

SCIENTIFIC NOTEBOOK

612-4E

by

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INITIAL ENTRIES

Scientific Notebook: #612E

Issued to: C. Scherer

Issue Date: September 17, 2003

Account Number: 20.06002.01.113

Title: TPA 5.0 Code Development

Participants: R. Janetzke
S. Mohanty
R. Rice
C. Scherer
O. Pensado
R. Benke
P. LaPlante
G. Adams
B. Winfrey
M. Smith

Objective:

This scientific notebook will document the work performed in the development of the TPA code.

9-17-2003 -

Started new notebook. Retired #170.

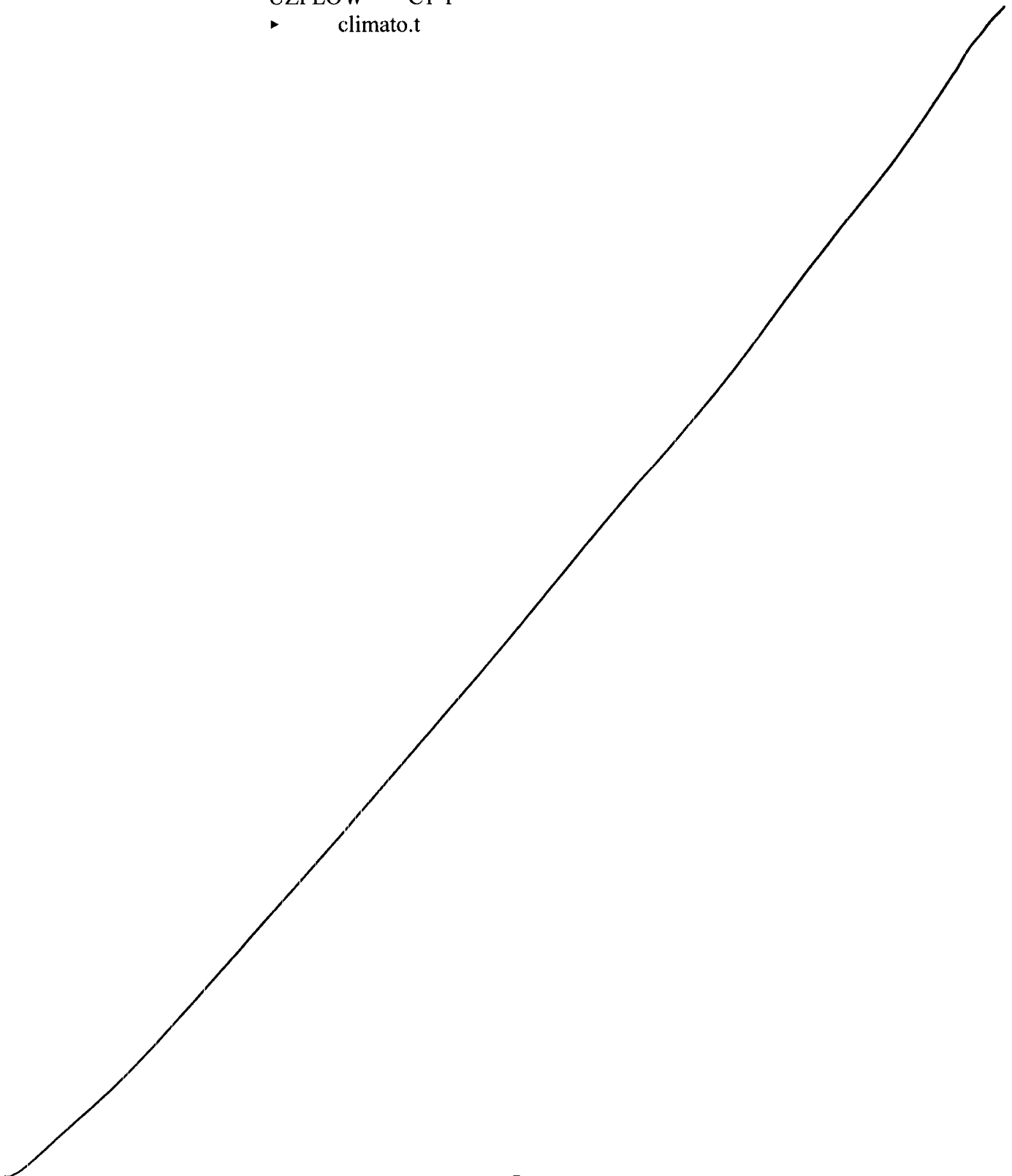
9-18-2003 - 11-3-2003

Worked on gathering data for the appendix to the TPA 5.0 Validation Test Report.
Process followed:

1. went through SVTR folders that Ron kept and answered following questions:
 - was there a hard copy of the SVTR in the folder?
 - was there a CD/floppy in the folder?
 - did the CD contain the SVTR in electronic format?
 - did the SVTR refer to the CD?
 - did the SVTR refer to any files not on the CD?
 - did the SVTR pass?
 - which SVTRs were supposed to be tested automatically?
 - later, after run, did tpa.out contain the automatic tests and did the printout contain enough information to replace a printed SVTR and was the output for the automatic tests consistent?
2. developed spreadsheet
3. read SVTRs and noted which should have auxiliary files
4. gathered files from testers
5. updated/modified automated test source files for:
 - ARRAY (major mods required - Rob didn't use the print utilities)
 - ▶ zero.t
 - ▶ zeroi.t
 - ▶ clearchar.t
 - ▶ initr.t
 - ▶ scale.t
 - ▶ scopy.t
 - ▶ scopy.t
 - ▶ addto.t
 - ▶ isoneoffset.t
 - ▶ checkinorder.t
 - ▶ checkforduplicates.t
 - ▶ icheckforduplicates.t (Brandi helped)

- ▶ sortqr.t (Brandi helped)
- ▶ maplist.t (Ron started this one)
- ▶ maptimeofevent.t
- ▶ ainterl.tl
- ASHPLUMO C14-1
 - ▶ ashplume.t
- DSFAIL C4-1
 - ▶ dsfail.t
 - ▶ setupCommons.t
 - ▶ getThickness.tl
- INVENT (moderate mods required to Andy's utilities - he didn't use the set that George and I put out) E3-4
 - ▶ newinventdb.t
 - ▶ setage.t
 - ▶ allchains.t
 - ▶ chains.t
 - ▶ chainsolver.t
 - ▶ decay43mol.t
 - ▶ decay43molglass.t
 - ▶ decayremove43mol.t
- MV E4-1 & E4-3
 - ▶ setconsmv.t
 - ▶ setconsmv_tc2.t
 - ▶ setconsmv_tc3.t
- NUMRECIP E9-1
 - ▶ gauleg.t
- PEAKFIND E10-1
 - ▶ peakfinder.t
- RAN1 E11-1
 - ▶ iranu.tl
 - ▶ ran1.tl
 - ▶ ran1seis.tl
 - ▶ setran.t
 - ▶ setranseis.t
- SAMPLER (moderate mods required to Andy's utilities - he didn't use the set George and I put out) E2-3 & E2-5
 - ▶ writesnllhsinp.t
 - ▶ newrealization.t
- SUBAREA (little or no modification required) E5-3
 - ▶ qchitsa.t
 - ▶ qlhitsa.t
 - ▶ qphitsa.t

- UZFLOW C1-1
 - climato.t



Summarized tasks in following spreadsheet (</net/spock/home/cscherer/validate/rptxref.xls>):

Test ID	SVTR #	electronic copy of SVTR	Folder contains svtr	Folder contains CD/floppy	CD contains SVTR doc	cross reference	auxiliary file(s) *1	mods needed to SVTR	automatic test	test reference in tpa.out	contact	NOTES	#
E1-1	1	x	x	x		E2-3 E3-4					Rice	READER	1
E1-2	2	x	x	x			x				Rice	READER	2
E1-3	3	x	x	x				x			Rice	READER	3
E1-4	4	x	x	x			x	x			Rice	READER	4
E1-5	5	x	x	x			x				Rice	READER	5
E2-1	6	x	x	x	x	E2-4	x				Peterson	SAMPLER	6
E2-2	7	x	x	x	x		x				Peterson	SAMPLER	7
E2-3		N/R	-	-		E1-1			x	x	Peterson	COVERED; SAMPLER	8
E2-4		N/R	-	-		E2-1					Peterson	COVERED; SAMPLER	9
E2-5		N/R	-	-					x	x	Peterson	SAMPLER	10
E3-1	8	x	x	x							Scherer	INVENT	11
E3-2	9	x	x	x							Scherer	INVENT	12
E3-3	10	x	x	x							Scherer	INVENT	13
E3-4		N/R	-	-		E1-*			x	x	Peterson	INVENT	14
E3-5	11	x	x	x							Scherer	INVENT	15
E4-1		N/R	-	x					x	x	Winfrey	MV	16
E4-2	12	x	x	N/A							Winfrey	MV	17
E4-3		N/R	-	x					x	x	Winfrey	MV	18
E5-1	13	x	x	x	-		x				Adams	SUBAREA	19
E5-2	14	x	x	x			x				Adams	SUBAREA	20

E5-3		N/R	-	x	-				x	x	Adams	SUBAREA	21
E6-1		N/R	-	-					x	x	Rice	ARRAY	22
E7-1	15	x	x	N/A							Winfrey	FILEUNIT	23
E7-2	16	x	x	x							Winfrey	FILEUNIT	24
E8-1		N/R										DELETED; FINDELEV	25
E9-1		N/R	-	-					x	x	Rice	NUMRECIP	26
E10-1		N/R	-	-					x	x	Peterson	PEAKFIND	27
E11-1		N/R	-	-					x	x	Rice	RAN1	28
E12-1	17	x	x	x								IAREADER	29
E12-2	18	x	x	x	-						Winfrey	IAREADER	30
E12-3	19	x	x	x	-						Winfrey	IAREADER	31
E12-4	20	x	x	x	-						Winfrey	IAREADER	32
E13-1	21	x	x	x							Adams	EXEC	33
C1-1		N/R	-	x	-				x	x	Adams; Fedors	UZFLOW	34
C1-2	22	x	x	x			x				Fedors	UZFLOW	35
C1-3	23	x	x	x			x				Adams	UZFLOW	36
C1-4	24	x	x	x							Benke	UZFLOW	37
C2-1	25	x	x	N/A			x				Codell	NFENV	38
C2-2	26	x	x	x		S1					Howard	NFENV	39
C2-3	27	x	x	x		S1					Howard	NFENV	40
C2-4	28	x	x	x		S1					Howard	NFENV	41
C3-1	29	x	x	x			x	x			Pensado	EBSFAIL	42
C3-2	30	x	x	x		C5-2	x	x			Pensado	EBSFAIL	43
C3-3	31	x	x	N/A			x				Csontos; Pensado	EBSFAIL	44
C3-4	32	x	x	N/A			x				Pensado; Grossman; Pensado	EBSFAIL	45
C3-5	33	x	x	x							Pensado	EBSFAIL	46
C4-1		N/R	-	x	-	S7	x	x	x	x	Winfrey	DSFAIL	47

C4-2	34	x	x	x		S7	x	x			Pensado	DSFAIL	48
C5-1	35	x	x	x		C3-1					Esh	WELDFAIL	49
C5-2		N/R	x	-		C3-2					Pensado	WELDFAIL; COVERED	50
C5-3	36	x	x	N/A			x				Csontos; Pensado	WELDFAIL	51
C6-1		N/R				S6					Mohanty	COVERED; SEISMO2	52
C7-1	37	x	x	x							Scherer	EBSREL	53
C7-3	38	x	x	x			x				Adams	EBSREL	55
C7-4	39	x	x	x			x				Adams	EBSREL	56
C8-1	40	x	x	N/A							Chichkov	EBSFILT	57
C8-2	41	x	x	x			x				Chichkov	EBSFILT	58
C8-3	42	x	x				x				Chichkov	EBSFILT	59
C8-4	43	x	x	N/A							Chichkov	EBSFILT	60
C9-1	44	x	x	N/A		S3	x				McCartin	UZFT	61
C9-2	45	x	x	N/A		S3	x				McCartin	UZFT	62
C9-3	46	x	x	x							Wittmeyer Scherer	UZFT	63
C10-1	47	x	x	x			x	?			McCartin	2/6 failed; SZFT	64
							x	x			Scherer	reran test; all passed	
C10-2	48	x	x	N/A			x				Povetko	SZFT	65
C10-3	49	x	x	N/A			x				Povetko	SZFT	66
C10-4	50	x	x	N/A			x				Povetko	SZFT	67
C10-5	51	x	x	x							Wittmeyer Scherer	SZFT	68
C11-1	52	x	x	x		S4 C16-1		x			Winfrey	DCAGW	69
11-1a	53	x	x			S4					LaPlante	DCAGW70	
11-1b	54	x	x			S4 C16-1					LaPlante	DCAGW	71

11-1c	55	x	x			S4 C16-1				LaPlante	DCAGW	72
C12-1		N/R									DELETED; FAULTO	73
C13-2	56	x	x	x	-					Winfrey	VOLCANO	74
C13-3	57	x	x	x						Winfrey	VOLCANO	75
C13-4	58	x	x	x			x			Winfrey	VOLCANO	76
C13-1	59	x	x	x			x			Smith	VOLCANO	77
C13-5	60	x	x				x			Smith	VOLCANO	78
C13-6	61	x	x				x			Smith	VOLCANO	79
C14-1	62	x	x	x	-		x			Winfrey	ASHPLUMO	80
C14-2	63	x	x	x	x		x			Rice; Mohanty	ASHPLUMO	81
C14-3	64	x	x	■						■ ■ ■ ■	■ ■ ■ ■	82
C14-4	65	x	x	■						■ ■ ■ ■	■ ■ ■ ■	83
C15-1	66	x	x	x			x			Smith	ASHRMOVO	84
C15-2		N/R	-	-							DELAYED until phase 3; ASHRMOVO	85
C16-1	67	x	x	x		C11-1b C11-1c			x	Winfrey	DCAGS	86
C16-2	68	x	x	x			x			Smith	DCAGS	87
C16-3	69	x	x				x			Smith	DCAGS	88
S1	70	x	x	x		C2-2, 3,4			x	Howard	FAILT	89
S2	71	x	x	x	x		x			Rice	RELEASET; EBSFILT	90
S3	72	x	x	■		C9-1, 2 C10-1				■ ■ ■ ■	■ ■ ■ ■	91
S4	73	x	x	N/A		C11-1				LaPlante	GENTPA	92
S5		N/R	-	-		C-14				Smith	COVERED by C-14; ASHPLUME	93
S6	74	x	x	x		C6-1				Adams	MECHFAIL	94

S7	75	x	x	N/A	C4-1 C4-2					Pensado	DSFAILT	95
S8	76	x	x	x	x		x			Rice	SNLLHS	96

*1 files contained on CD to be attached to Validation Test Report Appendix (some are ref'd in SVTR, some aren't)

LEGEND	
	haven't checked yet; N/A
-	missing; no
x?	should be one, where is it?
x	present; yes
wip	work in progress
N/A	not applicable
N/R	not required

.m files are Mathematica packages
 .nb files are Mathematica 4.1 notebooks
 .xls files are Excel spreadsheets

Current Status: checked automatic output

accounted for or replaced missing SVTRs/CDs
 sent SVTRs found in emails, local drives, etc., to Ruth
 retested C10-1; all tests passed; redid SVTR
 modified .t/.t1 files: update tests; SVTP -> SVT; add missing
 SVTR sections to output; change calls to outputstring to
 outputstring4; insert print utilities where needed
 marked up changes in SVTRs
 looked for ARRAY tests in Rob's old work - floppy ARRAY subdirectory empty
 ARRAY should be automated test but nothing shows in tpa.out - find out why?
 latest array.f w/ formatting & includes not there in TPA 5.0p; will be added to TPA 5.0q
 made CDs for C3-1, C3-2, C3-5, C4-2, and C10-1
 made CDs from floppies for E1-3 and E1-4
 made text files of VT lines from tpa.out for automated validation tests
 to be inserted into Appendix for Validation Test Report
 made CD of auxiliary files for Appendix to Validation Test Report
 Ron is checking w/ McCartin about files/CDs for C14-3, C14-4, & S3
 added tpa.out to CD of auxiliary files for the Appendix

Remaining questions:

C7-2 - Will this one be included? left as failed? other? Will it affect the SVTR numbers?
 C14-3, C14-2,
 S7 - Assume no auxiliary files and no CDs needed for these

NOTES:

C3-1 SVTR contains note about obsolete values in ebsfail.inp
C10-1 SVTR contains note about method of interpolating width over fractured path

Also, merged changes to dcags with the automatic testing and formatting changes.

Met with Ron and discussed SCRs for TPA 5.0. Discussed what we would be doing in the next several weeks. Prioritized list of tasks:

- clean up uzft.f (comments, organization, dead code)
- merge my notes/lists about changes that could be or need to be made to TPA and send to Ron
- look at releaset.f and how it processes colloids (calculate # of WPs in drift after backfill, colloid calculation)
- work on user's guide
- code characterization (determine coverage, efficiency; run w/ means as well as mins and maxs)
- parallel/multithread processing
- validation test abort runs
- file handling/intermediate data handling (std. format, binary files?; look at flow throughout TPA - both ci and dose - create binary file(s) to hold data so could be modified at discrete points for test purposes - user could override data in files by setting flag in tpa.inp)
- restrict data handling (only sample parameters that are actually used)
- phase 3 validation testing (models used)

Took tpa.out from the automated validation runs that Ron did and made a file for each SVTR that used an automated test. Found 2 more files to modify that I had missed earlier: buildInputFiles.t and raneseis.t.

11-04-2003 - 11-05-2003 -

Finished my input to the Validation Test Report Appendix. See cscherer/validate/tpa50q/appendix for files made from tpa.out.

Sent my list of changes to Ron. My merged list in cscherer/potential_changes.

Modified uzft.f - removed unnecessary comments and dead code (also did some general code cleanup for readability). We will need to do this for all the code, and Ron wanted to see what a file would look like as well as estimate how long it would take. Gordon also wants to see the file.

11-06-2003 - 11-11-2003 -

Ron gave me SCR450 to look at.

Started 10-K and 100-K, 1024-realization runs. All 4 Disruptive Scenario flags turned on. Otherwise, the runs will be base case runs.

The 10-K, 1024-realization run completed with no errors. Results in cscherer/tpa50r/10-Krun.

Ron is merging his notes and lists about potential changes to TPA with mine.

SCR # 450: Andy Jank did the testing on this one. Although he passed it, he apparently noticed an error or anomaly of some kind. He sent Ron a tar file with the test plan and a spreadsheet. There is a README file that says to run subarea 5 on TPA5.0m. I did this, but found no error to speak of. Andy doesn't remember this one, so I reran some tests to confirm that everything is OK.

Ron gave me SCR # 472 for testing. Needs to be finished ASAP. Includes changes to dcags and ashrmovo. Was worked on by Michael Smith and Rob Rice. Created directory cscherer/scr472. Copied TPA 5.0r to scr472. Created subdirectory cscherer/scr472/tpa50o and copied TPA5.0o to it. Subdirectory tests are the "before" situation and will be used for comparison purposes.

Met w/ Ron about code cleanup. George, Brandi, and Nathan are also going to be working on this task. We need to go through the code and clear out dead code, comments that aren't needed anymore (about past changes to the code). We will try to get it all done (TPA and standalones, including *.i and *.h files) in 3-4 weeks. Finishing SCR #472 is my priority, however.

11-12-2003 -

SCR # 472: Got SCRs for 384 and 460, earlier SCRs regarding dcags and ashrmovo to look at. Talked with Michael Smith about what to look for in the testing.

Andy Jank is joining the code cleanup team. He will be taking over some of the files from me and George.

11-13-2003 -

The 1024-realization run at 100,000 years that I started last Friday finally finished overnight. It ran to completion with no errors. Ron wanted me to start another one changing the

WindDirection 180 degrees. Started it going this afternoon.

Met with Andy Jank and passed on some of my assigned files to him for cleanup.

Added all the *.t, *.t1, and *.t2 files as well as tpa.out to the CD containing the auxiliary files for the Appendix for the Validation Test Report. Gave it to Ruth.

SCR # 472: Made several runs of the code (using both version 5.0o and 5.0r). Need to add print statements to dcags and ashrmovo to print out the intermediate/new values for comparison and graphing.

11-14-2003 -

Finished cleanup on array.f Put array.f and uzft.f in cscherer/clean_checkin. Cleanup team met with Ron this afternoon. Also need to cleanup the ITYM source code (Andy).

SCR # 472: Ran more tests. Got tpa.inp from Michael that NRC used when they found the anomalies. Started looking at output/intermediate files: airpkdos.res, arpkds_c.res, and ashrmovo.rlt. Along with the output from print statements and tpa.out, should contain enough data for analysis.

11-17-2003 - 11-21-2003 -

Ron asked me to help Osvaldo with his review of the Validation Test Report. Osvaldo needed to reviewed three of SVTRs for accuracy and completeness. I selected 3 SVTRs and provided Osvaldo with the SVTRs, automatic test output or CDs for him to review. Selected E3-1, C1-1, and S2.

SCR # 472: Emailed and talked with Michael Smith to get the details of the tests worked out. (See email below.) Test runs include a system level test to compare output between the two versions and to look at output files. There are three functional level tests to look at inside workings of ashrmovo and dcags to ensure that the new code functions as planned. Subdirectories slt1, flt1a, flt1b, and flt1c in both scr472 and scr472/tpa50o. Made spreadsheet for functional tests called scr472.xls. Graphed ash deposit against the 1-yr time steps that Rob added. All tests passed. Finished test plan and made CD. Turned in to Ron for shipping either late Friday or early Monday, Nov. 24th.

*From: Michael A. Smith [masmith@cnwra.swri.edu]
Sent: Tuesday, November 18, 2003 4:59 PM
To: 'Carol Scherer'
Subject: RE: SCR #472*

*Carol,
The large doses were seen in TPA5.0o file airpkdos.res. These large doses*

were correlated with initial small ash deposits as reported in both (take your pick) TPA5.0o file ashout.res as ashdensg/cm² or TPA5.0o file ashplume.out as xash(g/cm²). For example, a realization with a dose of 2.7164e12 rem/yr had an initial very small areal ash density of 3.2040e-10 g/cm². This correlation between initial small ash deposit and subsequent high dose was in error and should no longer be evident.

