
this differently. (LF90 didn't  
clamour about this when compiling though.)

Please give me a call if you have  
any questions at x5194 (I'm hiding  
upstairs in Room A244 this week).

Thanks,

Rob

Email from R. Janetzke:

All,

In order to meet the delivery schedule for the validated version of the  
TPA code, we need to complete all SVTRs by Thursday July 24, 2003. If  
you cannot complete the SVTR by then, please provide a justification as  
to why the test report could not be prepared as described in the SVTP.

Also, before delivery of the validated code we need to identify any  
SVTRs that differ markedly from what was proposed in the SVTP. If any  
of your SVTRs fall into this category please present a justification for  
the deviation from the plan outlined in the SVTP by COB Thursday.

thanks,

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ron j

**July 24, 2003**

Email to C. Scherer:

Carol,

I am trying to test tpa5.0m to see that SCR455 passes. This SCR is the one you gave me the modified tpa.inp file that has chains with up to 7 members. Well, your tpa.inp file will not work with the current version because there have been too many changes since version 5.0g. Can you show me just the section that I can cut-and-past into the current tpa.inp file for testing?

thank you,

**July 25, 2003**

Email from R. Janetzke:

Could you do one more SCR? It is a trivial inspection of repdes.dat.

The SCR mentioned in the above email is SCR468.

Email to R. Janetzke:

No problem. I'll have it back to you today.

Brandi

**July 28, 2003**

Email exchange between R. Janetzke and B. Winfrey:  
Yes, Ron it was completed. My electronic version has the completed (PASS) date as July 03, 2003). I'll print out a new SCR for you.

Brandi

-----Original Message-----

From: ron janetzke [mailto:rjanetzke@swri.edu]

Sent: Monday, July 28, 2003 8:59 AM

To: bwinfrey@swri.edu

Subject: Re: SVTP for c13-4

Brandi,

B. Winfrey            SCIENTIFIC NOTEBOOK No. 170-17e

This SVTR does not have a pass/fail status.    Was it completed?

thanks,

ron j

"Brandi L. Winfrey" wrote:

> Ron,  
>  
> Attached is the SVTP for c13-4 and the Excel spreadsheet results. I will  
> burn a CD of  
> SVTP and result files for c13-2, c13-3, and c13-4 for you today. I emailed  
> you e4-1  
> earlier and am waiting to see if it is acceptable before I burn it to CD.  
>  
> The sample SVTP was for FAULTO. Does this mean that you have already  
> completed  
> c12-1? Or do I need to come up with a test for it? Osvaldo and I were on  
> the team for  
> faulto, and I think he's under the assumption that it is already completed.  
>  
> Brandi

Email to R. Janetzke:

Ron,

George corrected the SCR and Test Plan to reflect the changes made. Attached are the two files that were modified: ial.i and iareader.f. Just search on SCR458 to find the changes.

**No entries made for the month of August.**

Entries into Scientific Notebook #170E for pages 1 -77 have been made by Brandi Winfrey 3/23/5.

No original text entered into this Scientific Notebook has been removed.

Brandi Winfrey for B. Winfrey 3/23/5.

I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding methods used for conducting tests,

Printed: March 23, 2005

B. Winfrey      SCIENTIFIC NOTEBOOK No. 170-17e

acquiring and analyzing data so that another qualified individual could repeat the activity.

James Winterle      11-9-05  
JRW