Thanks,
--Mike

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

From: Carol Scherer [mailto:cscherer@cnwra.swri.edu]
Sent: Tuesday, November 18, 2003 3:28 PM
To: masmith@cnwra.swri.edu
Subject: RE: SCR #472

See #1 below. Exactly, what file or result were you looking at when you found the 5 examples you talked about?

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

From: Michael A. Smith [mailto:masmith@cnwra.swri.edu]
Sent: Wednesday, November 12, 2003 5:36 PM
To: 'Carol Scherer'
Subject: RE: SCR #472

Carol,

Some background: The history involves the introduction of (SCR384) and subsequent fixes (SCRs 460, 472) for the ash redistribution model in TPA 5.0. The current testing is for SCR472. The ash redistribution model tracks the thickness over time of contaminated volcanic ash following an eruption and the concentration of radionuclides. The ash thickness changes over time due to redistribution by wind and water erosion and the radionuclide concentration changes due to radioactive decay and leaching; and with the introduction of clean ash/dust from distant sources. The ash redistribution model was added in October 2002 with the first version of TPA 5.0. In August 2003, following the validation testing, the NRC discovered a problem with the code.

The problem was that if the initial ash deposit was very thin or zero, subsequent doses would rise above 10e12 rem. The problem was that some of the time-dependent updates made in ASHRMOVO for the ash redistribution model were not carried through to calculations being performed in DCAGS. Mainly that an initially very thin ash deposit was maintained in the denominator of some later calculations, even though it increased in some cases over time with the ash redistribution (blowing the dose results up to 10e12 rem).

The high dose problem was easily corrected (updating DCAGS calculations to be time dependent), however, additional problems were discovered: divide by zero error in ASHRMOVO, array out of bounds error in INVENT, and peak dose not being captured (especially if volcanic event occurs in later years). The last problem occurs because most of the ash redistribution occurs within a short period of time (<100 years) and in late years (approaching 10,000 years) the TPA time steps are spaced further apart (too far to capture what

is happening with ash redistribution). As initially programmed, the ash thickness at the time of the volcanic event would drop to zero at the next TPA time step, making the initial ash thickness lead to the peak dose. With finer time resolution, the ash thickness usually rises slightly for a few steps following the event and then begins to decay away. The fix was to make a series of calculations with smaller time steps to find the actual peak ash thickness and time and then use that peak value at the previous available TPA time step.

Am I confusing things?

For testing, I would suggest the following and any other tests that you feel appropriate. Depending on how much time you were given to complete these tests, I believe it would be appropriate to conduct other general tests that you see fit, even if they cover areas of SCR384 and SCR460. Please pass on any test ideas that you may have. Implementation of the ash redistribution model was done on a short schedule, so additional tests would not be a waste of time. The 4 tests recommended below focus on SCR472.

1. Verify that TPA no longer produces exceedingly large doses. This was discovered by NRC when they sampled the volcanic event wind direction in tpa.inp (WindDirection[degrees]) from 0 to 180 degrees, instead of the default constant of -90 degrees. I was able to duplicate the NRC results in a 100 realization run, with 5 realizations greater than 10e8 rem (1 over 10e12 rem). It would be reasonable to have a peak dose around 10e2 to 10e4 rem. To speed things up, you can do these TPA runs without the groundwater pathway (DirectReleaseOnlyFlag(yes=1,no=0)).

2. Verify that there are no divide by zero errors and out-of-bounds arrays. This occurred when initial ash deposit thickness were zero and approached zero. This also occurred only when the wind direction was sampled between 0 and 180 degrees. You may be able to test for this as a part of #1 above. When we talked earlier I noted that the ipeak value in DCAGS might have been removed. This is true, but I noticed that it was added to ASHRMOVO, so ipeak is still in TPA (just not in DCAGS).

3. Verify that the loop in ASHRMOVO using 1-year time steps to calculate peak value and time for amassash() and other parameters is working properly and that the peak value is used in place of the TPA value at the previous available TPA time step.

4. Verify, qualitatively, that the dose curve in early TPA times (when time steps are smaller) rises following the initial volcanic event before decaying. Set the time of volcanic event at an early TPA time, say 100 years (TimeOfNextVolcanicEventinRegionOfInterest[yr]).

There are 19 parameters (the last 19 in ASHRMOVO section of tpa.inp) directly related to the ash redistribution model beginning with:
FractionOfQuicklyRedistributableAshMobilizedEachYear
and ending with:
DepositionRateOfSoilFromLongRangeSources[g/m2/yr]

Well, I got sidetracked doing a technical review, so didn't put as much detail as I had hoped. Let me know if you have any specific questions that I can help with. Maybe tracking down, as you mentioned, what output files that you will need to take a look at.

Thanks,
--Mike

Email stored in scr470/docs as Msmith_email.txt. Docs also contains scr472.wpd and tp_scr472 as well as a planning document from Rob Rice called DCAGS_ASRMOVO_proposed_changes_tpa5.0_b.doc.

100,000 year run w/ +90 WindDirection: Ran to completion.

100,000 year run w/o change in Winddirection: started this run again; files were accidentally overwritten. Should finish running early next week.

11-23-2003 - 11-29-2003 -

Working on SCR477:

From: ron janetzke [rjanetzke@cnwra.swri.edu]
Sent: Saturday, November 22, 2003 10:48 PM
To: Carol Scherer
Subject: SCRs

Carol,

Create and implement SCR 477 with these items:

- 1) Test the time-of-next-volcanic-event against the max simulation time. If it is a constant test the constant value, if it is sampled test both the min and max and give error message if equal.
- 2) Remove *DistanceCutoffForDoseConversionDualityInDCAGS*[km] if it is not used.
- 3) Correct the duplicate name error message in /reader/invent /where the line number of the nuclide is off by one.
- 4) Add checks for divide by 0 in /ebsrel/gsanwpglass/ for the 3 sampled parameters *WastePackagePayload*, *FractionOfRepositoryWasetInGlassForm* and *EquivalentMTUPayloadOfGlassPackage*.

You should use the 'checkin pending' versions of the files since I hope to put in /invent /and /dcags /before SCR477 when I return.

thanks,

ron j

Problem encountered trying to use the checkin pending version of invent.f. Ron made changes to invent.f to make Eric's automated test files work. But now invent.f in version r won't compile with my automated test files. Also, Eric's test files still contain implicit statements. Merged current version of invent with checkin pending one. Did cleanup. Added implicit none

and declarations to Eric's test files.

Searched for code containing the parameters mentioned in email above to see where changes needed to be made.

Made CD of 1024-realization runs. First CD contains 10-Krun and 100-Krun. Will need to do another yet to store 100K_wind+90 run.

12-1-2003 - 12-5-2003

On-hold: code cleanup version r, and SCR477. Right now, we need to do code cleanup on version 4.1jpd.

Worked on generating questionnaires on the tpa.inp parameters for Sitakanta. Learned how to use WordPerfect merge. Made .frm & .dat files to generate questionnaires designed by Bruce Goodwin. Started updating appA (from the User's Guide) using tpa.inp from TPA5.0r. Generated and distributed questionnaires for sampled parameters.

Worked on questionnaires for data files, currently covered in Apps. B, G, and H. Sent Bruce Goodwin an example of the PDF questionnaire, he will be sending me a questionnaire for data files. Sent him new data files or 1st pages of big files so he can make the data file questionnaire.

Made CD of last 1024-realization run.

Read sections of the Version 1 Performance Assessment report, including: Morris Method, Marty's directions and CH 4.

12-8-2003 - 12-12-2003 -

Constants questionnaires: Ron & Gordon helped me assign them to the correct expert. Updated constants.dat, consolidate multiple parameters to single questionnaire, printed and distributed questionnaires.

Finished merging invent.f and dcags.f for Ron to put into next version of software.

Working with Bruce Goodwin (consultant from Canada) via email.

12-15-2003 - 12-20-2003 -

Worked on data file questionnaires w/ Ron to assign them to the correct people. Then, printed and distributed them. Generated the missing constants questionnaires. Questionnaires for

the .def files are on hold until further research can be done into what data are not overwritten by code. If there isn't time, these won't be done.

Continued work on scr477.

12-21-2003 - 1-02-2004 -

Spock was down Jan. 2.

Questionnaires: mailed photocopies of returned questionnaires to Bruce Goodwin. Reassigned some questionnaires to different people and redistributed them. Asked Bruce to work on correlateinputs questionnaire.

1-5-2004 - 1-30-2004 -

Burned CD with 1024-realization ,100K_wind+90 run.

Spock down 1/5, 1/6 a.m., and most of 1/7 p.m. Up again 1/8.

Worked on SCR477.

Generated and distributed the correlated inputs questionnaire. Generated and distributed the reversible questionnaires - 81 questionnaires for David Pickett. Sorted the returned questionnaires and updated questionnaires2.xls.

Worked with Tom Glass on the preprocessor task. He needed help updating the supporting data files with the changes made to TPA between version 4.1j and version 5.0r.

Updated tpa_changes2.wpd.

Sitakanta's student, Juan Portillo, started this week, and he will be taking over the questionnaire task. Spent time bringing him up to speed and passed files related to the questionnaires to him.

February 2, 2004 - February 27, 2004 -

Continued working with Tom Glass on the preprocessor task.

Continued to help Juan on the questionnaires. David Pickett reminded us that we hadn't taken care of the parameters in reversibles.inp that are different from basecase tpa.inp. Generated 81 more questionnaires and delivered to David.

Reviewing the Sensitivity Analysis, version 1 document to learn how to generate the data and graphs in Chapters 3 & 4.

March 1, 2004 - March 26, 2004 -

Ron gave me a PC version of the TPA code. Ran it to test that it ran OK on the PC.

Continued working on SCR #477 whenever other tasks don't take me away from it. Merged in the cleaned up versions of invent.f and dcags.f, which hadn't made it into the new version of TPA yet. Working on automated tests for the new subroutines.

Continued helping Juan with questionnaires.

More review of the Sensitivity Analysis document.

March 29, 2004 - April 2, 2004 -

Proofread TPA Sensitivity Analysis changes for version 2. Returned markups to Ruth.

Finished SCR477 test plan/report. Made CD and gave to Ron.

April 12, 2004 - April 16, 2004 -

Looked at Version 2 of the Sensitivity Analysis again. Working on ensuring that changes are getting into the final product.

Started working on SCR # 470, using TPA 5.0s. Also reviewing a memo from Keith Compton regarding the cleaned up version of TPA. There are still some sections of code that may need changes in comments or headers added, etc.

April 19, 2004 - April 23, 2004 -

Continued working on SCR#470, adding tpamin.out and tpamax.out files (similar to tpameans.out). Analyzed reader.f and identified additions that need to be made to the code. Continued reviewing Compton memo.

April 26, 2004 - April 30, 2004 -

Completed review of Compton memo and send summary to Ron. Modified reader.f for SCR # 470. While testing the new tpamin.out and tpamax.out, ran into two small bugs in the code.

May 3, 2004 - May 7, 2004 -

Finished SCR# 477 changes requested by Ron and updated the SCR document and the test plan/report. Burned new CD of test directories; turned it in to Ron.

Finished modifications for SCR#470. Started on the test plan/report. Generated SCR# 485 for the bugs discovered while testing tpamin.out and tpamax.out..

May 10, 2004 - May 14, 2004 -

Analyzed the bugs in SCR# 485. The bug uncovered by running tpamax.out as tpa.inp was due to a conditional statement in releaset.f that compared WP fill start and stop times when it should have used the bathflow flag. Running tpamin.out as tpa.inp uncovered a bug in exec.f where there needed to be a check of values used in the denominator of a divide statement to prevent a divide by zero. Made the changes and turned the SCR and modified code into Ron. Also made a test plan and burned a CD for Ron until someone else can test the fix.

Started working on SCR#486, an SCR generated by B. Ibrahim about a step increase in total dose at the last time step of a run. Ron made code modifications to correct the problem and I'm going to test his changes.

May 17, 2004 - May 21, 2004 -

Continued with SCR# 486. Making 300-realization runs with the base case (TPA 5.0t) before changes were made and with the modified code (TPA5.0u). Created Excel spreadsheets to compare. Worked out a filter with Ron to determine what percentage of runs showed a step increase at the last time step for both versions of the code.

Spent some time helping Zbigniew Wojcik come up to speed with TPA while Ron was in a training seminar.

Met with Ron, Al Lozano, and Zbigniew Wojcik (a new consultant working on changes to near field specified by Osvaldo. He is going to turn nfenv into two routines. Al is working with George Adams on mechfail, which will also become two routines. We discussed the current effort of completing SCRs and getting version 5.0.1 ready for delivery to NRC. I will be doing testing of the code modifications.

May 24, 2004 - May 28, 2004 -

Finished SCR# 486 testing, updated SCR, generated test plan/report and made CD. All turned in to Ron Janetzke for his files. In subdirectory *scr486*.

Helped Zbigniew with TPA and Juan with getting information about changes to TPA between 4.1j and 5.0u so he could work on Appendix A for the User's Guide and a sensitivity report for Sitakanta.

June 1, 2004 - June 4, 2004 -

Made modifications requested by Ron Janetzke to the test plan/report for SCR #486 and burned a new CD.

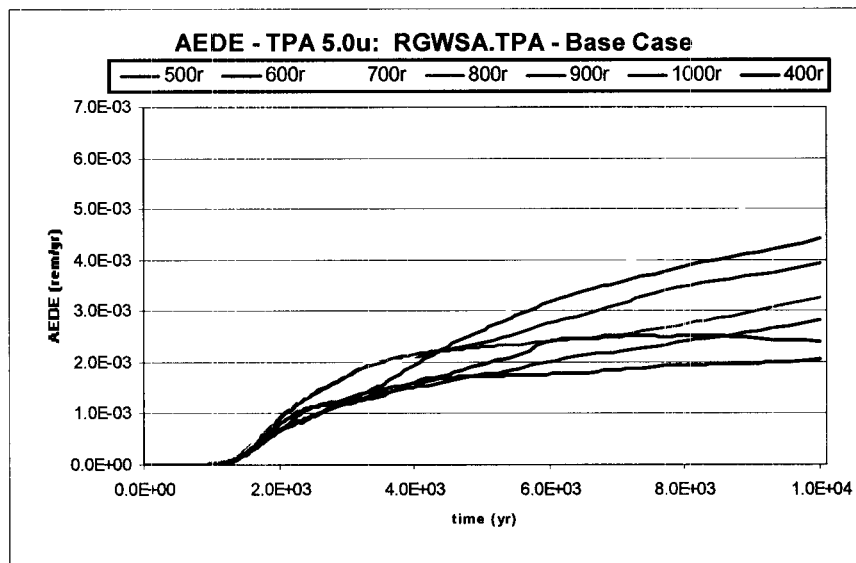
COMPRESS & ARCHIVE FILES & DIRECTORIES: (UNIX NOTES). Space on spock was getting low, so I compressed files in directories from older tasks. These are now stored in subdirectory *tarbzip_files*. Cleared up 2 - 3 % of space, but need some of the larger users to archive files, too. Used the following commands to 1) make a tar file of a directory and 2) zip the tar file to compress the data and clear up space. Still need to burn compressed files onto a CD.

- 1) tar cvf <directoryname.tar> <directoryname>
- 2) bzip2 <directoryname.tar>

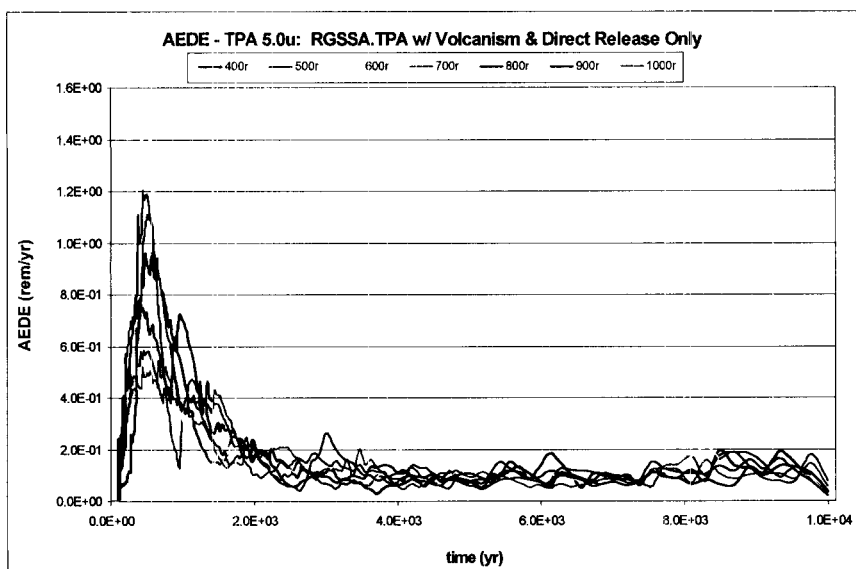
Brett Dobbs is now working with Tom Glass on the TPA preprocessor. Sitakanta had Brett load the newest preprocessor software onto my PC and Juan's, so we can help test it. The preprocessor requires that the PC have JAVA version 1.4, at least. LAUNCH isn't working as expected on my PC. Brett is analyzing the problem.

Created directory *testTPA2004* to perform tests on **TPA 5.0u**. Created subdirectory *basecase* and subdirectory *volcano_dro* to test for convergence on runs of varying numbers of realizations. Basecase runs were run on the basecase tpa.inp. One run was made at 400, 500, 600, 700, 800, 900, and 1000 realizations. In the case of volcano_dro, the basecase tpa.inp was modified to turn on VolcanismDisruptiveScenario and DirectReleaseOnly was set to 1. The same number of runs at the same number of realizations were run. Excel spreadsheets were created from rgssa.tpa and rgwsa.tpa, which contain Annual Effective Dose Equivalent (AEDE) values summed over all nuclides and averaged over all realizations. The runs were plotted (see below); graphs and data were saved in files */net/spock/home/cscherer/testTPA2004/basecase/rgwsa_allr.xls* and */net/spock/home/cscherer/testTPA2004/volcano_dro/rgssa_allr.xls*. There appears to be convergence, but it doesn't show up well in the way I graphed the data. Ron will come up with other tests that might show the information better.

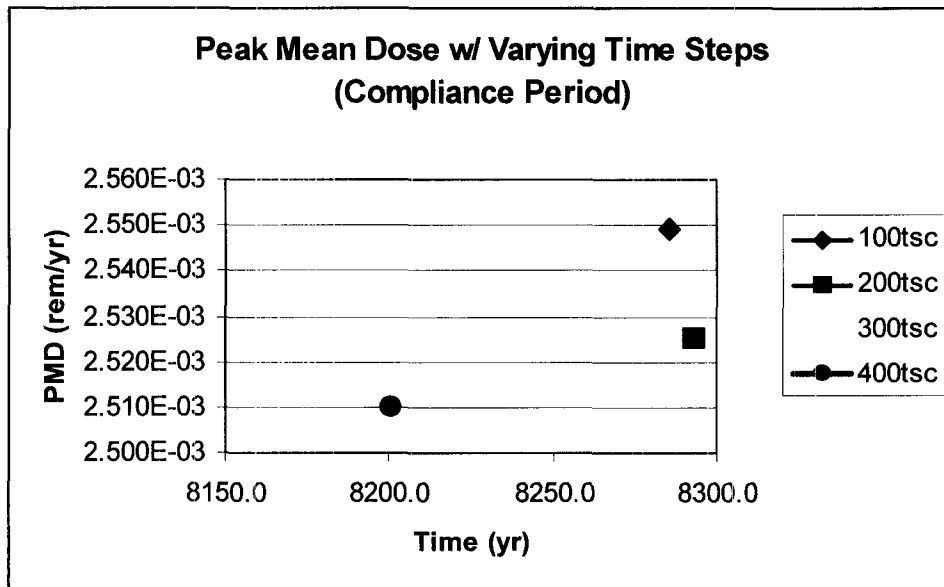
The 1000-realization run of the volcano/direct release scenario generated some "NaN" values in several files (totdose.res, totds_c.res, rgssa.tpa, rgssr.tpa, rgsnr.tpa, rgsna.tpa, gmedia.out, genv.out, gs_cb_ad.dat, gs_cb_ci.dat, gs_pb_ad.dat, and gs_pb_ci.dat). Determined that it was realization 668 where the trouble occurred. I've asked Ron to run the tpa.inp with the debugger, to help us determine where the problem occurs.



convergence diagram

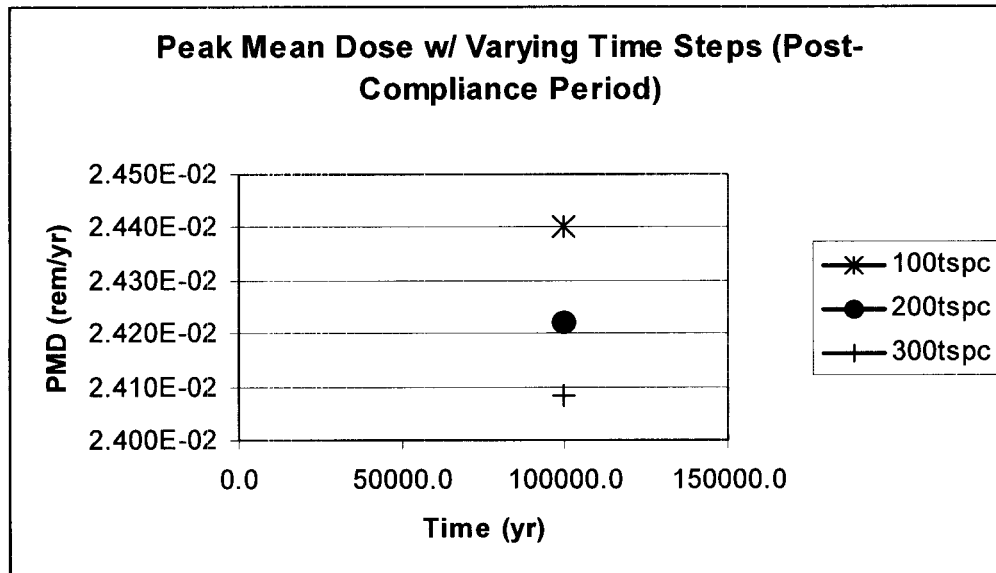
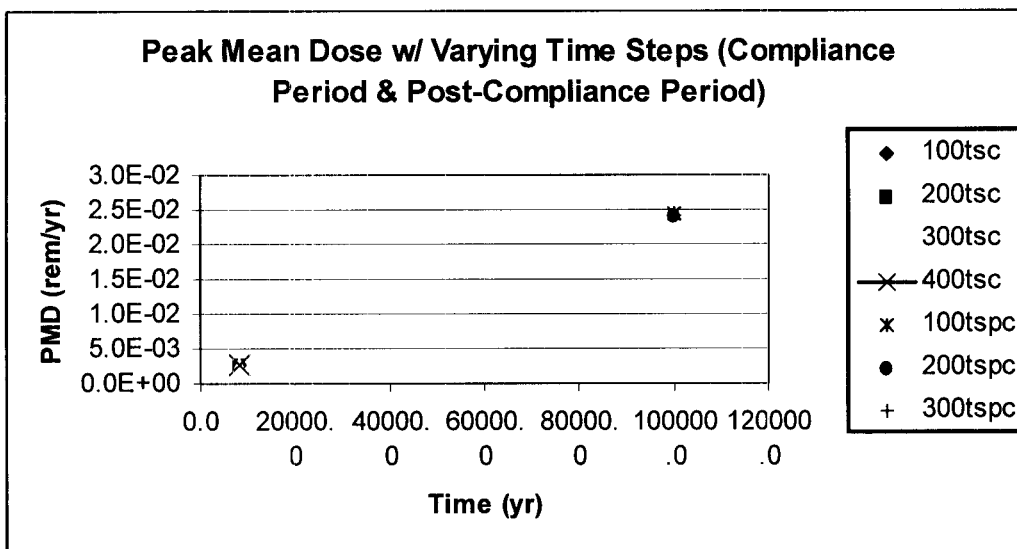


convergence diagram



June 7, 2004 -

Started runs Friday that completed over the weekend for time step tests. The first set, 400 realizations at 10,000 years, varied NumberOfTimeStepsInCompliancePeriod with runs at 101, 201, 301, and 401 time steps. NumberOfTimeStepsAfterCompliancePeriod was set to 0 in all 4 runs. The second set, 400 realizations at 100,000 years, varied NumberOfTimeStepsAfterCompliancePeriod with runs at 100, 200, and 300 time steps. NumberOfTimeStepsInCompliancePeriod was set to 101 for all 3 runs. The output from the runs is stored in */net/spock/home/cscherer/testTPA2004/timesteps10K* and */net/spock/home/cscherer/testTPA2004/timesteps100K*. An Excel spreadsheet, *pmd_timesteps.xls* was created to list the Peak Mean Doses (PMDs) of each run and the times at which the PMDs occurred. These were graphed.



These graphs show convergence better.

Brett came over with another upgrade for the preprocessor LAUNCH software. Still having trouble getting tpa.exe to run via the LAUNCH button even though tpa.exe will run if I execute it from a dos window. Also having trouble LAUNCHing on Juan's PC. There may be a memory (RAM) problem with Juan's PC. His problem looks different than mine.

June 8, 2004 - June 18, 2004

The preprocessor doesn't run on Tom Glass' PC either; it has the same problem as Juan's. It will run on Brett's PC, however; he is looking into the problem.

Started working on tests based on repository geometry. Ron wants several runs where one subarea is divided into finer pieces. Ran time steps tests in repository geometry tests. The first set, 400 realizations at 10,000 years, varied NumberOfTimeStepsInCompliancePeriod with runs at 101, 201, 301, and 401 time steps. NumberOfTimeStepsAfterCompliancePeriod was set to 0 in all 4 runs. The second set, 400 realizations at 100,000 years, varied NumberOfTimeStepsAfterCompliancePeriod with runs at 100, 200, and 300 time steps. NumberOfTimeStepsInCompliancePeriod was set to 101 for all 3 runs. These runs showed convergence better.

Worked on excel spreadsheet to determine proper coordinates for subarea 2 divided into 4, 8, and 16 smaller subareas. Started making test runs (subarea 2 as 1, 4, 8, or 16 subareas, 10K and 100K years, 400 realizations).

Started work on scr487 (divide by zero and listing of NaN in output files), but it was put on hold pending resolution of a related problem when glass fraction is set to a value besides zero. This one is similar to the problem identified when the tpamin.out and tpamax.out were used as tpa.inp files.

Ran test runs for Ron to look at wpsfail.res for versions 4.1j and 5.0u. Buck Ibrahim had reported that failed WPs (by seismic activity) that appeared in 4.1j did not show up with 5.0u. My runs showed no difference, but showed no WPs failed by seismic events at all. Apparently, this is the way the code is structured now.

June 21, 2004 - July 2, 2004 -

Working on more test runs for subarea repository geometry. The longer runs are taking several days to complete. One long run didn't finish - an Invalid Operation occurred and the run aborted in NEFTRAN. Since I don't have the debugger, I'll need to work with Ron to find out where the Invalid Operation (likely a divide by zero) occurred. I'm checking now to see if smaller subareas created from a single previous subarea result in the same processing path (e.g., are the same streamtubes selected? - see streamtubes.xls). [NOTE: to determine which streamtube is selected, run 1 subarea at a time for one realization; look at nefii.inp (2nd leg) and

distance between first two nearfield streamtube coordinates] I'm also comparing temperatures calculated in smaller subareas against one larger subarea. Runs are stored in cscherer/testTPA2004/rep_geom.

Brett Dobbs came by with more fixes for LAUNCH in the TPA preprocessor. They've been able to get it to work on everything except machines running NT - like mine.

Helped Zbigniew Wojcik understand what was going on in the code for scr487 and SCR485. Zbigniew was testing them for Ron.

Finished runs for Buck Ibrahim's reported problem with WPs. Graphs of the results of runs showed what looked like outlier points at the tail of the graphs, but they were actually correct, the values leading up to the points were incorrect; colloid values hadn't been added back in yet. Ron corrected the problem.

The repository geometry testing has been put on hold. Ron wants me to implement the changes for SCR # 484 (change mechanism for calculating reversible colloids). Met with Ron and Scott Painter. Changes are required to tpa.inp, uzft.f, szft.f and nefmks.f. Scott provided a writeup of the required changes - see scr_488.wpd in cscherer/scr488/docs on Spock.

July 6, 2004 - July 16, 2004 -

Continued working on SCR484. Deleted 8 parameters from tpa.inp and added 41 new ones. Met with Scott to determine initial values for the new parameters. Added routine to uzft.f (mod_kd) to modify KD/RD values (excepting those calculated by David Turner's method, the actinides Am, Np, Pu, Th, and U). This routine will approximate the effects the presence of reversible colloids has on release and dose. Started on new routine for szft.f (mod_rdrdi). Scott has already made the necessary changes to NEFMKS. After talking to Scott, he modified the algorithm for fracture Rds.

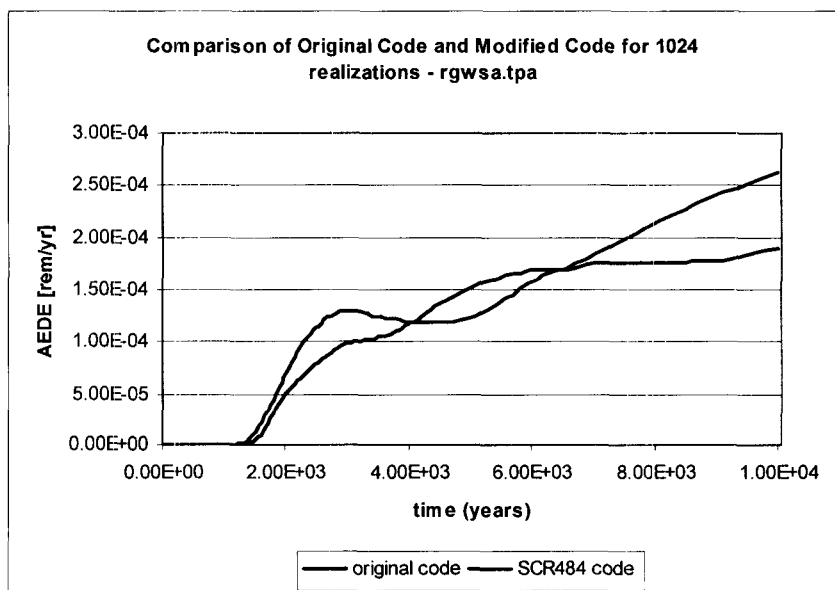
Also made several TPA runs for Scott Painter and Alex Sun to establish the dispersivity range for uzft.f (see cscherer/dispersivity_range) on Spock. Three initial runs vary FractureLongitudinal DispersivityFraction[FractionOfLayer]. After Alex and Scott have a chance to look at the results, they'll let me know what other data they need to look at.

Met with Ron, Zbigniew, and Al Lozano to discuss status of current changes and testing. Working toward TPA5.0.1 release.

July 19, 2004 - July 30, 2004 -

Finished code changes for SCR484 and started debug and testing. Scott made more

algorithm changes. He will update his original document to attach to the scr_488.wpd. Made a spreadsheet (cscherer/scr488/AEDEsr.xls) to check Excel calculations against programmatic results. Graphed results from rgwsa.tpa. Added more new parameters and deleted obsolete ones from tpa.inp (see scr_488.wpd for a list).



Worked on updating scr_488.wpd and updating the Kd/Rd calculation table (created when Turner's calculations were added to the code) for Ron. Scott still needs to review the results to see if the results are accurate. Scott provided update to his original algorithm for attachment to the SCR.

Attachment A

COLLOID-FACILITATED TRANSPORT: EQUILIBRIUM SORPTION ON COLLOIDS

For that part of the heterogeneous colloid population with rapid desorption rates relative to the transport time scale, equilibrium partitioning of radionuclides among solution, colloids, and porous matrix is an adequate approximation. The effect of those colloids can be modeled using the single-component advection dispersion equation with appropriately defined transport parameters.

For the alluvium, colloid-facilitated transport has the net effect of reducing the effective retardation factor. Neglecting colloid filtration and defining a new coefficient K_0 for partitioning between colloids and solution, the advection dispersion equation becomes

$$R^{eff} \frac{\partial C}{\partial t} + \mathcal{I} C = - \lambda R^{eff} C \quad (1)$$

where T is the transport operator and

$$R^{eff} = \frac{R + K_0 R_c}{1 + K_0} \quad (2)$$

is the new effective retardation that takes into account the effects of colloids. Similarly, the equations describing transport in the fractured tuff become

$$R_f \frac{\partial C}{\partial t} + \mathcal{T} C = -\beta_0^{eff} (\omega C - C') - \lambda R_f C \quad (3)$$

$$R_s^{eff} \frac{\partial C'}{\partial t} = \beta_0^{eff} (\omega C - C') - \lambda R_s^{eff} C' \quad (4)$$

where

$$R_s^{eff} = \frac{R_s}{1 + K_0} \quad (5)$$

$$\beta_0^{eff} = \frac{\beta_0}{1 + K_0} \quad (6)$$

and

$$R_f = \frac{1 + R_c K_0}{1 + K_0} \quad (7)$$

Thus, equilibrium partitioning to colloids reduces the mass exchange coefficient and the immobile retardation factor, with the net effect of reducing matrix diffusion. In addition, retardation in the fractures is introduced, with retardation coefficient given by Eq. (7).

Equation 1 is in the form used by NEFTRAN in the fractured alluvium and in each of the fracture and matrix continua in the unsaturated zone. Equations 3 and 4 are in the form used by NEFTRAN in the saturated tuff. The net effect of reversible sorption to colloids is simply to modify the transport parameters.

The parameter K_0 in the equations is a dimensionless partitioning coefficient for radionuclides on colloids. Pickett and Dam (2003) following Contardi et al. (2001) write

$$K_0 = C F K_d \quad (8)$$

where C is the colloid concentration in water, F is a dimensionless factor accounting for surface area differences between matrix and colloid (equal to 590; Contardi et al. 2001), and K_d is the distribution coefficient for radionuclides on the porous matrix.

The required modifications are as follows:

(1) The colloid concentration C and the colloid retardation factor R_c should be made input parameters. Different values for each hydrostratigraphic unit are required. For the unsaturated zone, separate matrix and fracture values are needed.

(2) After the current calculation of the K_d for each unit, the new parameters defined by equations 2 and 5-8 should be calculated. Equation 2 with 8 applies to the alluvium, and to the unsaturated zone. Equations 5-8 applies to the saturated tuff.

(3) The new retardation values should be written to the NEFTRAN input file. R^{eff} defined by Equation 2 simply replaces the current retardation factor written to NEFTRAN. The same is true for the parameters defined in Equations (5) and (7). These are the element- and unit-specific values of retardation used in NEFTRAN.

(4) Element specific values of the mass transfer coefficient are not currently allowed in NEFTRAN. The parameter b_0 should be written to the NEFTRAN as before, and a new element-specific mass-transfer

modification factor $\frac{1}{1 + K_0}$ should be written to the NEFTRAN input file. This modification factor is

element- and unit-specific. It should be written as a new field at the end of the input line for the element- and unit-specific retardation factors.

(5) NEFTRAN should be revised to read the new mass-transfer modification factor. The modification factor should be used in the mass-transfer calculation in NEFTRAN.

Colloids with irreversibly attached radionuclides

(6) For the fraction of radionuclides that are attached irreversibly to colloids, the new colloid retardation factor R_c should be used as the retardation factor. The separate input for retardation factors is not needed for these species and can be removed. However, the filtration factors and the irreversible fraction should still be read.

Matrix							
Unsaturated Zone				Saturated Zone (Alluvium)			
Quantity	Symbol	Units	Source	Quantity	Symbol	Units	Source
matrix porosity	Φ	-	sampled	matrix porosity	Φ	-	sampled
matrix grain density	ρ	kg/m ³	sampled	matrix grain density	ρ	kg/m ³	sampled
matrix pore radius	r	m	sampled	matrix pore radius	r	m	sampled
specific surface area	ssa	m ² /kg	$= \frac{3 \Phi}{\rho r}$	specific surface area	ssa	m ² /kg	$= \frac{3 \Phi}{\rho r}$
K _a	K _a	mL/m ²	table lookup	K _a	K _a	mL/m ²	table lookup
K _d	K _d	m ³ /kg	$= K_a \text{ ssa } (10^{-6} \frac{\text{m}^3}{\text{mL}})$; or sampled	K _d	K _d	m ³ /kg	$= K_a \text{ ssa } (10^{-6} \frac{\text{m}^3}{\text{mL}})$
				moisture content	n	kg/m ³	1
				mobile Rd immobile Rd	R _{d,m} R _{d,i}	m ³ /kg	$= 1 + \frac{\rho(1-\Phi)}{n} K_d$; or sampled
modify Rd to approximate effect of reversibles:							
colloid concentration	C _c	kg/m ³	sampled	colloid concentration	C _c	kg/m ³	sampled
surface area factor	F	-	590	surface area factor	F	-	590
colloid retardation factor	R _c	m ³ /kg	sampled	colloid retardation factor	R _c	m ³ /kg	sampled
radionuclide partitioning coefficient	K ₀	-	$= C_c \times F \times K_d$	radionuclide partitioning coefficient	K ₀	-	$= C_c \times F \times K_d$
effective retardation	R ^{eff}	m ³ /kg	$= (R_d + (K_0 \times R_c)) \div (1 + K_0)$	effective retardation mobile	R ^{eff} _m	m ³ /kg	$= (R_{d,m} + (K_0 \times R_c)) \div (1 + K_0)$
				effective retardation immobile	R ^{eff} _i	m ³ /kg	$= R_{d,i} \div (1.0d0 + K_0)$
mass transfer factor		-	0.0d0	mass transfer factor tuff		-	$= 1.0d0 \div (1.0d0 + K_0)$
				mass transfer factor alluvium		-	0.0d0

Fracture							
Unsaturated Zone				Saturated Zone (Tuff)			
Quantity	Symbol	Units	Source	Quantity	Symbol	Units	Source
specific surface area	ssa	m ² /kg	1	specific surface area	ssa	m ² /kg	1
K _a	K _a	mL/m ²	table lookup	K _a	K _a	mL/m ²	table lookup
K _d	K _d	m ³ /kg	$= K_a \text{ ssa } (10^{-6} \frac{\text{m}^3}{\text{mL}})$	K _d	K _d	m ³ /kg	$= K_a \text{ ssa } (10^{-6} \frac{\text{m}^3}{\text{mL}})$
fracture aperture	A	m	sampled	fracture aperture	A	m	sampled
R _d	R _d	m ³ /kg	$= 1 + \frac{2}{A} K_a$; or sampled	mobile RD immobile RD	R _{d_m} R _{d_i}	m ³ /kg	$= 1 + \frac{2}{A} K_a$; or sampled
modify R _d to approximate effect of reversibles:							
colloid concentration	C _c	kg/m ³	sampled	colloid concentration	C _c	kg/m ³	sampled
surface area factor	F	-	590	surface area factor	F	-	590
colloid retardation factor	R _c	m ³ /kg	sampled	colloid retardation factor	R _c	m ³ /kg	sampled
radionuclide partitioning coefficient	K ₀	-	$= 2.0d5 \times A \times C_c \times (R_d - 1.0d0)$	radionuclide partitioning coefficient	K ₀	-	$= C_c \times F \times K_d$
effective retardation	R ^{eff}	m ³ /kg	$= (R_d + (K_0 \times R_c)) \div (1.0d0 + K_0)$	effective retardation mobile	R ^{eff_m}	m ³ /kg	$= (R_{d_m} + (K_0 \times R_c)) \div (1 + K_0)$
				effective retardation immobile	R ^{eff_i}	m ³ /kg	1.0d0
mass transfer factor		-	0.0d0	mass transfer factor tuff		-	$= 1.0d0 \div (1.0d0 + K_0)$
				mass transfer factor alluvium		-	0.0d0

August 2, 2004 - August 13, 2004 -

Scott requested some changes to uzft.f and szft.f for SCR 484. Those were made. More changes may be required after Scott looks at results from these changes.

Met with Michael Muller. He will be doing the testing for SCR 484. Michael will also be testing SCR 489, changes made by Zbigniew to uzft.f and szft.f. Ron wants us to integrate our code changes.

Reviewed validation test plan/results to see what changes are needed due to these SCRs.

We are getting a lot of aborted TPA runs (NEFMKS aborting due to array out of bounds - the same old error we get when runs get too complex for NEFMKS to handle). Ron, Scott, Michael & I are looking for a solution or a workaround for the problem. Received new basecase parameter values for the new sampled parameters for SCR 484.

August 16, 2004 - August 27, 2004 -

Helped Juan with his questionnaire task and Michael with testing SCR484.

Scott identified another problem with the modified code. Came in on Saturday to debug and correct the problem. Also merged my modifications with Zbigniew's.

Updated the documentation for SCR 484 and turned it in to Ron.

Started working on the test plan for SCR 488 - code changes to nfenv.f and uzflow.f as well as data changes to tpa.inp (2 new parameters that used to be hardcoded in uzflow.f) and climato2.dat. Ran initial test run to compare results of modified code to previous code. Will show results to Randy Fedors for his opinion.

August 30, 2004 - September 17, 2004 -

SCR484 completed and turned in. Michael says tests are passing except for the NEFTRAN abort problem.

SCR 488: Re-ran basecase tests for TPA5.0x and TPA5.0y, using the corrections indicated in Ron's email:

*From: Ron Janetzke [rjanetzke@cnwra.swri.edu]
Sent: Tuesday, September 07, 2004 7:43 PM
To: carol; marty menchaca; M muller; alozano@swri.edu
Subject: TPA error
All,*

An error has been found in the data files for TPA versions 5.0w,x,y. If you are having trouble with any of the test results for SCRs 483, 476, 478, 480, 481, or 488, make the following modifications.

FILE: data/nuclides.dat

Set base year to 2008.

FILE: data/burnup.dat

Set base year to 2008.

FILE: tpa.inp

Set CalendarYearOfEmplacement to 2033.

Let me know if this affects any of our tests.

thanks,

ron j

Used the tpeans.out from the basecase runs for TPA5.0x and TPA5.0y as tpa.inp for each version. Modified the mean value tpa.inp for subsequent runs.

Ron has come up with a modification to uzft.f that looks like it will fix the NEFTRAN abort problem. He showed it to Tim McCartin and Tim has agreed with it. This change will be made in SCR # 518, an SCR that will update some parameter names, change gwtmin from 10.0 to 20.0 (Ron's fix), correct an error in burnup.dat that affects the results for SCR488. Once implemented, will need to rerun the test for SCR 488 again. SCR 518 also corrects a couple of compile warnings and removes two divides by 100.0 in nfenv.f that caused errors in the values for seepage threshold and repository temperature written out to nfenv.rlt. Made all changes. SCR 518 is complete unless more "cleanup" items come up. Turned changed files and scr_518 (on Guardian PC: d:\css\tparun\scr518\docs).

Sitakanta wants us to move development and testing work over to the PC. One problem is that Guardian doesn't have the latest version of Lahey FORTRAN so the make file doesn't work. I'll either have to compile on a PC in the GIS lab or at home if I do development on the PC.

Made 3 runs varying GroundSurfaceTemperature from 17.38 to 10.0, 15.0, and 20.0. Randy Fedors says a realistic range would be from 10.0 to 17.38. Also, made two runs varying CurrentAnnualPrecipitation from 162.8 to 100.0 and 200.0. However, itym used the default temperature (17.38) and precipitation (162.8) when it was executed to generate the smaydtbl.dat, maidtbl.dat, and maydtbl.dat files. If we really wanted to get accurate results from varying GroundSurfaceTemperature, Randy says we should regenerate those data files for each temperature value of interest. Same for Current Annual Precipitation. However, at this point, we just want to see the general trends of varying the input parameters on the results, so the existing files are adequate. Made one run varying FactorForVentilationHeatloss from .7 to .86. Made one run changing CalendarYearOfEmplacement from 2033 to 2034. Made one run with TPA5.0y executable but using the TPA5.0x version of climato2.dat.

Graphed the results of the runs from infilper.res and ebsfail.ech in spreadsheets ebsfail_ech.xls and infilper_res.xls. Results are reported in the test plan/report tp_scr488.wpd. All tests passed. It might be a good idea to look at why we get the first spike in the relhumwp graph from relhumwp results in ebsfail.ech. This existed before the current changes were made, so is out of scope of this test plan. Randy also suggested that it might be a good idea to revisit the values generated from itym sometime just to confirm the values or possibly to generate a set of files for other temperatures or precipitations.

Documentation for SCR # 488 is stored on Guardian (d:\css\tparun\scr488\ in the files scr_488.wpd and tp_scr488.wpd). All earlier questions were resolved. Copies of the spreadsheets (ebsfail_ech.xls and infilper_res.xls) were sent to Randy Fedors for him to look at one more time.

September 20, 2004 - September 21, 2004 -

Turned in paperwork for SCR488 and CD to Ron Janetzke 9/20/04. Although, after I did that, Randy looked at the results and he has a couple of more concerns which I passed on to Ron. Randy thinks infiltration is too high and reflux too low and that the overall temperatures are

about 20 degrees too high.

Started work on SCR # 517. Testing changes to Kds/Rds made by Femi Osidele.

September 22, 2004 - September 30, 2004 -

Turned in Electronic Scientific Notebook for period ending September 17, 2004 to Ron Janetzke.

SCR#517: Ran basecase runs for TPA5.0z and TPA5.0.0a on the PC (Guardian). Results from runs are stored on Guardian - d:\css\tparun\scr517. Then, ran means case run for 5.0.0a. Starting with means case, ran additional runs varying the two new sampled parameters. Ran with AlluviumTotalPorosity_SAV set to 0.15 and 0.3 (min and max values; mean = 0.225) Ran with AlluviumMatrixSpecificSurfaceArea set to 2000 and 10000 m²/Kg (min and max values; mean = 6000). Discussed the mods made with Femi Osidele, who did the programming, and Paul Bertetti, who is the Subject Matter Expert (SME) for this scr. Once the results are done and organized, Paul will look at them to make sure the mods do what was wanted.

Ran TPA5.0.0a basecase with 100 realizations.

Making comparisons for SCR517 using actinide_kdrd.out and the tpa*.out files from the runs. Looks like the mods cause a decrease in PMD overall. Varying the two sampled parameters do not affect Peak Mean Dose at all.

Running tests for SCR517 on PC. Cannot compile new versions of TPA on Guardian because the installed version of Lahey 95 (v. 5.5) is too old. The make bat file requires version 7.? (1, maybe). Hollen says there are no more available versions of the current Lahey to install on Guardian. If I want to compile a PC version, I'll have to do it on one of the GIS lab computers or at home on my laptop. Ron looking into having Hollen install a license on Guardian that isn't being used where it is installed currently.

Randy has some new concerns about the results from SCR488: he says that, in general, the infiltration is too high, reflux is too low, and temperatures are about 20 degrees too high. Passed this on to Ron to see if he wants more testing at this time. It may have to be a part of the validation testing for TPA 5.0.1, which should start soon.

Paul looked at results from runs. He determined that the last values for input parameters that he gave Femi weren't being used. So, we are now modifying tpa.inp again; see following email:

*From: Olufemi Osidele [oosidele@cnwra.swri.edu]
Sent: Tuesday, September 28, 2004 4:41 PM
To: Carol Scherer
Subject: Re: SCR517 testing - TPA parameter updates and basis*

Carol,

Per the forwarded message, Paul Bertetti has requested a revision of three sampled parameters in tpa.inp. Ron plans to implement them in a subsequent

SCR. In the meantime, please include them in your tests for SCR517.

Regards Femi.

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

From: "Paul Bertetti" <pbertetti@cnwra.swri.edu>

To: "Olufemi Osidele" <oosidele@cnwra.swri.edu>

Cc: "Ronald Janetzke" <rjanetzke@cnwra.swri.edu>

Sent: Tuesday, September 28, 2004 4:23 PM

Subject: TPA parameter updates and basis

Femi,

After meeting with Carol today, there seemed to be a little confusion over the ranges for pH, CO₂ and specific surface area for alluvium. As a result, I am resending this note from Sep 15 with a request to enter these changes in the base TPA input file. (correlation between pH and CO₂ added)

Paul

Femi,

As I mentioned a few minutes ago:

The alluvium specific surface area distribution should be a uniform distribution from 1.9 to 12.1 m²/g (or 1900 to 12100 m²/kg). These values are based on mineralogical and surface area analyses of well cuttings and sonic core samples from EWDP wells, NC-EWDP-02D, NC-Washburn-1X, and NC-EWDP-19PB.

Our final analysis of recent groundwater chemical data indicate that the range and distribution for pH and CO₂ should be modified for TPA. We recommend a TRIANGULAR probability distribution for both pH and CO₂.

For pH the values are: minimum = 6.7, maximum = 9.2, and mode = 7.8 For CO₂ the values are: minimum = -4.0, maximum = -1.0, and mode = -2.5

>>pH and CO₂ should be correlated at -0.95

These probability distributions for pH and CO₂ are based on analysis of sampled groundwater chemistries from the saturated zone within the DOE site-scale model boundary. The values are listed in BSC, 2004 and Bertetti et al., 2004.

References:

Bechtel SAIC Company, LLC. Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing, and Recharge at Yucca Mountain, Nevada. ANL-NBS-HS-000021, Rev. 01. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2004.

Bertetti, F.P., J.D. Prikryl and B.A. Werling. Development of Updated Total-system Performance Assessment Parameter Distributions for

*Radionuclide Transport in the Saturated Zone. CNWRA Report (in review).
San Antonio, Texas: CNWRA. 2004.*

Then, I need to re-run the runs I've already done; compare the results (see scr517.xls in d:\css\tparun\scr517). Running the 100-realization and 500-realization runs on Spock (home/cscherer/scr517); the PC takes too long. Ran 100K run on PC - need to look at how Np behaves.

Juan Portillo is leaving. He gave me the status on the questionnaires and related tasks. He plans to leave me with CDs containing all his files, a directory list that tells me where things are, and some work with stickies on them to tell me what still needs to be done. Checking with Sitakanta to see what he wants me to take on.

October 5, 2004 - October 7, 2004 -

Per Ron's direction, SCR517 is on hold until after I complete the mods to the files for the preprocessor.

Identified the changes in tpa.inp from TPA5.0r to TPA5.0.0d. Started work on modifying tpa.sys and tpa.mod for Brett. All work for TPA going on hold temporarily.

October 18, 2004 - October 20, 2004 -

Found some deleted sampled parameters that I didn't catch before. Added to table (see below). Used writeups from SCR478, 480, 481, and 482 to develop new categories for preprocessor hierarchical tree structure in tpa.mod. Found some errors in the scr documents and errors in the implementation of the scrs, including a list of sampled parameters that should have been deleted from tpa.inp, but weren't yet.

Talked to Brett about the tpa.sys and tpa.mod files. Sampled parameters that are userdiscretaempirical or usersuppliedpwiscdf need special handling (special view). They are identified in tpa.mod by using '[' instead of '\$' in the first columns. They also appear twice; they are also listed in tpa.sys under 'Special Distributions'. Finished modifying the files tpa.sys and tpa.mod; sent them to Brett Dobbs for him to try out in the preprocessor. The user supplied pdfs are:

```
usersuppliedpwiscdf:
  EnvironmentII_Cl [mol/L]
  EnvironmentII_pH []
  EnvironmentII_NO3 [mol/L]
  FractureColloidRetardationFactor_TSw_ [m3/kg]
  FractureColloidRetardationFactor_CHnv [m3/kg]
  FractureColloidRetardationFactor_CHnz [m3/kg]
  FractureColloidRetardationFactor_PPw_ [m3/kg]
  FractureColloidRetardationFactor_UCF_ [m3/kg]
  FractureColloidRetardationFactor_BFw_ [m3/kg]
  FractureColloidRetardationFactor_UFZ_ [m3/kg]
  MatrixColloidRetardationFactor_TSw_ [m3/kg]
  MatrixColloidRetardationFactor_CHnv [m3/kg]
  MatrixColloidRetardationFactor_CHnz [m3/kg]
  MatrixColloidRetardationFactor_PPw_ [m3/kg]
  MatrixColloidRetardationFactor_UCF_ [m3/kg]
```

MatrixColloidRetardationFactor_BFw_ [m3/kg]
 MatrixColloidRetardationFactor_UFZ_ [m3/kg]
 ColloidRetardationFactor_SAV_ [m3/kg]
 ColloidRetardationFactor_STFF [m3/kg]
 NumberOfMagmaInducedMechanicalFailuresRemainingInDrift []

userdiscreteempirical:

ThresholdDisplacementforFaultDisruptionofWP [m]

Updated spreadsheet (tpa50r-500d_diff.xls) that lists the changes in tpa.inp from TPA5.0r to TPA5.0.0d. There are 225 mods.

Ron asked me to provide the new tpa.inp modifications table for SCRs 478, 480, 481, and 482 (the ones that contain information about the changes to tpa.inp from TPA5.0r and TPA5.0.0d). Found file on Juan Portillo's CD (AppendixA/AppendixA_Additions.xls that contains pertinent information. Copied to WordPerfect file and checked against my spreadsheet for the preprocessor changes. Juan's information is incomplete; had to update it with information from the SCR documentation and from tpa.inp itself.

October 21, 2004 -

Made "Update Requirements for Tpa.inp" documents for SCRs 478, 480, 481, 482, and 517. Gave them to Ron. Updated my spreadsheet to indicate which SCRs affected the changes to parameters (see below):

CHANGES IN SAMPLED PARAMETER NAMES FROM TPA5.0r TO TPA5.0.0d**				
Sampled Parameter	type of change	tpa section	SCR	order
AverageCalendarYearAssumedForEmplacement [A.D.]	name change - new (1)	SETUP	518	1
SelectThermalModel (1,2)	new	NFENV	480	2
FractionAllowedToDegrade []	new	NFENV	480	3
SelectParticleModel (1,2)	new	NFENV	480	4
KinematicViscosity [m ² /s]	new	NFENV	480	5
ThermalDiffusivity [m ² /s]	new	NFENV	480	6
VolumeOfThermalExpansion [1/K]	new	NFENV	480	7
BackfillParticleDiameter [m]	new	NFENV	480	8
BackfillPorosity []	new	NFENV	480	9
ThermalConductivityOfAir [W/(m-C)]	new	NFENV	480	10
TortuosityOfBackfill []	new	NFENV	480	11
SortingCoefficient []	new	NFENV	480	12
SkewnessOfDistribution []	new	NFENV	480	13

CoefficientOfVariation[]	new	NFENV	480	14
IndriftEvaporationTemperature [C]	deleted	NFENV	478	15
EnvironmentI Fl [mol/L]	new	NFENV	478	16
EnvironmentI Cl [mol/L]	new	NFENV	478	17
EnvironmentI pH[]	new	NFENV	478	18
EnvironmentI NO3 [mol/L]	new	NFENV	478	19
EnvironmentI CO3 [mol/L]	new	NFENV	478	20
EnvironmentI SO4 [mol/L]	new	NFENV	478	21
EnvironmentI Wastepackage DeltaECrit [VSHE]	new	NFENV	478	22
EnvironmentII Fl [mol/L]	new	NFENV	478	23
EnvironmentII Cl [mol/L]	new	NFENV	478	24
EnvironmentII pH[]	new	NFENV	478	25
EnvironmentII NO3 [mol/L]	new	NFENV	478	26
EnvironmentII CO3 [mol/L]	new	NFENV	478	27
EnvironmentII SO4 [mol/L]	new	NFENV	478	28
EnvironmentII Wastepackage DeltaECrit [VSHE]	new	NFENV	478	29
EnvironmentIII Fl [mol/L]	new	NFENV	478	30
EnvironmentIII Cl [mol/L]	new	NFENV	478	31
EnvironmentIII pH[]	new	NFENV	478	32
EnvironmentIII NO3 [mol/L]	new	NFENV	478	33
EnvironmentIII CO3 [mol/L]	new	NFENV	478	34
EnvironmentIII SO4 [mol/L]	new	NFENV	478	35
EnvironmentIII Wastepackage DeltaECrit [VSHE]	new	NFENV	478	36
SeepageThresholdT [C]	new	NFENV	478	37
FlagSeepageThreshold[]	new	NFENV	478	38
RewettingHumidity[]	new	NFENV	478	39
Indrift Cl PreTemperaturePeak [mol/L]	deleted	NFENV	478	40
Indrift Fl PreTemperaturePeak [mol/L]	deleted	NFENV	478	41
Indrift pH PreTemperaturePeak[]	deleted	NFENV	478	42
Indrift CO3 PreTemperaturePeak [mol/L]	deleted	NFENV	478	43
Indrift Cl PostTemperaturePeak [mol/L]	deleted	NFENV	478	44

Indrift Fl PostTemperaturePeak[mol/L]	deleted	NFENV	478	45
Indrift pH PostTemperaturePeak[]	deleted	NFENV	478	46
Indrift CO3 PostTemperaturePeak[mol/L]	deleted	NFENV	478	47
AgeOfWaste[yr] (was changed to CalendarYearOfEmplacement[A.D.] for SCR 490	name change - old (1)	NFENV	518	48
CurrentAnnualPrecipitation[mm/yr]	new	NFENV	488	49
GroundSurfaceTemperature[C]	new	NFENV	488	50
EmissivityOfBackfill[-]	new	NFENV	480	51
Wastepackage DeltaECrit PreTemperaturePeak[VSHE]	deleted	DSFAIL	478	52
Wastepackage DeltaECrit PostTemperaturePeak[VSHE]	deleted	DSFAIL	478	53
TransitionLowHighpH	new	EBSFAIL	478	54
OuterChargeTransferCoefReductionReactHighpH	new	EBSFAIL	478	55
OuterChargeTransferCoefReductionReactLowpH	new	EBSFAIL	478	56
OuterReferenceCurrReductionReactHighpH[C/(m2*yr)]	new	EBSFAIL	478	57
OuterReferenceCurrReductionReactLowpH[C/(m2*yr)]	new	EBSFAIL	478	58
OuterActivationEnergyReductionReactHighpH[J/mole]	new	EBSFAIL	478	59
OuterActivationEnergyReductionReactLowpH[J/mole]	new	EBSFAIL	478	60
OuterEffectiveReactionOrderHHHighpH	new	EBSFAIL	478	61
OuterEffectiveReactionOrderHLowpH	new	EBSFAIL	478	62
InnerChargeTransferCoefReductionReactHighpH	new	EBSFAIL	478	63
InnerChargeTransferCoefReductionReactLowpH	new	EBSFAIL	478	64
InnerReferenceCurrReductionReactHighpH[C/(m2*yr)]	new	EBSFAIL	478	65
InnerReferenceCurrReductionReactLowpH[C/(m2*yr)]	new	EBSFAIL	478	66
InnerActivationEnergyReductionReactHighpH[J/mole]	new	EBSFAIL	478	67
InnerActivationEnergyReductionReactLowpH[J/mole]	new	EBSFAIL	478	68
InnerEffectiveReactionOrderHHHighpH	new	EBSFAIL	478	69
InnerEffectiveReactionOrderHLowpH	new	EBSFAIL	478	70
OuterActivationEnergyPassiveCurrDens[J/mol]	new	EBSFAIL	478	71
InnerActivationEnergyPassiveCurrDens[J/mol]	new	EBSFAIL	478	72
RefTemperaturePassiveCurrDens[K]	new	EBSFAIL	478	73
OuterInhibitingNitrateToCl	new	EBSFAIL	478	74
OuterInhibitingCarbonateToCl	new	EBSFAIL	478	75

OuterInhibitingSulfateToCl	new	EBSFAIL	478	76
OuterDeltaEcritInh [mV]	new	EBSFAIL	478	77
InnerInhibitingNitrateToCl	new	EBSFAIL	478	78
InnerInhibitingCarbonateToCl	new	EBSFAIL	478	79
InnerInhibitingSulfateToCl	new	EBSFAIL	478	80
InnerDeltaEcritInh [mV]	new	EBSFAIL	478	81
WeldCritChlorideConc [mol/L]	new	EBSFAIL	478	82
WeldInhibitingNitrateToCl	new	EBSFAIL	478	83
WeldInhibitingCarbonateToCl	new	EBSFAIL	478	84
WeldInhibitingSulfateToCl	new	EBSFAIL	478	85
WeldDeltaEcritInh [mV]	new	EBSFAIL	478	86
ExponentForLocCorrOfOuterOverpack (from Exponet)	spelling	EBSFAIL	518	87
OuterWPBetaKineticsParameterforOxygen	deleted	EBSFAIL	478	88
InnerWPBetaKineticsParameterforOxygen	deleted	EBSFAIL	478	89
OuterWPRateConstantforOxygenReduction [coulomb-m/mole/yr]	deleted	EBSFAIL	478	90
OuterWPActivationEnergyforOxygenReduction [J/mole]	deleted	EBSFAIL	478	91
InnerWPRateConstantforOxygenReduction [coulomb-m/mole/yr]	deleted	EBSFAIL	478	92
InnerWPActivationEnergyforOxygenReduction [J/mole]	deleted	EBSFAIL	478	93
StandardExchangeCurrentDensityforOxygenReduction [C/(m ² yr)]	deleted	EBSFAIL	478	94
EquilibriumPotentialOxygenReduction [VSHE]	deleted	EBSFAIL	478	95
ContactAngle [degrees]	new	SEISMO	481	96
DeflectionDepth [m]	new	SEISMO	481	97
BulkheadThickness [m]	new	SEISMO	481	98
WastePackageOuterBarrierUltimateTensileStrength [MPa]	new	SEISMO	481	99
MatrixKD TSw Ja [m3/kg]	deleted	UZFT	484	100
MatrixKD CHnvJa [m3/kg]	deleted	UZFT	484	101
MatrixKD CHnzJa [m3/kg]	deleted	UZFT	484	102
MatrixKD PPw Ja [m3/kg]	deleted	UZFT	484	103
MatrixKD UCF Ja [m3/kg]	deleted	UZFT	484	104
MatrixKD BFW Ja [m3/kg]	deleted	UZFT	484	105

MatrixKD UFZ Ja [m3/kg]	deleted	UZFT	484	106
MatrixKD TSw Jc [m3/kg]	deleted	UZFT	484	107
MatrixKD CHnvJc [m3/kg]	deleted	UZFT	484	108
MatrixKD CHnzJc [m3/kg]	deleted	UZFT	484	109
MatrixKD PPw Jc [m3/kg]	deleted	UZFT	484	110
MatrixKD UCF Jc [m3/kg]	deleted	UZFT	484	111
MatrixKD BFW Jc [m3/kg]	deleted	UZFT	484	112
MatrixKD UFZ Jc [m3/kg]	deleted	UZFT	484	113
MatrixKD TSw Jp [m3/kg]	deleted	UZFT	484	114
MatrixKD CHnvJp [m3/kg]	deleted	UZFT	484	115
MatrixKD CHnzJp [m3/kg]	deleted	UZFT	484	116
MatrixKD PPw Jp [m3/kg]	deleted	UZFT	484	117
MatrixKD UCF Jp [m3/kg]	deleted	UZFT	484	118
MatrixKD BFW Jp [m3/kg]	deleted	UZFT	484	119
MatrixKD UFZ Jp [m3/kg]	deleted	UZFT	484	120
MatrixKD TSw Jt [m3/kg]	deleted	UZFT	484	121
MatrixKD CHnvJt [m3/kg]	deleted	UZFT	484	122
MatrixKD CHnzJt [m3/kg]	deleted	UZFT	484	123
MatrixKD PPw Jt [m3/kg]	deleted	UZFT	484	124
MatrixKD UCF Jt [m3/kg]	deleted	UZFT	484	125
MatrixKD BFW Jt [m3/kg]	deleted	UZFT	484	126
MatrixKD UFZ Jt [m3/kg]	deleted	UZFT	484	127
FractureRD TSw Ja	deleted	UZFT	484	128
FractureRD CHnvJa	deleted	UZFT	484	129
FractureRD CHnzJa	deleted	UZFT	484	130
FractureRD PPw Ja	deleted	UZFT	484	131
FractureRD UCF Ja	deleted	UZFT	484	132
FractureRD BFW Ja	deleted	UZFT	484	133
FractureRD UFZ Ja	deleted	UZFT	484	134
FractureRD TSw Jc	deleted	UZFT	484	135
FractureRD CHnvJc	deleted	UZFT	484	136

FractureRD CHnzJc	deleted	UZFT	484	137
FractureRD PPw Jc	deleted	UZFT	484	138
FractureRD UCF Jc	deleted	UZFT	484	139
FractureRD BFW Jc	deleted	UZFT	484	140
FractureRD UFZ Jc	deleted	UZFT	484	141
FractureRD TSw Jp	deleted	UZFT	484	142
FractureRD CHnvJp	deleted	UZFT	484	143
FractureRD CHnzJp	deleted	UZFT	484	144
FractureRD PPw Jp	deleted	UZFT	484	145
FractureRD UCF Jp	deleted	UZFT	484	146
FractureRD BFW Jp	deleted	UZFT	484	147
FractureRD UFZ Jp	deleted	UZFT	484	148
FractureRD TSw Jt	deleted	UZFT	484	149
FractureRD CHnvJt	deleted	UZFT	484	150
FractureRD CHnzJt	deleted	UZFT	484	151
FractureRD PPw Jt	deleted	UZFT	484	152
FractureRD UCF Jt	deleted	UZFT	484	153
FractureRD BFW Jt	deleted	UZFT	484	154
FractureRD UFZ Jt	deleted	UZFT	484	155
SurfaceAreaFactor TSw []	new	UZFT	484	156
SurfaceAreaFactor CHnv []	new	UZFT	484	157
SurfaceAreaFactor CHnz []	new	UZFT	484	158
SurfaceAreaFactor PPw []	new	UZFT	484	159
SurfaceAreaFactor UCF []	new	UZFT	484	160
SurfaceAreaFactor BFW []	new	UZFT	484	161
SurfaceAreaFactor UFZ []	new	UZFT	484	162
FractureColloidRetardationFactor TSw [m3/kg]	new	UZFT	484	163
FractureColloidRetardationFactor CHnv [m3/kg]	new	UZFT	484	164
FractureColloidRetardationFactor CHnz [m3/kg]	new	UZFT	484	165
FractureColloidRetardationFactor PPw [m3/kg]	new	UZFT	484	166
FractureColloidRetardationFactor UCF [m3/kg]	new	UZFT	484	167

FractureColloidRetardationFactor BFW [m3/kg]	new	UZFT	484	168
FractureColloidRetardationFactor UFZ [m3/kg]	new	UZFT	484	169
MatrixColloidRetardationFactor TSw [m3/kg]	new	UZFT	484	170
MatrixColloidRetardationFactor CHnv[m3/kg]	new	UZFT	484	171
MatrixColloidRetardationFactor CHnz[m3/kg]	new	UZFT	484	172
MatrixColloidRetardationFactor PPw [m3/kg]	new	UZFT	484	173
MatrixColloidRetardationFactor UCF [m3/kg]	new	UZFT	484	174
MatrixColloidRetardationFactor BFW [m3/kg]	new	UZFT	484	175
MatrixColloidRetardationFactor UFZ [m3/kg]	new	UZFT	484	176
FractureColloidConcentration TSw [kg/m3]	new	UZFT	484	177
FractureColloidConcentration CHnv[kg/m3]	new	UZFT	484	178
FractureColloidConcentration CHnz[kg/m3]	new	UZFT	484	179
FractureColloidConcentration PPw [kg/m3]	new	UZFT	484	180
FractureColloidConcentration UCF [kg/m3]	new	UZFT	484	181
FractureColloidConcentration BFW [kg/m3]	new	UZFT	484	182
FractureColloidConcentration UFZ [kg/m3]	new	UZFT	484	183
MatrixColloidConcentration TSw [kg/m3]	new	UZFT	484	184
MatrixColloidConcentration CHnv[kg/m3]	new	UZFT	484	185
MatrixColloidConcentration CHnz[kg/m3]	new	UZFT	484	186
MatrixColloidConcentration PPw [kg/m3]	new	UZFT	484	187
MatrixColloidConcentration UCF [kg/m3]	new	UZFT	484	188
MatrixColloidConcentration BFW [kg/m3]	new	UZFT	484	189
MatrixColloidConcentration UFZ [kg/m3]	new	UZFT	484	190
FractureRDLog10 STFF Ja	deleted	SZFT	484	191
AlluviumMatrixRDLog10 SAV Ja	deleted	SZFT	484	192
FractureRDLog10 STFF Jc	deleted	SZFT	484	193
AlluviumMatrixRDLog10 SAV Jc	deleted	SZFT	484	194
FractureRDLog10 STFF Jp	deleted	SZFT	484	195
AlluviumMatrixRDLog10 SAV Jp	deleted	SZFT	484	196
FractureRDLog10 STFF Jt	deleted	SZFT	484	197
AlluviumMatrixRDLog10 SAV Jt	deleted	SZFT	484	198

SurfaceAreaFactor SAV []	new	SZFT	484	199
SurfaceAreaFactor STFF[]	new	SZFT	484	200
ColloidRetardationFactor SAV [m3/kg]	new	SZFT	484	201
ColloidRetardationFactor STFF[m3/kg]	new	SZFT	484	202
ColloidConcentration SAV [kg/m3]	new	SZFT	484	203
ColloidConcentration STFF[kg/m3]	new	SZFT	484	204
AlluviumTotalPorosity SAV	new	SZFT	517	205
AlluviumMatrixSpecificSurfaceArea [m2/kg]	new	SZFT	517	206
ImmobileRDLog10 STFF Ja	deleted	SZFT	484	207
ImmobileRDLog10 STFF Jc	deleted	SZFT	484	208
ImmobileRDLog10 STFF Jp	deleted	SZFT	484	209
ImmobileRDLog10 STFF Jt	deleted	SZFT	484	210
DiameterOfVolcanicConduit [m]	new	VOLCANO	490	211
DiameterOfVolcanicCone [m]	deleted	VOLCANO	490	212
DistanceCutoffForDoseConversionDualityInDCAGS [km]	deleted	DCAGS	477	213
DepthOfResuspendibleLayer[cm] (from Suspendable)	spelling	DCAGS	518	214
AshEvolutionMode[0=no ashremob,1=ashremob]	new	ASHREMOB	482	215
AshPlumeRealizationIndex[]	new	ASHREMOB	482	216
WeightingFactorInitialDeposit[]	new	ASHREMOB	482	217
WeightingFactorFluvial[]	new	ASHREMOB	482	218
AmbientSedimentYieldVolumeFromBasin [m/event]	new	ASHREMOB	482	219
AreaDrainageBasinFluvial [m2]	new	ASHREMOB	482	220
TimeBetweenFlowEvents [yr]	new	ASHREMOB	482	221
PostEruptionYieldVolumeFluvialAsh [m/event]	new	ASHREMOB	482	222
WeightingFactorEolian[]	new	ASHREMOB	482	223
DensityOfDistalAsh [g/m3]	new	ASHREMOB	482	224
AreaEolianSourceRegion [m2]	new	ASHREMOB	482	225
** This table contains only changes/additions/deletions of parameter names. It does not include changes to PDF type or paramter values.				

Ron has requested a write up of the changes to uzft and szft, particularly those that may affect NEFTRAN. Tim McCartin at NRC wants an update. Began reviewing the code changes.

October 22, 2004 -

Worked on uzft.f/szft.f writeup for Ron. Talking about the changes from SCR 484, 489, and 517.

October 27, 2004 - October 29, 2004 -

Finished uzft/szft writeup and gave it to Ron. Complete unless changes requested.

Spock is at 99+% again. Perry says I am one of 5 people with over 12Gig in my account, so archived files. Copied the *.tar.bz2 files I had in the cscherer/tarbz2_files directory onto CD. These are code_cleanup, compton_memo, scr445, scr450_50m_recheck, scr471, scr472, scr473, scr476, tpa50q_merge, tpa50q_testdcags, and validate directories tarred and zipped into files (unix commands: *tar cvf <directoryname>.tar <directoryname>; bzip2 <directoryname>.tar*). Then tarred and zipped the following directories: IHI_Buffer, Marty_SA, preprocessor01-2004, checkin_102904, dispersivity_range, scr470, scr477, scr478, scr485, scr486, and scr487. Copied all but Marty_SA onto one archive CD. Marty_SA is too big for a CD; I'd have to unzip it and redo it in smaller chunks to get it on CDs. Deleted the rest of the directories that made it to CD. Copied Marty_SA.tar.bz2 to Guardian for storage to clear up the space on spock. Tarred and zipped the following directories: scr484, scr488, and scr518. Tarred and zipped the following directories under testTPA2004: convergence, glass, timesteps100K, timesteps10K, seismo_changes, rep_geom, and streamtubes. Original directories were removed from spock. About 5% of total disk space cleared up (not all necessarily from my files - Ron, Sitakanta, and Marty were also freeing up space).

Continued with testing for SCR517. Re-ran all TPA runs with the updated tpa.inp (see comments for September 20, 2004), and updated scr517.xls. Need to look at results and finish test plan/report.

November 1, 2004 - November 10, 2004 -

Worked on the test plan/report for SCR517. Analyzed results from the TPA runs using TPA5.0.0d and the modified values in tpa.inp.

Brett Dobbs has errors or discrepancies in some of the files I sent him for the preprocessor. Made more mods and sent him back tpa500d.inp, tpa.sys, tpa.opt, and tpa.mod.

Asked Paul Bertetti to check results from my runs for SCR517. Accumulating PMDs and some other numbers in a spreadsheet.

A 400-realization run TPA run aborted. NEFTRAN - BF array bounds exceeded again. There were NaNs in nefii.inp.

Found error, 2nd call to calc_rd in SZFT, porosity and density values are for alluvium, not tuff. This will require code changes, so Ron says to say test failed and refer to SCR523, where this will be fixed.

Put finishing SCR517 test plan/report on hold until after delivery of 4.1jpdlsbeta4 next

week. This is the first task I've had for the long simulation software (1,000,000 years). Ron and Sitakanta want me to work on the SDP for this TPA version (long simulation).

November 11, 2004 - November 12, 2004 -

Guardian, my pc here, cannot run the long simulation (not enough RAM). I need to run on spock. Copied tpa.e from Marty for TPA41jpdls_beta3.

Rob had a run abort of the long simulation tpa.e. Started a 400-real, 1000000years, StopAtReal 165 run to double check that it will abort. Running sal only. The typical NEFTRAN-related abort problem. Need to figure out why. SDP will have to wait until afterwards.

A new chain was added to tpa.inp and the problem seems to be related to isotopes in that chain. Tried to modify Rds and velocity in NEFII.VEL to get it to run; unsuccessful. Removed 14900 time step in NEFII.VEL; still unsuccessful. Modified NEFII.VEL again - got rid of 14950-year step; replaced with a time-step every 5000 years and distributed velocity change from 10K to 1000K over the time steps. Still unsuccessful. Ron says Rob has had another

There is a divide by zero that occurs in snllhs.exe. This is a problem that has happened before, but has been fixed since TPA 4.1jpd. To test snllhs.e, need to provide the input from tpa_lhs.lgd. Just type it in with carriage returns.

Brett still had a few problems with the preprocessor files, so I went through them again and made a few more mods for him.

November 15, 2004 - November 19, 2004 -

Back to working on the SDP - there is no SRD available. Getting the requirements from Rob's notes of what had to be changed to make it work.

Ron told me that the SDP has been cancelled.

New task: try TPA4.1jpdls_beta4 (copy from Remington) on Guardian to see if it runs. Still won't get message: "The system cannot execute the specified program." Made a spock version from the Remington PC version. This runs. Ron wants me to run as many runs as I can changing the iflag parameters in tpa.inp. It will sent to NRC Thursday this week.

Updated "Changes to UZFT and SZFT in TPA5.0.1" writeup for Ron.

Rob Rice won't be here next week. He has been working on changes to the RARI to address concerns by NRC legal counsel. So, I need to drop everything and talk to Rob about the status of the RARI so I can continue his work next week. Made list of Figures that need to be revised. Sitakanta wants a list of just the figures that belong to NRC authors. Here's the entire list:

- Figure 2-1: add the word "Estimated" to the beginning of the y-axis label
- Figure 2-2: add the word "Estimated" to the beginning of the y-axis label

- Figure 2-3: change y-axis label to "Estimated Mean Number of Waste Packages Failed"
- Figure 2-4: change y-axis label to "Estimated Mean Number of Waste Packages Failed"
- Figure 3-2: change "TPA 5.0q" to "code"
- Figure 3-3: change "TPA 5.0q" to "code"
- Figure 4-1: add the word "Estimated" to the beginning of the y-axis label
- Figure 4-2: add the word "Estimated" to the beginning of the y-axis label
- Figure 4-3: add the word "Estimated" to the beginning of the y-axis label
- Figure 4-4: add the word "Estimated" to the beginning of the y-axis label and 2nd y-axis label; add the word "Estimated" before "Probability Weighted Dose" and "Conditional Dose" in the legend
- Figure 4-5: add the word "Estimated" to the beginning of the y-axis label and 2nd y-axis label
- Figure 4-6: add the word "Estimated" to the beginning of the y-axis label; change " $\text{cm}^2/\text{s}^{5/2}$ " to " $\text{cm}^2/\text{s}^{2.5}$ "
- Figure 7-1: change "modified coefkdeq.dat" to "modified basecase"
- Figure 7-3: add the word "Estimated" to the beginning of the y-axis label
- Figure 8-3: add the word "Estimated" to the beginning of the x- and y-axis labels
- Figure 8-4: add the word "Estimated" to the beginning of the x- and y-axis labels
- Figure 8-5: change "New" to "Alternative"
- Figure 8-7: change the y-axis label to "Estimated Peak Dose(Sv) - Alternative"
- Figure 8-8: change "Original" to "Current" and "Revised" to "Alternative" in the legend; change y-axis label to "Estimated Mean Dose (mSv/yr)"
- Figure 9-2: change "TPA profile (burnup.dat)" to "TPA input data profile"
- Figure 10-2: add the word "Estimated" to the beginning of the y-axis label
- Figure 10-4: delete "Effect of Natural Backfill on the Eruptive Risk for the Dog-Leg Alternative Conceptual Model"
- Figure 11-3: add the word "Estimated" to the beginning of the y-axis label
- Figure 11-4: add the word "Estimated" to the beginning of the y-axis label
- Figure 11-5: add the word "Estimated" to the beginning of the y-axis label
- Figure 11-6: add the word "Estimated" to the beginning of the y-axis label
- Figure 13-3: add the word "Estimated" to the beginning of the y-axis label
- Figure 13-5: add the word "Estimated" to the beginning of the y-axis label
- Figure 13-6: add the word "Estimated" before "Fluoride" in the y-axis label
- Figure 13-7: add the word "Estimated" to the beginning of the y-axis label
- Figure 13-8: add the word "Estimated" to the beginning of the y-axis label
- Figure 13-9: add the word "Estimated" to the beginning of the y-axis label
- Figure 13-10: add the word "Estimated" to the beginning of the y-axis label

November 22, 2004 - November 24, 2004 -

Took Rob's 1st and 2nd markups for the RARI and made sure that all his changes were in the document. Corrected a few minor omissions and tense mistakes. Gave new markup to Ruth. Took list of Figures that needed changed. With Marty's helped, we determined which figures we already had electronic files for from previous changes. Gave list of remaining figures from NRC authors to Sitakanta to send memo to them. Marty is working on changes for the NRC figures we have from Codell. I went around to the CNWRA authors and got electronic files where I could or left messages. Made changes to 13 figures and put in directory under `s:/cscherer/UpdateFiguresForRARI_11242004`. Other files, .xls, .doc, and copies of .wpd are in

subdirectories under the authors name. Couldn't get a hold of Mike Smith (on vacation) for the figures from Chapter 7. Other than those, all CNWRA-authored figures are changed. We still need 6 figures from Compton and 2 from Codell at NRC. Sitakanta says the deadline for the changes is next Monday. Got a hold of Paul Bertetti about the figures from Chapter 7. He isn't actually here. He will look at them and try to get them modified for me Monday morning.

Sitakanta sent the request for changes/files to Codell's and Compton's PM. He (?) said that as long as the change was just adding "Estimated" to the axis labels, then, as long as "Estimated" is in the caption, that is sufficient. The only "must change" figures then from NRC are Fig 8-5 and Fig 8-8. Those are figures that Marty has files for, thankfully. I also need to get Fig 7-1 (Smith/Bertetti) Monday at the latest. Need to check with Rob to see when he plans to come in Monday.

Ron needs some more changes to the Changes to UZ/SZ document. He also wants me to re-run current tpa after removing the fix to gwtmin and modifying Cm KD values in tpa.inp to 4.1j values. Will have to wait for next week, after RARI.

November 29, 2004 - December 3, 2004 -

Received two figures from Paul Bertetti (7-1 & 7-3) for the RARI. All CNWRA figures were updated; couldn't update all the NRC figures because we didn't have the electronic files and NRC couldn't provide them. So Figure update is complete as much as possible. Passed task back to Rob Rice Monday.

NEFTRAN is bombing again (TPA 5.0.0d & e), call from szft. Tested TPA4.1jpdls_beta4 values for Cm (Rob did this for the long simulation runs when he had problems with NEFTRAN and the mods "fixed" the problem). Cm MatrixKD values are the same as Am in TPA4.1jpdls_beta4. But it didn't work here. Also tried changing gwtmin back to 10.0d0. In uzft.f, gwtmin had been changed to 20.0d0 instead of 10.0d0 when NEFTRAN problems surfaced after SCR #484. In szft.f, gwtmin is still 10.0d0. Set off original, 400-realization run in directory tpa500e. Set off modified, 400-realization run in directory tpa500e/testmodCmKD. Original runs bombed at realization 12, subarea 7. Modified runs bombed at realization 123, subarea 6.

George Adams reported problems running TPA 5.0.0d and TPA 5.0.0e, aborting during NEFTRAN run, calling szft.

Test: modified szft and changed gwtmin to 20.0d0. Run 400 realizations: outcome aborted at realization 12 of 400 in subarea 7 after calling szft.

Looked at intermediate and output files from TPA 5.0.0e runs to try to determine which chain and perhaps element was being processed when the array boundaries were exceeded..

December 6, 2004 - December 10, 2004 -

NEFTRAN bombs, this time in szft. Why? Tried raising gwtmin in szft.f from 10.0 to 20.0, but that's not it. Tested the use of modified Cm KD values in uzft (from tpa4.1j, using Am

values instead of defaults. Didn't help. NEFTRAN bombed processing colloidal chain 5 (Jt230,Ra226,Pb210). Usual error, BF array out of bounds.

I finished updating tp_scr517.wpd scr_517.wpd. Made CD of test directories, and turned them all in to Ron.

I go SCR #490 from Ron for testing.

I went over what I know about the questionnaire stuff w/ Rob. He is supposed to organize it and come up with a final status. TPA5.0.0d has changes to tpa.inp that Juan Portillo identified, but there may be errors, typos, etc.

New top priority: verify data set for TPA 5.0.0e. Rob, Marty, and I will be working on this. We know there are inaccuracies. Need to look at Juan's and Bruce Goodwin's last Appendix A spreadsheet and compare it against the current tpa.inp, as well as updates identified in SCRs. Started organizing the files.

December 13, 2004 - December 17, 2004 -

Worked on TPA final data set verification with Rob Rice and Marty Menchaca. We're using tpa.inp from TPA5.0.0e. Organized file container with questionnaire folders - made sure all had hanging files and that all folders were marked with a name. Put folders in alphabetical order. For each file folder, we are checking tpa.inp against the App A spreadsheet (from Juan Portillo and Bruce Goodwin) and against the questionnaire. The goal is to confirm the values for all parameters. So far, I've done folders for Ahn, Bertetti, Browning, Codell, Gute, Jain, Janetzke, and LaPlante. I'm working on Osvaldo Pensado's folder. Once we've gone through the folders in the black plastic file container, we'll go through the unfiled stacks of questionnaires. Then we'll check against typed-in questionnaires (for those with hard copies missing), and against the SCRs that modified tpa.inp parameters.

I haven't figured out why some questionnaires are filed and some not. Some questionnaires are "missing". I don't know where they are. I sent an e-mail to Juan asking him if he knows where they might be. Juan called to reply - it seems that he didn't necessarily print out all the hard copies if the responder responded electronically. So, after we've gone through all the hard copies we have, we'll have to sit down with the list and try to find the remainder on Juan's CD.

Four parameters in tpa.inp aren't used, exactly. They are read in by ebsrel and written out to ebsrel.inp, which is read by releaset. Releaset reads the values but does nothing with them. They could be deleted but that would require code changes. Ron suggests we add comments to ebsrel saying all this, but not actually do code changes right now. The parameters are: SFC-14InventoryPerKgSF[ci], CladC-14InventoryPerKgSF[ci], ZyrOxideAndCrudC-14InvPerKgSF[ci], and GapAndGrainBoundaryInventoryPerKgSF[ci]. In ebsrel and releaset, they are also CFUEL, CZMETAL, CZOXIDE, and CGAP.

December 20, 2004 - December 22, 2004 -

Continued with verification of the final data set for TPA; finished going through

questionnaire folders for Pensado, Pickett, Smith, and Menchaca. Started going through piles of stuff Juan left. Can't resolve all of them; will need to talk to Ron, Rob, Sitakanta, or Mike Smith to complete. Cannot access Juan Portillo's mailbox; the account was deleted when he left, so missing attachments will have to come either from originator or forwarder of emails that Juan printed out and left with instructions. Worked with Marty Menchaca.

I had to retrieve my directories for SCR #484 to print out a clean version of scr_484.wpd to use for data set verification. I had compressed the files earlier when space when needed. Used these commands in tarbzip_files directory:

```
bunzip2 scr484.tar.bz2  
tar xvf scr484.tar
```

Talked to Ron. When we update the tpa.inp files, we will delete all comments about changes due to SCRs and deleted parameters, except those related to Turner's calculations for actinide Kds and Rds. Those will be grouped together at the end of the UZFT and SZFT sections and commented w.r.t. "turning off" Turner's calculations and using the old default values for Am, Np, Pu, Th, and U. Turning off the calculations would require that the commented out values be un-commented out and the number of elements set in coefkdeq.dat (currently 5) be set to zero.

Ron sent me SCR # 519 to implement if I need additional work before he returns from winter break at the end of the second week in January. Sitakanta is out until the beginning of the second week in January.

Looked up how some parameters are used because questionnaires said they were not used, were obsolete, or some other variation meaning the same thing.

December 27, 2004 - December 30, 2004 -

Finished with folders and unfilled questionnaires for Bertetti, Benke, Wittmeyer, and Winterle. Went through all of Juan's loose stacks of papers. Put all unanswered questions and problems in one stack. Worked with Marty Menchaca. Marty is working on converting Turner's given values from Kds to Rds (or vice versa?) and generating the shape parameters for the beta distributions for Turner's values.

Went through recent SCRs (SCR # 480, 481, 482, 517, 518) along with Marty (SCR # 478, 484) to make sure modifications to tpa.inp were included. Separated out data file questionnaires. All file folders have been checked. Started looking for "missing questionnaires" (questionnaires that were sent out but no hard copy has been found; there are parameters and other data in tpa.inp for which no questionnaires were generated in the first place).

January 5, 2005 - January 7, 2005 -

I took the AppA spreadsheet files from the folders and went through them to determine which questionnaires had been sent out but for which we have no hard copy responses. I made a list of "missing questionnaires". Some may be misfiled or they may have been in the folders but weren't checked off when we went through the folders previously. I know that some

questionnaires were filled out electronically but were not printed out. Some questionnaires disappeared because the responder considered the parameter(s) to be obsolete and suggested deletion. However, if the parameter is still being used in viable code, we need to include the parameter along with description, value, and justification.

Some of the missing questionnaires were just not checked off on the AppA spreadsheets. Those are resolved. Found electronic copies of LaPlante's missing questionnaires. Those are resolved. The rest are still up in the air; I haven't been able to find an electronic version indicating any changes. I've added them to the pile of questions/problems to be resolved. Sitakanta said we're not going to send more questionnaires to Bruce or have any more typed, so I was able to pull those out of the questions/problems to be resolved pile and file them.

January 10, 2005 - January 14, 2005 -

Continued with final data set verification. Made another search through Juan's CD looking for modified electronic versions of questionnaires.

Talked to the following people to resolve outstanding questions and issues:

- ▶ Ron talked to LaPlante (see e-mail).
- ▶ Marty talked to George Adams to verify that data files submitted are the latest.
- ▶ Mike Smith
- ▶ Sitakanta
- ▶ Paul Bertetti

Started updating & testing tpa.inp.

January 17, 2005 - January 21, 2005 -

Finished updating tpa.inp (1/21/2005) except for some outstanding questionnaires. Worked on updating Appendix A.

The first run with verified tpa.inp at 400r bombed - new SeedForRandomNumber out of range; need to change range check in code from $10^8 - 10^9$ to $2^{30} - 2^{31}$. This change will be part of SCR #519 and requires 2 code changes each in reader.f, sampler.f, ran.f. The same range check is done for SeedForRandomNumber and SeedForRandomNumberSEISMO.

The next run at 400 realizations ran to completion. The next run was for 400 realizations at 100,000 years. It also ran to completion. Also made the following runs, with some problems as noted:

- 400r 10K no ash remobilization (400r 10K no ash remobilization geometric volcano model volcanism off) - same .out as with ash remobilization turned on
- 400r 10K no ash remobilization geometric volcano model volcanism on
- 400r 10K ash remobilization on geometric volcano model volcanism on - ran to completion BUT there is a divide by zero

- 400r 10K no ash remobilization distribution volcano model volcanism on - bombed!
- 400r 10K ash remobilization on distribution volcano model volcanism on
- 400r 10K ash remobilization on distribution volcano model volcanism off - ran to completion

January 24, 2005 - January 28, 2005 -

Passed the verified tpa.inp and updated Appendix A to Marty who will double check my changes to tpa.inp and will modify the reference/justification column in Appendix A.

Modified ran.f, reader.f, and sampler.f to change the range check for the SeedForRandomNumber and SeedForRandomNumberSEISMO value, which Ron changed via questionnaires. Otherwise the code bombs with the new values.

Met with Ron (1/24), Rob, Marty, Femi, Razvan (George on vacation) new tasks. I'm implementing SCRs #519, #524, and #552. Also need to finish SCR #523. Marty will be testing mine. I won't be testing SCR #490 anymore - it goes to Raz. These have to be finished in February for a delivery of a beta version of the code March 1st.

Finished updating App. A columns for name, pdf type, range of values, contact, module, and order. That still leaves Description and Comments/Justification. Looks like we'd need to go through all the questionnaires again and update those columns.

There is a question about whether the final data set should include just tpa.inp or data files from data subdirectory. We haven't finished those questionnaires yet because Rob, Marty, and I have been concentrating on tpa.inp. Ron says Brett Leslie/NRC wants us to send out all the data to authors for their final review. Ron is deciding how to go about doing that.

January 31, 2005 - February 4, 2005 -

Made a copy of App A for Ron sorted by module - he needs to send it out to NRC per B. Leslie.

Updated tpa.inp with Turner's new beta distributions for Kds now that Mary has figured out the shape parameters. Now, TPA hangs in snllhs. Seems to be in a loop - massive processor usage.

Have finished all code changes for SCR #523. The code compiles and runs but the data isn't formatted quite right yet.

Looked at SCR #524 to start it. Mailed George about what is wanted. He referred me to David Ferrill (should have been David Farrell) and Randy Fedors. There seems to be confusion about what should be done and who should decide what to do. This SCR is on hold until it's determined what's going on. See emails:

*From: George Adams [gadams@cnwra.swri.edu]
Sent: Monday, January 31, 2005 5:18 PM
To: 'Carol Scherer'
Subject: RE: SCR #524*

Carol,

Ron and I met with Randy Fedors, Bobby Pabalan, and Osvaldo several months ago (around October). One of the concerns during the meeting was the reflux model that is in the code (by default reflux 3). The parameter list doesn't include a repository temperature as an input parameter. There were e-mails just after the meeting in which there was some discussion between David Ferrill, Randy, and I think Alexander Sun (but I could be wrong about Alexander). I think the point of discussion at that time was to develop a new reflux model or possibly evaluate the current one to determine if it is doing what is needed in the tpa code. I thought David assigned the work to Alexander. I think it would be best to ask David, if he remembers this. I think the nature of the SCR 524 may be to update the reflux model. The question came up when I was validating the NFENV code.

George

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

From: Carol Scherer [mailto:cscherer@cnwra.swri.edu]
Sent: Monday, January 31, 2005 12:52 PM
To: gadams@cnwra.swri.edu
Subject: RE: SCR #524

Thank you. Hope you had a good trip. Did you learn anything?

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

From: George Adams [mailto:gadams@cnwra.swri.edu]
Sent: Monday, January 31, 2005 12:34 PM
To: 'Carol Scherer'
Subject: RE: SCR #524

Hey there Carol,

I just got back from DC, so I'm trying to get caught up. I'm not certain about that SCR, but I need to talk to Ron today anyway, so I'll try to determine what needs to be done in it.

George

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

From: Carol Scherer [mailto:cscherer@cnwra.swri.edu]
Sent: Monday, January 31, 2005 11:06 AM
To: George Adams
Subject: SCR #524

I've assigned SCR #524 to implement. All the information I have is that it is supposed to "Verify temperature for reflux3 is temp of repository." I was told this idea came from you. What can you tell me about it?

From: Randy Fedors [rfedors@cnwra.swri.edu]
Sent: Tuesday, February 01, 2005 12:47 PM
To: 'Carol Scherer'
Cc: 'David Ferrill'; David Farrell
Subject: RE: SCR #524

Carol,

Maybe George is referring to these emails.
Also, he meant David Farrell, not David Ferrill.

--Randy

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

From: Carol Scherer [mailto:cscherer@cnwra.swri.edu]
Sent: Tuesday, February 01, 2005 11:28 AM
To: David Ferrill; Randall Fedors
Subject: FW: SCR #524

Do either of you have the emails George is talking about?

From: David Farrell [dfarrell@cnwra.swri.edu]
Sent: Wednesday, October 06, 2004 10:50 AM
To: asun@cnwra.swri.edu; rfedors@cnwra.swri.edu
Cc: 'George R. Adams'; 'Osvaldo Pensado'
Subject: RE: George's validation test results

We don't really have an alternative ... the rest of us are tied up with reviews ... if you want to do a review then I can get some one else to do the analysis. Review response are due at the end of the month. By the way Sitakanta will assign your GoldSim task to some one else.

David

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

From: Alexander Sun [mailto:asun@cnwra.swri.edu]
Sent: Wednesday, October 06, 2004 10:23 AM
To: rfedors@cnwra.swri.edu
Cc: 'George R. Adams'; 'Osvaldo Pensado'; 'David Farrell'
Subject: RE: George's validation test results

Randy,

I have not used TPA before. I think it'll save a lot time if you ask someone with TPA experience to run the reflux module. I hope there is an alternative.

Regards,

Alex

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

From: Randy Fedors [mailto:rfedors@cnwra.swri.edu]
Sent: Wednesday, October 06, 2004 9:57 AM
To: Ronald Janetzke
Cc: 'George R. Adams'; Osvaldo Pensado; David Farrell; Alexander Sun
Subject: George's validation test results

There were three things I was responsible for from our meeting Tuesday afternoon on George's validation testing of nfenv module in TPA 5.0.0d.

Before commenting on the 3 items, do I remember correctly that George used the first realization of parameters and subarea 1? Is it possible to use basecase parameters and subarea 1? I am still wondering why George's results for TPA 5.0.0d validation were approx 20 C cooler than Carol's results in TPA 5.0.0y validation testing (Carol used subarea 7, but there is no reason for subarea 7 to be hotter than subarea 1; if anything, subarea 7 should be slightly cooler at later times).

1. The late time response of relative humidity
I agree with the TPA results after checking some of the calculations. I now see that my uneasiness with the RH response was caused by familiarity with RH response when no rubble pile was present. The response at late times differs markedly when a rubble pile is present.

2. Reflux3

I talked with Barbados about Alex exercising the reflux3 module in the next couple weeks. The goal would be to identify parameter ranges that lead to thermal seepage results that TEF can justify based on "expert" consensus, whatever that is. Barbados talked with Sitakanta about freeing up Alex's time to work on the reflux3 parameter input distributions. [This task falls outside the realm of George's validation testing, especially if TPA 5.0.0d results using reflux3 agree with TPA 4.1j results.]

3. Distribution of vaporization barrier seepage threshold temperature
TEF still needs to talk about this one, specifically what distribution to use instead of a constant value of 100 C. I anticipate using some of the results of Birkholzer's work to provide some basis for a distribution. We have not done any thermal seepage numerical modeling ourselves.

--Randy

From: George Adams [gadams@cnwra.swri.edu]
Sent: Monday, October 04, 2004 9:28 AM
To: rfedors@cnwra.swri.edu
Subject: RE: TEMP-RH PLOTS

Randy,

I'm sure glad I sent the plot to you. I saw the obvious blip at closure and was curious about the stair stepping, but the rest of it pretty much went past me. In the base case tpa.inp there is a seepage flag, FlagSeepageThreshold[] {iflag, 1}, and a seepage threshold temperature, SeepageThresholdT[C] {Constant, 100 C}, parameter. In Nfenv, if the flag is true {1} and rock wall temperature is above the seepage threshold temperature, then the flow hitting the waste package is added into the flow missing the waste package and then is zeroed. Also, in the basecase, there is a parameter TimeOfBackfillEmplaced[yr] which probably should be renamed, but is used to indicate the change from Preclosure to Postclosure. It is set to 10,000 years and this will then generate a blip at 10,000 years. At 10,000 years, it also eliminates the natural backfill effects, so I set it to what was in tpa.inp previously (50 years). I'll look into the areas that you mention and then talk to you about the plot.

George

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

From: Randy Fedors [mailto:rfedors@cnwra.swri.edu]
Sent: Monday, October 04, 2004 8:18 AM
To: gadams@cnwra.swri.edu
Subject: RE: TEMP-RH PLOTS

George,

You are getting better temperatures than Carol was getting with her testing on TPA 5.0y (after fixing obvious problems, the temperatures were ~20 C to high; the temperatures you show are closer to what we expected).

The RH blip at closure (ventilation turned off) is probably not realistic and was suppose to be eliminated when Osvaldo put in the smoothing between preclosure and postclosure RH. The smoothing doesn't appear to work anymore (disabled because of recent changes) or doesn't work as expected.

The other part of the RH curve that looks different from what I expected is from 1400 to 10,000 years. It's like there is a different model calculating RH for this later period. Why doesn't it rise up to near saturation anymore? Why the inflections at 1400 and 2000 years? Did someone try to link RH to the climate model?

The flux plot has the peculiar stair-stepping. I don't know why? Also, I have to look into what parameters are controlling the seepage during the thermal period. It appears that all seepage is eliminated when the wallrock is above 100 C. I did not realize that was the basecase model used by TPA.

--Randy

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

From: George Adams [mailto:gadams@cnwra.swri.edu]
Sent: Friday, October 01, 2004 4:18 PM
To: Randall Fedors
Subject: TEMP-RH PLOTS

Randy,

I'm doing some validation work on the NFENV module, and I wondered if you would take a look at the first plot which shows the relative humidity. This is a base case tpa5.0.0d for subarea 1. I include the drift degradation from mechfail and the default wedge of 25%. The point at 51 years stands out, but I also wanted to have your thoughts on this rh plot overall.

George

February 7, 2005 - February 11, 2005 -

Finished SCR #523 and updated scr_523.wpd Put changed files (tpa.inp, uzft.f, szft.f, exec.f, prenefmks.h) in checkin directory for Ron and Marty.

Finished modifications for SCR #552. Updated changes to ran.f, reader.f, and sampler.f. Updated scr_552.wpd. Fixed snllhs bug. Had to modify Makefile4.2 in the codes subdirectory and add "-xtypemap=real:64,double:64,integer:64" to snllhs.e section. Then code doesn't hang. It never hung on the PC and default compiler running on spock.

Started SCR #519.

Questionnaires: Razvan returned his. Paul is out sick. He gave 7 of his to Jude McMurry. I emailed her about them. Paul will work on the questionnaires when he gets back.

Paul has:

AlluviumMatrixGrainDensity__SAV[kg/m3]
AlluviumMatrixPorosity__SAV

ImmobileGrainDensity_STFF
AlluviumMatrixPoreRadius__SAV DELETED

Jude has:

FractureAperture_TSw
FractureAperture_CHnv
FractureAperture_CHnz
FractureAperture_PPw
FractureAperture_UCF
FractureAperture_BFw
FractureAperture_UFZ

Razvan had: RelativeRateOfBlanketRemoval[1/yr]

February 14, 2005 - February 18, 2005 -

Jude finished the questionnaire on Fracture Apertures and put it in Sitakanta's mailbox. Got it today. No changes to parameter values, but new description and justification.

Continued working on SCR #519.

Attended meeting (2/15 at 3:30 p.m.) with Sitakanta, Ron, Marty, Rob, and Bruce Goodwin (telecon). Ron will send Bruce the current copy of the Appendix A spreadsheet. Bruce will review it (check contents against the questionnaires he has) and make comments. He'll send it back to me. I'll resolve any issues Bruce brings up, and update the descriptions, comments/references/justifications, etc.

Ron has sent appropriate portions of the spreadsheet to the KTI leads at NRC. They will then send appropriate rows to selected points of contact. The POCs will review, comment, and return comments to Ron. They have until 3/18/2005. If changes are indicated, I'll incorporate them into the spreadsheet.

February 21, 2005 - February 25, 2005 -

Bruce worked over the weekend on the spreadsheet and returned App A. I asked him to put his & Juan's status column back in. He sort of incorporated his comments and status on top of the values we had in the PDF Type and Value(s) columns. I copied the columns and moved

them to the end of the spreadsheet. Then I deleted his mods from column B and C. The first 6 columns are intended to be the final form of the spreadsheet and will be copied over to Word Perfect when we need to finalize the Appendix for the new version of the User's Guide. I added a set of columns after Bruce's for my comments, etc. Need to review all of Bruce's markups and resolve any questions, issues. Need to go through questionnaires again and update any information provided. Worked on reformatting and started resolving questions and updating cell information.

Discovered bug in ebsfail/failt. Code was using Inner Inhibiting values for sulfate and carbonate when should have been using outer. Weld inhibitors were not being used at all when they should have been. Effective weld inhibitor vector needs to be calculated, written out to ebstrhc.inp, read by failt and then passed to the calculateWeldFailure subroutine instead of InhEff which should be used to calculate WP failure. Worked with Osvaldo on solution and implemented it.

Completed SCR #519. Updated scr_519.wpd. Passed all modified files (ashremob.f, dcags.f, ebsfail.f, ebsrel.f, exec.f, failt.f, nfenv.f, and tpa.inp) to Ron and Marty, who will be testing my mods.

Asked for some clarifications from Bruce; emails follow:

#1

From: Bruce Goodwin [goodwinb@mts.net]
Sent: Saturday, February 19, 2005 6:34 PM
To: Carol Scherer
Subject: Comments/justification column

Carol:

I updated the information in the comments/justification column for every parameter in my version of the spreadsheet for Appendix A. My entries were based on an evaluation of the questionnaire responses plus some additional information generated by Juan.

1. For responses that were 'satisfactory', the comments column contains the essential summary and the status column is highlighted green to indicate that everything is fine.

2. For all responses that were not 'satisfactory', the response sometimes indicates that a data update is coming (often dependent on data in the forthcoming DOE submission). The comments column is loaded with whatever is pertinent and the status column is flagged with orange with a note to the effect that a data update is coming or expected.

3. For all responses that were not 'satisfactory', I have put some useful information in the comments column and indicate what information is lacking in the status column. An "S" indicates that the data source is not specified and a "J" that the data is not justified. These cases also use an orange highlight.

4. There are a few more serious cases where there is no available data. I have used red highlighting in the status column with a D to denote data is needed.

5. Juan emailed me some additional information where some people had responded to my questionnaire evaluations. Pabalan and LaPlante are two such people, and another might be Janetzke or Fedors. For most parameters, this extra information made for a satisfactory response. I do not know whether Juan included the extra information with the original response, but the comments/justification column should include any cited references and key points and the status column will be highlighted green.

6. Juan emailed me some information on additional parameters, sometimes with parameter data. Those entries have been added, but often the comments column simply states "No information". I have not seen questionnaire responses for these parameters and the status column should be orange and note that S, J and sometimes D are needed.

7. Juan also created a version of Appendix A which appears to contain everything he knew about every parameter. It was somewhat unwieldy and, where I had no information from a questionnaire response etc., I condensed some of his description and inserted into the comments column. These parameters invariably have an orange highlight of course.

The above covers off what I recall and have rediscovered on the spreadsheet "AppendixA_V10.xls" which was generated to capture what we knew about the TPA parameters and auxiliary files. Does it answer your questions?

Bruce

#2

From: Bruce Goodwin [goodwinb@mts.net]
Sent: Sunday, February 20, 2005 11:54 PM
To: Carol Scherer
Cc: Sitakanta Mohanty
Subject: Review of spreadsheet for the TPA input file

Carol:

I have now finished a first complete pass through the current spreadsheet for the TPA input file ("Appendixa012805_sortSectionContact-1.xls").

1. I have checked the PDF types and attributes and other information in the spreadsheet against the entries in all hard and electronic copies of questionnaires responses in my possession. There are a few obvious problems and a larger number of probable corrections (for instance some parameters were apparently assigned to the wrong TPA modules).

2. I have also identified parameters for which I have no questionnaire responses. I last received a batch of responses near the start of September 2004. I do not know if I received all responses up to that time or if additional responses have been turned in since that time.

3. I reinstated the parameter 'status' information based on the questionnaire evaluations that were documented in my spreadsheet from September 2004.

4. I am now in the process of modifying this status information by identifying and evaluating changes since September 2004 to the parameter PDF type, PDF attributes and comments. This will yield an up-to-date picture of where problems may remain in identifying the source and justification for parameter data.

I expect to finish early tomorrow and will email you the results. Should we discuss the results on your return Tuesday, starting just after lunch?

Bruce

#3

From: Bruce Goodwin [goodwinb@mts.net]
Sent: Monday, February 21, 2005 2:07 PM
To: Carol Scherer
Subject: RE: Clarification

Carol:

I have attached a revised version of the Appendix A spreadsheet. I have used colour coding to indicate problems and added text to clarify.

1. "PDF type" column --> PDF type and attributes comparison

Green highlighting indicates that the PDF and data agree with the questionnaire responses that I have.

Orange highlighting indicates differences which might arise because the PDF type has changed or because I do not have a questionnaire response to check against. The inserted text comments will state which case holds.

2. "Values" column --> Status of documented support for the parameter

Green highlighting indicates that the PDF and its attributes have been sufficiently supported IN MY VIEW. The "comments" column will describe the source of the data and the justification of the data.

Orange highlighting indicates that further support is needed IN MY VIEW. The inserted text will indicate whether Source or Justification is needed. Sometimes new data has been installed into the spreadsheet and I have presumed that the existing (from last September) comments applied only to the old data, and hence new S&J is needed.

NOTE: The adequacy of the source and justification is essentially my judgement based on:

- a. my evaluation of the information presented in the questionnaire responses;
- b. my evaluation of follow-up comments from the experts forwarded to me by Juan;
- c. my evaluation of comments and data provided by Juan for those parameters that had no questionnaire response; and
- d. my assumption that all parameters that are used as program control features (e.g. all IFLAG type and other related parameters) do NOT need any support.

I strongly recommend a further review by the experts who supplied the data. They should be asked to confirm that S&J is correctly documented in the comments column. Some experts might also point out that the existing comments actually do provide the required support so that the S&J deficiency claim can be revoked.

3. "Comments" and "CNWRA Contact" columns: a few potential problems have been highlighted.

Finally, most of the changes noted above are consistent with the spreadsheet that I produced last September. However, I have also attempted to identify and evaluate all recent changes to determine whether the parameter status has changed. You will

find a few such cases. For instance, if the parameter PDF type or PDF attributes have changed since last September, I have indicated that S&J is required since the old S&J pertained to the old data (some comments have been deleted, but no new information has been added).

Let's talk Tuesday after lunch to decide the next step?

Bruce

#4

From: Bruce Goodwin [goodwinb@mts.net]
Sent: Thursday, February 24, 2005 10:03 PM
To: Carol Scherer
Subject: RE: question
Carol:

Both are abbreviations used in the questionnaire.

Exp - sparse data but practical experience and knowledge of similar systems

Alog - known behavior of analogous situations

Is everything else okay? Did you find many mistakes/glitches etc. and do my notes help?

Bruce

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

From: Carol Scherer [mailto:cscherer@cnwra.swri.edu]
Sent: February 24, 2005 3:07 PM
To: 'Bruce Goodwin'
Subject: question

What does [EXP, ALOG] mean?

February 28, 2005 - March 4, 2005 -

Met with Ron, Sitakanta, Marty, Al, Raz, and Brandi (George couldn't make it & Rob wasn't here) to discuss SCRs. The schedule has changed; we have March now to finish. There are also more SCRs. SCRs need to be finished by mid-March so there is time for the testing. My tasks are complete - SCRs 519, 523, & 552 are in the code. Marty is working on testing them. TPA5.0.01 is the current version.

Worked on verifying data in the Appendix A spreadsheet.

Also, Paul Bertetti returned some questionnaires that need to be reviewed and potentially incorporated into the spreadsheet.

March 7, 2005 - March 11, 2005 -

Continued work on Appendix A. Sitakanta has brought Brandi Winfrey onto the task. Spent time with her to show her what we've all been working on with the questionnaires, tpa.inp, and the Appendix. She and Lane Howard are working on justifications/references for the rows

where these cells are blank. Bruce Goodwin is working on updating comments with full References and any missing details from the questionnaires that he has.

Worked on verifying data in the Appendix A spreadsheet. Finished going over all the rows and verifying that the data we had from the Questionnaire Review in Dec./Jan. is the latest correct value or has been overwritten by an SCR. Not all SCRs have been completed and turned in to Ron so there may still be a few changes to make. Otherwise, I am done with my 1st task (see email).

From: Carol Scherer [cscherer@cnwra.swri.edu]
Sent: Wednesday, March 02, 2005 10:20 AM
To: Sitakanta Mohanty; Ronald Janetzke
Subject: Plan for finishing App. A. Sitakanta - you will want to read this one.

My goal is to have a spreadsheet containing App. A for the new User's Guide at the end of all checking and re-checking. This is what I suggest we do.

Current task:

Starting with Bruce's spreadsheet that he reviewed and returned 2-22-05, resolve all of his questions/issues. Update spreadsheet with information from current SCRs, so everyone is working with the latest information about tpa.inp parameters (about 1300 of them). I am in the middle of doing these things and expect to be finished by middle of next week. I have added columns to keep track of previous values, manner of changes, dates of changes, who made the change, etc. When this is done, we keep a snapshot copy of spreadsheet for documentation purposes, along with a copy of the spreadsheet as we sent it to Bruce and a copy of the spreadsheet as Bruce sent it back to us. Two problems to resolving all Bruce's comments: 1) a bunch of parameters are marked "data needed", "data expected", or "data possible" (I think these comments refer to comments on the questionnaires along the lines of "data needs to be updated after DOE turns in the license application"); 2) can't complete the "J, S needed" without getting more information from SMEs. This is mostly typing and rechecking out work from Dec./Jan. or questionnaires. It is pretty much a linear task and not conducive to sharing. It would be difficult for someone unfamiliar with the work we did during Dec./Jan. to work efficiently on this task. This is the task I gave the 80-hour estimate on; it looks like it won't take quite that long.

Next task:

Using a new copy of the spreadsheet after the changes listed above, update spreadsheet with information returned from Ron's request to SMEs to check and agree on values. After skimming the responses that I have copies of so far, two items are relevant to the task of approaching SMEs to update sources, justifications, descriptions, etc. 1) two of the responses DO contain information appropriate for justification, source, etc. 2) Names of contact people are changing. I think that information should be updated in the spreadsheet so we don't bug the wrong people and so we don't ask for info that someone has already given us. Once the spreadsheet is updated with this information, save snapshot copy of spreadsheet. This task is possibly shareable, as long as there is only one master copy of the spreadsheet around. Someone else could be entering data when I'm not here working on it. We would just have to agree on how we handle the task, so it wouldn't matter which of us did the work. I anticipate that this task will take 24 - 40 hours, depending upon number of changes identified. Calendar date for task completion dependent on when all people respond.

Third task:

Approach SMEs to fill in missing information. I could use help here, definitely. I would sort the spreadsheet by Contact, highlight the deficient areas, provide specific comments, if necessary, about what we

need. People would receive a generic set of instructions on what to review, update. It would be helpful, here, if we had an updated Reference list to give to people. We are getting source references such as (SAIC, 2003). I don't know if the specific reference intended is already included in the old App. A. reference list (I'm sure some aren't) or if there is the possibility for confusion without the entire source reference given. It would be more efficient to check this during this task than waiting until the User's Guide is ready for final review. Someone could start on this reference list update immediately; it is a separate although related task. We have references listed on questionnaires that need to be checked against and possibly added to the list. We'll need to ask the SMEs if existing references are now obsolete or superseded and should be removed. Duration of task will depend on SMEs availability. At the end of this task, App. A should be ready for the User's Guide, although I recommend keeping it in spreadsheet format until the User's Guide is ready for review. I would also recommend keeping a working copy of App. A. in spreadsheet form for easy updates as other changes are made to code during beta testing, etc. Someone could periodically review SCRs and update App. A. as indicated.

So, all that remains to Task One is to finish up with any outstanding questionnaires that have come in and any SCRs turned in after 3/11/05 (or after I left for the day). Will need to freeze the spreadsheet (AppendixA_working.xls for now; will change name to AppendixA_BG review.xls).

The next task is to update Appendix A with responses to Ron's email for the value checks (Concurrence Review). Responses are due by 3/18/05, although some have already come in.

March 14, 2005 - March 18, 2005 -

Ron has asked for Scientific Notebooks to be turned in covering 9/3/04 - 2/5/05. Made CD and hard copy. Gave them to Ron.

Received updates from Bruce Goodwin - he went back through the questionnaires he had and updated references. He checked the Reference list from Appendix A in the old User's Guide and updated it. He gave full references where needed in the spreadsheet. Updated AppendixA_working.xls with new info.

Received updates from Brandi and Lane - they were trying to fill in empty cells for Descriptions and Comments. Updated AppendixA_working.xls.

Since I had a little lag time waiting for SCRs to be finished, Ron gave me a task to look at tempwp from thermal.dat. When tempwp is plotted against Log Time, there is a glitch in the data. What's causing it? Didn't finish with analysis.

Ron out today, so froze spreadsheet (d:\css\appA\frozen\AppendixA_preConcurrenceReview_031805.xls). No more SCRs with new data can come in since Ron is out.

Sitakanta - look up parameters; how article implemented; SelectParticleModel(1,2) - change default to 2. comment Sorting Coefficient - only used in 1, but insufficient data for now - use model 2.

March 21, 2005 - March 25, 2005 -

App. A Concurrence Review updates made for all parameters with responses. There were

about 247 parameters for which there were no responses. Re-sorted so no-response parameters isolated and saved in d:\css\appA\backups\noresponse-ConcReview.xls. The updated version of the spreadsheet will be frozen Monday as d:\css\appA\AppendixA_ConcurrenceReview1.xls after I clean up the file (put columns where they belong, make sure cells are highlighted appropriately).

Meeting with Sitakanta, Ron, Lane, and Brandi. Lane is going to update tpa.inp when the values seem to be stable. Brandi is co-ordinating the Appendix A update task.

March 28, 2005 - April 1, 2005 -

App. A update late responses; consolidate comments; get ready to send out for desc/comments review; added new column to AppendixA_working.xls that specifies questions or missing information from cells for the current parameter (row).

Meeting Friday with Sitakanta, Ron, Lane, and Brandi to go over status and plans for Appendix A. Plan to send out rows of spreadsheet per Contact person next week asking for review of and updates for each parameter in spreadsheet.

April 4, 2005 - April 8, 2005 -

Finished going through the comments column and the questions column of the Appendix A spreadsheet. Handed it off to Brandi and Lane.

Started and completed implementing SCR # 564 - remove two Extrusive parameters from tpa.inp and added ExtrusiveEventFlag instead. Modified volcano.f to use new flag instead of old parameters. Created scr_564.wpd. Ran several tests. Code changes with ExtrusiveEventFlag and VolcanismDisruptiveScenarioFlag turned on gets same results as original (TPA5.0.0o) code, as long as you ensure same lhs outputs. Sent document and modified files to Ron.

If the geometric volcano model is the "old" model and distribution is the "new" model, shouldn't VolcanoModel default to 2 (geometric) instead of 1 (geometric)? Talked to Britt Hill. He says no. Turns out that the geometric is not the "old, obsolete, never going to use it anymore" model. It is still viable, except that when the code went from 3.0 to 4.0, the geometric model wasn't changed as intended. Britt says that for geometric, the source term comes from Conduit and NormalizedMagmaInducedMechanicalFailuresRemainingInDrift[] and the Dike-related parameters shouldn't be used at all. For distribution, the source term comes from NormalizedMagmaInducedMechanicalFailuresRemainingInDrift[] and NumberOfWPsEntrainedByEjecta[]. Ron thinks we may have kept the Dike area calculations for Sitakanta in order to keep a "true" geometric model. We all need to talk about this and figure out what should be in volcano.

Britt's email:

From: Brittain Hill [bhill@cnwra.swri.edu]
Sent: Tuesday, April 05, 2005 1:38 PM
To: Carol Scherer
Subject: Re: FW: VolcanoModel

Just so we're absolutely clear on this, the "geometric or distribution"

option only affects the number of waste packages that fail during an extrusive event (i.e., HLW source-term for ASHPLUMO calculations). This should default to the geometric distribution (=1), with the distribution distribution (=2) a selectable option for an alternative conceptual model for extrusive events.

For the intrusive event, however, the number of WP failed for hydrologic release should always be calculated from the distribution for NumberOfMagmaInducedMechanicalFailuresRemainingInDrift. This distribution should always be sampled, regardless of VolcanoModel =1 or =2. Previously, the "dike area" was used to calculate the intrusive source term for model=1, which is not a supportable model. Use NumberOfMagmaInducedMechanicalFailuresRemainingInDrift sampling for either VolcanoModel =1 or =2.

Thanks-
Britt

Carol Scherer wrote:

> Britt, we need your agreement if we do this. Do you want VolcanoModel to default to geometric or distribution?

>

> -----Original Message-----

> From: Ron Janetzke [mailto:rjanetzke@cnwra.swri.edu]

> Sent: Tuesday, April 05, 2005 11:38 AM

> To: Carol Scherer

> Subject: Re: VolcanoModel

>

> yes

>

> Carol Scherer wrote:

>

> >VolcanoModel still defaults to 1 (geometric). Were we going to change it to 2 (distribution)?

> >

> >

Decision to make changes based on email above pending discussions with Ron, Britt, & Sitakanta.

Started work testing SCR # 530 - long simulations. A one million-year run (basecase, 1 realization, all subareas, 4800 time steps after compliance period) is taking approximately 5 hours on Spock. The same thing, but mean case, took 47 minutes to run. Started several 1M-year runs. Also ran TPA500m runs for 10- and 100-K years, both base and mean cases. Started a 430-realization run for 1M years and 4800 times steps post compliance period. Started 10-K, 100-K, and 1M-year runs with a 2-line climato2.dat (0 and 1000000 years with the same numbers). Hope to compare *_c. files and have them come out the same. Running 100-K years with 200 time steps post compliance; should get the same outputs . . .

April 11, 2005 - April 15, 2005 -

Received SCR # 549 (time-dependent Fwet parameter for releaset.f) from Ron for testing. Set up working area for tests, but waiting until SCR 530 is finished before doing this one.

Continued testing SCR #530 (long simulations). Comparing TPA 5.0.0o runs with TPA5.0.0m runs. Testing space requirements for million-year runs will all append files turned

on, the restart option, and different climato2 files. Had to archive more files and remove them from spock. All space has been used up twice while running tests, not from long simulations but from other work going on. A single-realization run is taking 4-5 hours at one million years. Started analyzing results.

April 19, 2005 - April 22, 2005 -

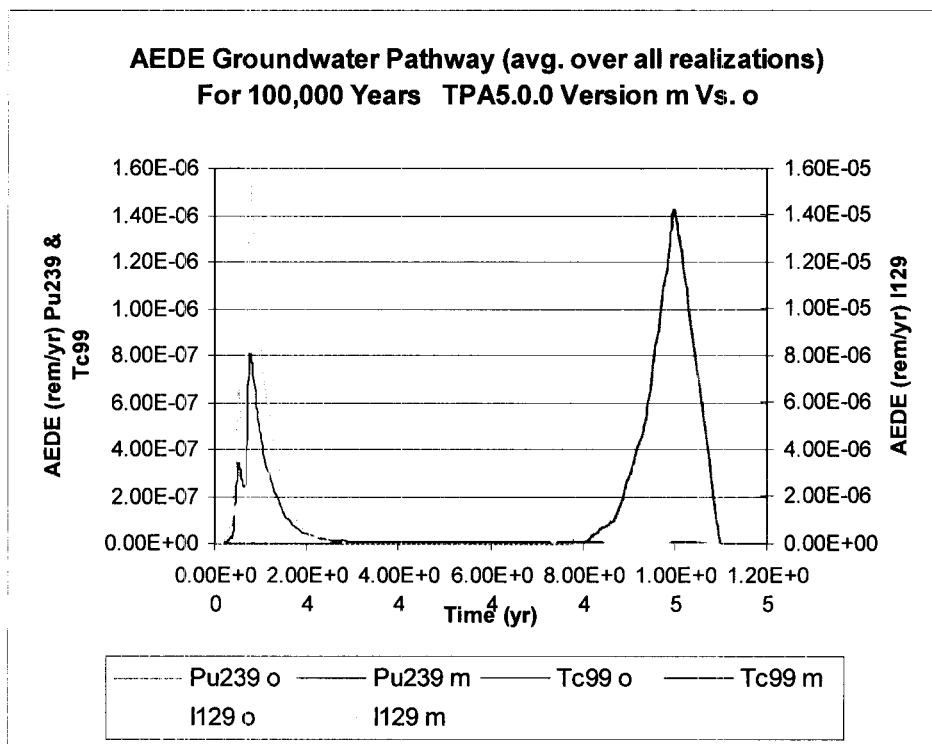
Monitor went kaput over weekend - Hollen brought up a different one and installed it.

Talked with Ron about the VOLCANO model. Decided to remove WidthOfVolcanicDike[m] from tpa.inp. Removed code from volcano.f that used width of dike and calculated area of dike. Also removed code that calculated position of conduit w.r.t. dike and overlap. Not interested in dike area any more, only in where dike intersects drifts. Ran a test for Ron where DiameterOfVolcanicConduit[m] was set to constant, 280.0 m, the maximum size of the conduit. This run determined that 123 WPs (max) would be ejected, a number that all the subareas could handle. Then, changed XlocationInRegionOfInterest to uniform[547900.0, 548360.0] and YlocationInRegionOfInterest to uniform [4078950.0, 4080875.0]. Also, modify exec.f to report WPs ejected in subarea identified by SubareaOfVolcanicEvent[] instead of hardcoding it to 2. This allows the center of the conduit and dike to vary within the repository. Can't use entire subare, because of odd shape and the break between subareas 1-6 and 7. Using a rectangular area that encompasses parts of subareas 2, 3, 5 & 6. This was part of SCR # 564. Finished the new mods and send tpa.inp and volcano.f to Ron. updated scr_564.wpd and sent him that. too. Ron and Rob are also making changes to drifts, so that they will be segmented instead of one long tube. That will affect results also.

Continued working on SCR # 530 - long simulations. Had to re-run some comparison runs between TPA5.0.0o and TPA5.0.0m to make sure data files used were the same (climato2.dat, wpflow.dat). Modified version m so that maxseismic events in seisadj.i was the same as version o (7100 instead of 1500) because that influenced numbers generated using seismichazard curve. Also modified refluxend in nfenv.f in version m to set refluxend to 20,000 instead of 10,000 years. Modified the tpa.inp in version o to leave out U233 and Th229 from the nuclide chains. The MatrixKds per layer for Cm were already the same. With these adjustments, the results for the 100000 years could be compared on a relatively level playing field.

Archived more older SCR directories. Space on spock is at a minimum. One million year runs with all files being generated and restart turned on (check.pnt files) can use over 1.1G.

SCR530 test to compare versions m and o at 100,000 years; see chart (NOTE: copy image of graph or chart, select chart, shift-Edit, copy Picture):

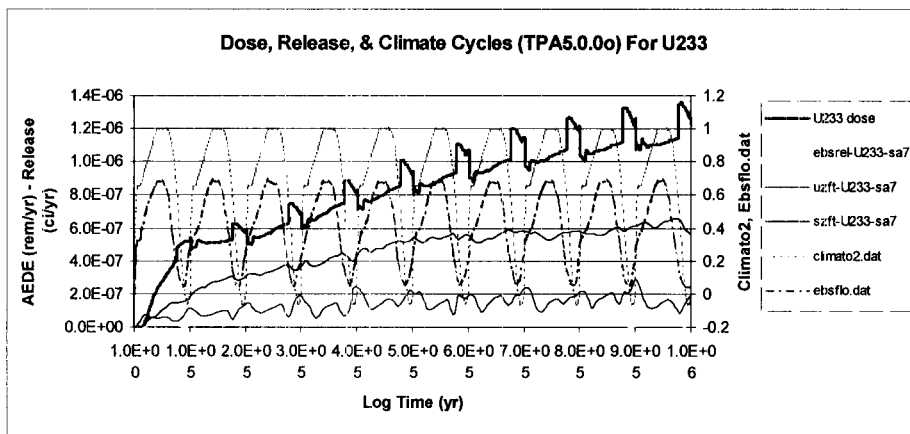


SCR530 - slt1 will compare versions m and o at 10,000 years while slt2 will compare at 100,000 years. Flt 1 (functional level test) will be a visual inspection of the changes listed in SCR530 (scr_530.wpd). This test failed due to the missing members of the 2nd colloidal chain. Sl1 - 3 (system level test) all pass. Sl4 is a test for multiple realizations (430 because there are 429 sampled parameters; this test fails - the TPA run bombs in realization 5 due to NEFTRAN problems. Sl5 is a test for resources and the restart option. All files are turned on, 4 realizations are run, execution is aborted after the 1st realization to test the check.pnt file and the restart option. This test fails also; there is no problem with restart at 10,000 years, but it doesn't work at 1,000,000 years (file dimensions ???). The subdirectory that contains the check.pnt file and output from 1 realization takes 1.2 G (not including source code and data). The subdirectory containing output from a completed 4-realization run takes 1.1 G (not including source code and data).

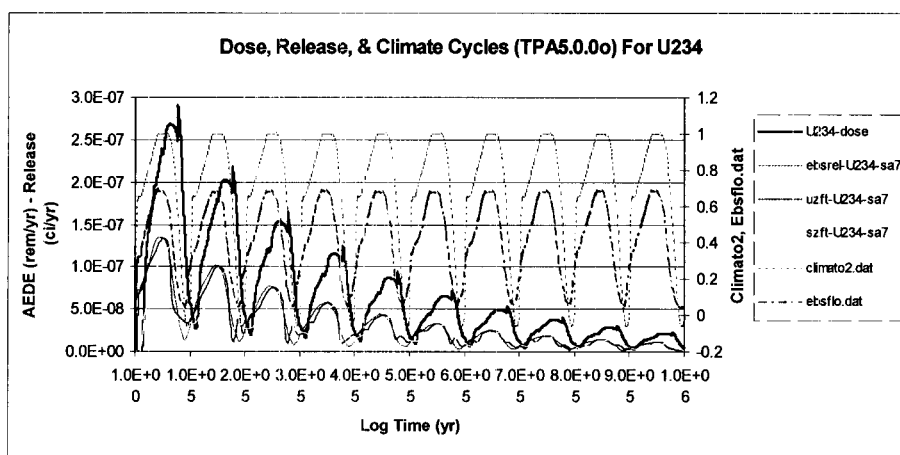
April 25, 2005 - April 29, 2005 -

Finished looking at results from TPA runs for SCR # 530 (long simulations). Graphed results for slt3 in spreadsheet containing rgwna.tpa data for 10,000, 100,000, and 1,000,000 years in rgwna-mean-alltimes.xls in spock: cscherer/scr530/test-report. Also included data from climato2.dat, ebsflo.dat, ebsrel.rlt, uzft.rlt, and szft.rlt. Only included data from subarea 7 and for the three uranium nuclides (U233, U234, and U238). The three graphs for these nuclides compare the cyclic dose output to the cycles in climato2.dat, ebsflo.dat and output from ebs, UZ, and SZ. See graphs a), b), and c) on next page.

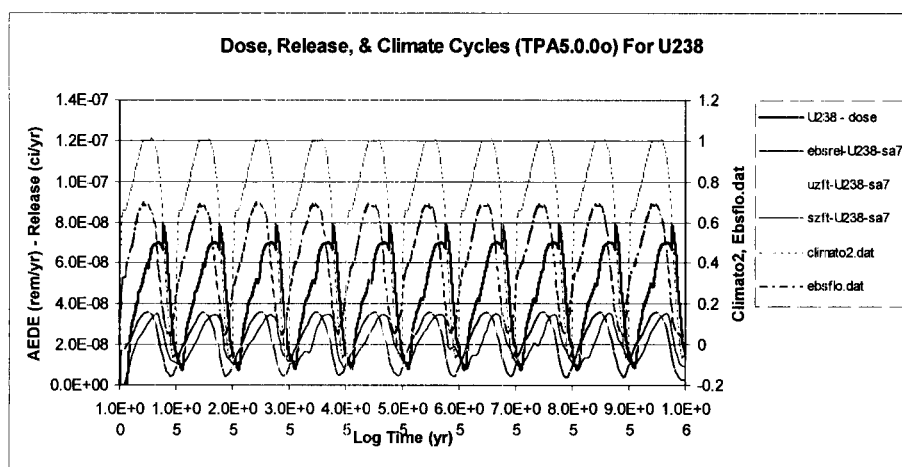
a) U233



b) U234



c) U238

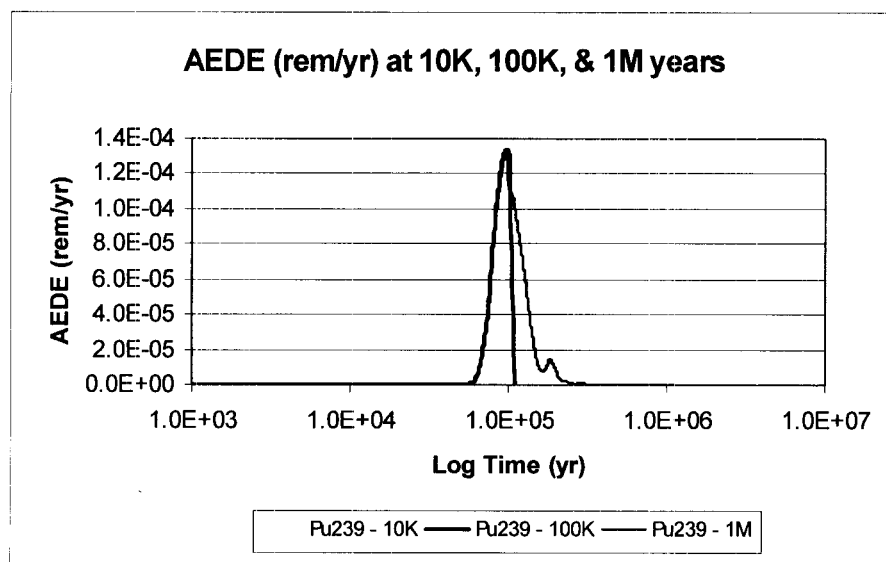


One question about the U-species graphs: what creates the “spike” shown right after the down turn of the dose cycles? Gave copies of graphs to Ron. Whatever causes the spike, it was around before the addition of long simulations and figuring out what it is more correctly belongs to validation testing than acceptance testing for SCR 530.

NOTES about *.tpa files:

1. last two lines are added for graphing purposes - years and data are “made up”; this was done for ease of graphing multiple realization runs; ignore the last two “time steps”/rows.
2. zero, values less than $1.0\text{e-}15$ are set to $1.0\text{e-}15$; so Nb94 shows $1.0\text{e-}15$ or “zero” dose for all time periods; all other elements showed some release (or dose).

For those nuclides that have dose/release beyond 100,000 years, the data trend follows the cycles from climato2.dat. (See uranium graphs above.) Cycles are also evident in flow (ebsflo.dat) and release data from EBS (ebsrel.rlt), UZ (uzft.rlt), and SZ (szft.rlt). Retardation of nuclides is shown by the shift or delay in the “peak” of the cycle as water flows down through the layers. Dispersion is shown by the “spreading” of the peaks. U-233 cycles are “muddy” due to the ingrowth of the radionuclide (U233 is a daughter product from the decay of 2nd aqueous nuclide chain (Cm245->Am241->Np237->U233->Th229). All nuclides were graphed from the 10K, 100K, and 1M runs. This was a check for continuity and to see if the results at 1M years seemed reasonable based on the results from the shorter duration runs. These tests passed. Pu239 is an example of a good test here. Pu239 dose peaks at approximately 100,000 years, so the graph of Pu239 at 100,000 years drops off sharply at 100,000 years. At 1M years, however, the dose falls more gradually and seems to be both continuous and meets the expectations of reasonable results.



Working on completing tp_scr530.wpd. All files necessary for the test report were copied to cscherer/scr530/test-report. There is a subdirectory for each functional level test (flt) and each system level test (slt). The run directories are all under cscherer/scr530/testruns. These directories were compressed (tar then bzip2) to free up space; spock went from 92% full to 88% full afterwards.

May 2, 2005 - May 6, 2005 -

Finished SCR530 and turned in everything to Ron. Compressed files. Archived as much as I could from Spock and Guardian:d:\. Supposed to get new computer next week. Hope it has enough oomph to run the new TPA for 1,000,000 years.

Started SCR # 549. Making runs.

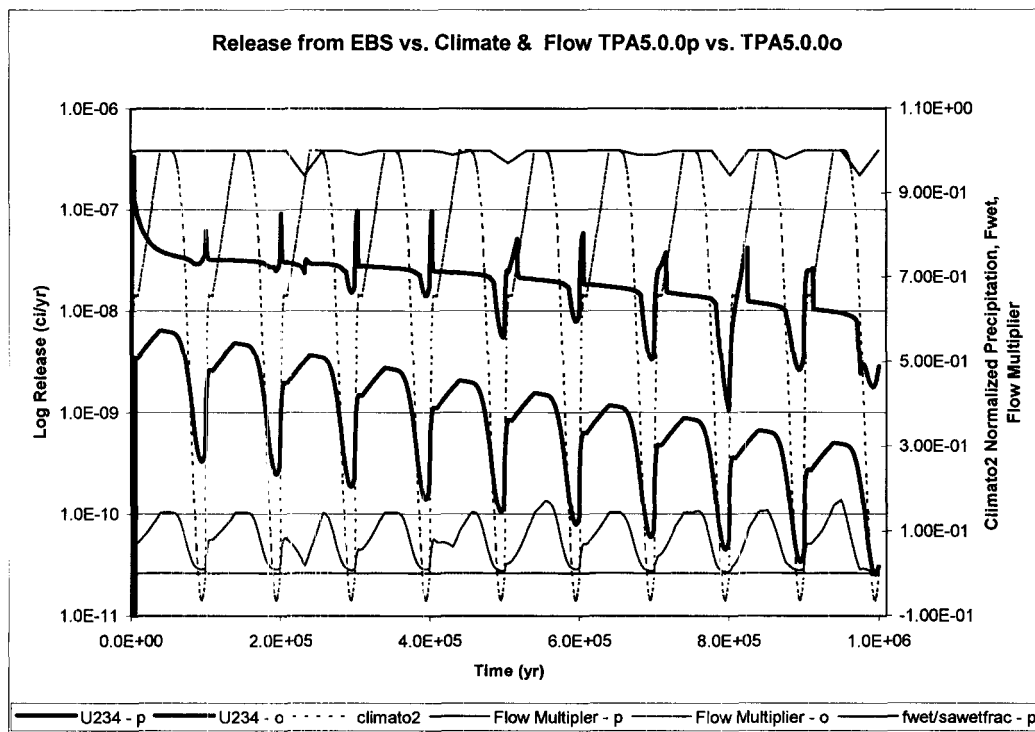
Left for the weekend with a 100,000-year run with all files appended for 430 realizations. Also started run for 1,000,000 years with all files appended for 1 realization.

In ebsnef.dat, 4 aqueous nuclides are listed twice (U238, Np237, Ra226, and Pb210). The 22 aqueous nuclide releases are listed first, then the 11 colloidal nuclide releases (including the 4 aqueous nuclides listed above which occur in both aqueous and colloidal chains). Using ebsnef.dat output as the System Level Test (slt1) for SCR549. Using a million year run to get the on/off solubility limited flag action.

May 9, 2005 - May 13, 2005 -

The 100,000-year run with all files appended and for 430 realizations took up 7.1G space on spock. Deleted the *.ech and *.rlt as well as nefiuz.cum and nefiisz.cum. That took it below 1G.

A one million-year run produces some very large file, e.g., ebsnef.dat is 4.9 M and is too large to fit entirely into an Excel spreadsheet (ebsnef-dat.xls). For SCR549, using the 3 uranium species from the aqueous release columns for TPA5.0.0p. Only used U234 from TPA5.0.0o. Graphed release (ci/yr) from ebsnef.dat against climato2.dat (for the climate cycles), fwet or sawetfrac from the new wpflow.def file, and "flow multipliers" from each run. Flow multiplier is drip/wp, fmult, fow, and flow factor from ebsflo.dat, all multiplied together.



May 16, 2005 - May 20, 2005 -

Finished tp_scr549.wpd. Made CD, updated scr_549.wpd, and turned everything in to Ron.

Rob found what he calls double counting of colloids when he implemented . Talked to David Pickett about the problem.

From: David Pickett [dpickett@cnwra.swri.edu]
Sent: Friday, May 20, 2005 2:43 PM
To: Carol Scherer
Subject: Colloid release

Carol,

As we discussed, I concur with the EBSREL implementation of the colloid release factor that results in enhanced radionuclide release. A comment line in the code stated, "Do not diminish solute nuclides when releasing colloids." This has, in fact, been a concern of mine, i.e., that in assigning a fraction of the released radionuclide mass to colloids with irreversible attachment, we were lowering the dissolved concentration. Colloids can enhance release, allowing total water concentrations to exceed solubility limits. Therefore, keeping the dissolved concentration unchanged is appropriate.

Of course, we need to ensure that, for each radionuclide, the additional mass being added in the form of the colloidal species is accounted for in the calculation of remaining wasteform inventory. That is, we should not be creating mass out of nothing.

Thanks,

David

Met with Ron Janetzke and Rob Rice to discuss validation testing for exec and system-level tests.

May 23, 2005 - May 25, 2005 -

Met with Ron and Rob again. We went through a list of tests Rob drew up when he was testing long simulations for TPA4.1jpdls. We added several tests to the system level validation testing.

David Pickett has been thinking about what he wants to do to correct the “double counting” problem for colloids. He wants to maintain the current method of adding the colloid releases without diminishing the aqueous amounts because colloids don’t count toward the solubility limit for nuclides. SCR 567 is to correct the “double counting” problem; also to fix the missing AF column for the last 3 nuclides in ebsrel.rlt.

May 31, 2005 - June 3, 2005 -

David has a solution for the “double counting of colloids”.. We’re going to calculate an “enhanced solubility limit” for the aqueous nuclides that have colloids associated with them (Am, Cm, Pu, and Th). The enhanced solubility limit will be written out to ebspac.nuc instead of the Solubility from tpa.inp. The enhanced solubility factor will be the old solubility times $1 + \text{ColloidReleaseFactor}$ divided by $1 - \text{ColloidReleaseFactor}$. The colloid release factor is the proportion of the mass of an element that is in colloidal form. Subtracting the colloid release factor from 1 gives the proportion of the element mass that is in aqueous form. Releasest reads the solubility limit from ebspac.nuc and will use it in its processing. This will allow for the more rapid depletion of the element due to the presence of colloids.

Finished coding the double colloid fix. Added a fix to uzft.f to SCR567. Femi discovered that the media printed out in uz_revers.out was incorrect. I used media from a previous loop, but it was always set for the last layer processed in the loop. That would be UFZ - the unsaturated fracture zone which is always going to be fracture. Legs retained for NEFMKS are more likely to be always matrix. Anyway, added an array, parallel to nefrd, called nefrd_media to save the media for each retained leg.

Completed SCR567 and gave modified files to Ron: uzft.f, exec.f, and ebsrel.f. Ron generated a new SCR580 to look at the checkpoint/restart problem I found testing SCR530. Restart works at 10K years, but not at 1M years. Probably a dimensioning problem; next guess would be some data needs to be saved that isn’t being saved currently.

June 6, 2005 - June 10, 2005 -

Multiple realizations, MatrixKD_Cm changed to Am values from TPA 4.1jpd.

List of system-level validation tests & SVTRs:

5/25/05

After 2nd meeting with R. Janetzke, R. Rice and C. Scherer, modified the following initial list of tests for Task ID 11 (Checkpoint/restart; system tests) for TPA 5.0.1 Module Validation to include some tests from R. Rice's 10/20/04 tests for TPA4.1jpdls. This list of tests includes verifying the correct functioning/specification of the following:

1. Checkpoint/restart for times beyond 100,000 yrs
2. WP counting (i.e., intrusive VOLCANO, INITIAL, FAULTING, SEISMIC, and CORROSION) for the number of WPs in a subarea - note that extrusive VOLCANO WP failures are intended to be double counted with the GW pathway WP failures
3. With VOLCANO activated, use a switch to select (i) the new ASHREMOB model and (ii) the previous model to compute GS dose; perform simulations with and without the DirectReleaseOnly switch activated
4. Determine consistency in output and convergence of results based on the number of time steps and the maximum simulation time (i.e., up to 5,001 time steps and a maximum simulation time of 1,000,000 yrs); run with a Compliance Period different than 10,000 yrs; and run with 1 large subarea with the about the same area that covers roughly the same region as subareas 1 through 6
5. Consistency in subarea coordinates in the tpa.inp file; repository outline, panels, and emplacement blocks in the repdes.dat file; and drift endpoints in the drifts.dat file - also, consistency in the number of WPs assigned to each subarea based on the information in these 3 files; perform tests using tpa.inp subarea coordinates and repdes.dat information with known outcomes
6. Select 1 subarea, divide that subarea (i.e., into 4 pieces), and examine TPA code output for the two cases
7. Activate the switch to run SZFT NEFTRAN twice using separate TUFF and ALLUVIUM legs and compare with the switch not activated (i.e., one SZFT NEFTRAN execution with two legs)
8. Functioning of the tpa.inp file flags (perform using one-on and all-others-off approach)
9. Failure to execute any of the TPA code standalone code results in stopped execution of the TPA code
10. Using a data code modification for calculating RDs, the values in the tpa.inp file are used in TPA code calculations. Turn off calculating KDs/RDs using coefkdeq.dat by setting number of actinides from 5 to 0. Former values for KDs/RDs for Am, Np, Pu, Th, and U are commented out in tpa.inp. Remove the comment

*indicators "***" for these values in tpa.inp.*

(Related to #10 - Note: maybe call Paul to ask about the information in the data file coefkdeg.dat to calculate RDs and whether this has been tested and is a part of the RARI Progress Report - or whether these values have been updated since then - this will determine the extent of needed testing for these values - I think, by looking at the comments, this information is included in the Progress Report and has been tested a lot already)

- 11. Run mean (tpameans.out), max (tpamax.out), and min (tpamin.out) runs at 10,000, 100,000, and 1,000,000 years.*
- 12. Check how TPA handles duplicate nuclides in the aqueous and colloidal chains.*
- 13. Run with TPA with a single nuclide, e.g., Tc99 or I129.*
- 14. Do time history plot for Np237.*
- 15. Check that TimeOfNextFaultingEventinRegionOfInterest[yr] and TimeOfNextVolcanicEventinRegionOfInterest[yr] are handled correctly.*
- 16. Test that dilution models have intended effect for both current climate and pluvial. Include test when DistanceToReceptorGroup[km] = 1 meter.*

My tests are 1, 3, 7, 8, and 10-16. That leaves 2, 4-6, and 9 for Rob Rice.

June 13, 2005 - July 8, 2005 -

Working on validation testing. Started with SVTRs 1, 7, 10, & 11 and TPA 5.0.1betaA. Redoing SVTRs as necessary as TPA updated to TPA 5.0.1betaD. Starting 12-14.

Disk space used has been sitting in the high 90s (e.g., 98, 99) and even 100%. Can't do 1M year runs or multiple realizations with so little space available. Having to archive work almost immediately. Jim Winterle looking into getting some space freed up. Spock down to 56% capacity, at least temporarily!

July 11, 2005 - July 15, 2005 -

Spock has a lot of space right now, which may not last, so decided to run the rest of the SVTR runs: # 12, 13, 14, 3, 8, 15, & 16. Got started on the runs. Worked on analysis and updating reports while waiting for runs to finish.

Attended meeting Thursday to hear PA discuss differences (S. Mohanty) in outputs between TPA4.1j and TPA5.0.1betaD. Also presentation (J. Winterle, R. Janetzke) on how subareas are represented and what the new subareas look like. NRC has some concerns about parameters that haven't been updated and whether or not the new subareas adequately deal with thermal issues.

July 18, 2005 - July 22, 2005 -

Worked mostly on SVTR11-3, Volcano-related flags. Ran 16 permutations of flag combinations at 10,000 and 1,000,000 years. Test results passed. Also worked on SVTRs 13 & 14.

Met with Ron and Al Lozano to discuss testing the most recent colloid-related changes to TPA.

Met with Paul Bertetti and Ron about fixing some things in `uz_kdrd.out` and `uz_revers.out`. Paul needs the changes to complete his validation testing, so will temporarily interrupt my validation testing to make modifications to `uzft.f` and maybe `exec.f`.

July 25, 2005 - July 29, 2005 -

Worked on SCR590. Finished modifications to `uzft.f` and `exec.f` to correct some formatting and content problems with `uz_kdrd.out` and `uz_revers.out`. Also updated the FAULTO parameters in `tpa.inp`. Working on the maxudist task.

New version out: TPA5.0.1betaF. Set up new directory for validation. Moved remaining tasks there. Trying to finish validation tasks in the next two weeks, provided there are no major changes to TPA that require tests to be re-run.

August 1, 2005 - August 5, 2005 -

Paul wants more changes to `uz` AND `sz` output files for SCR590. One of them may be trickier than all the others. Probably will make new subroutine to handle outputting `uz_kdrd.out`.

Sat in on meetings about how to handle colloids in TPA, how ash remobilization is abstracted in TPA and what, if any, changes may be required. Sounds like more changes will be coming to TPA that will probably affect our validation efforts.

September 21, 2005

Scott Painter gave me a copy of a 2-page draft Proposed Refinement for Irreversible Colloids Abstraction in TPA dated 8/16/2005, which contains the following information for proposed TPA code changes to colloid handling (retyped):

Overview of the abstraction:

Consider iron-oxide type corrosion products as dominant in waste package. Focus on release abstraction – transport model remains unchanged.

Physical picture is fast irreversible sorption with competition until all sorption sites on colloids are filled.

Pu, Am, Th, and Cm compete for available sorption sites on colloids. U also competes. Evaluate later whether U needs to be tracked as a colloidal species.

Assign radionuclide mass to colloids until *finite sorption capacity* is reached.

Remainder of radionuclide mass is dissolved (limited by solubility or dissolution rate).

Abstraction is conservative. Additional competition with stationary corrosion products may reduce releases, but this will require more detailed model and technical basis is more difficult to develop.

Dataflow:

(1) Before calling RELEASET, sample sorption capacity (colloid concentration * specific surface area * number sites per unit area). This is a new parameter S_X .

(2) For each of the five elements, sample *relative affinity* γ for corrosion product colloid. A K_d for sorption on hematite is adequate here. [My note, $\gamma_{Pu} = 1$]

(3) Sample solubility limit C_S for each radioelement.

(4) Calculate an *effective solubility limit* by assuming that Pu, Am, U are solubility limited and that sorption is described by a competitive Langmuir-like sorption model. Effective solubility limit is then

$$C_{\text{seff, Pu}} = C_{S, \text{Pu}} + S_X \frac{\gamma_{\text{Pu}} C_{S, \text{Pu}}}{\gamma_{\text{Pu}} C_{S, \text{Pu}} + \gamma_{\text{Am}} C_{S, \text{Am}} + \gamma_{\text{U}} C_{S, \text{U}}} \quad \text{and similar for Am.}$$

Solubility for Th and Cm are unchanged.

(5) Call RELEASET with the effective solubility limits.

(6) Using concentrations C_j as calculated by RELEASET, set the "J" species concentrations:

$$C_{J, \text{Pu}} = S_X \frac{\gamma_{\text{Pu}} \text{Min}(C_{\text{Pu}}, C_{S, \text{Pu}})}{\sum \gamma_j \text{Min}(C_j, C_{S, j})} \quad \text{where sum is over Pu, Am, Th, Cm, and U.}$$

(7) Dissolved concentration in water leaving waste package is the $C_{\text{Pu}} - C_{J, \text{Pu}}$.

Notes:

Final dissolved concentrations may be slightly above true solubility limit, but this is relatively unimportant.

At later times, when releases from waste package are limited by dissolution rate, colloids may take all released Pu. This is consistent with Los Alamos sorption experiments that show strong uptake and little desorption of Pu and Am and is not important for performance.

Required TPA modifications are minor.

Work needed on two parameter distributions, but we have distributions for other

parameters. Need to look at possible correlations in Kd values.

October 14, 2005 -

Scott made some changes to the above algorithm because RELEASET deals with ci/yr, not concentrations. So, releases need to be converted to concentrations for new calculations and the result converted back to releases. (6) - (7) above becomes:

(6) Convert release rate to concentration:

$$C[\text{kg/m}^3] = 2.795\text{e-}9 * \frac{\text{Release}[\text{ci/yr}] * t_{1/2}[\text{yr}]}{Q_{\text{out}}[\text{m}^3/\text{yr}]} * A[\text{AMU}]$$

where A is atomic weight, $Q_{\text{out}} = Q_{\text{in}}$ (for bathtub model, Q_{in} after bathtub fills, 0 before) and $t_{1/2}$ is the half-life

(7) Using concentrations C_j as calculated above, set the "J" species concentrations:

$$C_{\text{JPu}} = S_x * \frac{Y_{\text{Pu}} \text{Min}(C_{\text{Pu}}, C_{\text{S,Pu}})}{\sum Y_j \text{Min}(C_j, C_{\text{S,j}})} \quad \text{where sum is over Pu, Am, Th, Cm, and U.}$$

(8) $C_{\text{JPu}} = C_{\text{JPu}} * A / 1000$, where A is Atomic weight; converts from moles/m³ to kg/m³

(9) $C_{\text{JPu}} = \text{Min}(C_{\text{Pu}}, C_{\text{JPu}})$

(10) Dissolved concentration in water leaving waste package is the $C_{\text{Pu}} - C_{\text{JPu}}$.

(11) Convert from concentration back to release rate before written to output files.

Scott also provided the following "working" sampled parameters and values:

Sorption Capacity [moles/m³]
usersuppliedpwisecdf

(3 significant digits only)

3.93115E-6, 0.0
0.000116645, 0.05
0.00022018, 0.1
0.000462612, 0.2
0.000817224, 0.3
0.00142776, 0.4
0.0025857, 0.5
0.00462584, 0.6

0.00858462, 0.7
0.0164876, 0.8
0.034794, 0.9
0.0539524, 0.95
0.0938, 0.99
0.144244, 1.0

Affinity Factors: (γ 's) [m³/kg]

U
loguniform
0.1, 50.0

Pu
usersuppliedpwisecdf
10.0, 0.0
50.0, 0.15
100.0, 0.35
500.0, 0.85
1000.0, 1.0

Am
usersuppliedpwisecdf
100.0, 0.0
500.0, 0.15
1000.0, 0.35
5000.0, 0.9
10000.0, 1.0

November 8, 2005 -

Today, Scott modified step 1 and deleted step 8 in the above series of steps. Now, the entire thing looks like this:

Overview of the abstraction:

Consider iron-oxide type corrosion products as dominant in waste package. Focus on release abstraction – transport model remains unchanged.

Physical picture is fast irreversible sorption with competition until all sorption sites on colloids are filled.

Pu, Am, Th, and Cm compete for available sorption sites on colloids. U also competes. Evaluate later whether U needs to be tracked as a colloidal species.

Assign radionuclide mass to colloids until *finite sorption capacity* is reached.

Remainder of radionuclide mass is dissolved (limited by solubility or dissolution rate).

Abstraction is conservative. Additional competition with stationary corrosion products may reduce releases, but this will require more detailed model and technical basis is more difficult to develop.

Dataflow:

(1) Before calling RELEASET, sample sorption capacity (colloid concentration * specific surface area * number sites per unit area). This is a new parameter S_X . Convert S_X from moles/m³ to kg/m³ by multiplying S_X by 240/1000, where 240 is a rough average atomic weight and 1000 is number of moles in 1 kg.

(2) For each of the five elements, sample *relative affinity* γ for corrosion product colloid. A K_d for sorption on hematite is adequate here. [My note, $\gamma_{Pu} = 1$]

(3) Sample solubility limit C_S for each radioelement.

(4) Calculate an *effective solubility limit* by assuming that Pu, Am, U are solubility limited and that sorption is described by a competitive Langmuir-like sorption model. Effective solubility limit is then

$$C_{\text{seff, Pu}} = C_{S, \text{Pu}} + S_X \frac{\gamma_{\text{Pu}} C_{S, \text{Pu}}}{\gamma_{\text{Pu}} C_{S, \text{Pu}} + \gamma_{\text{Am}} C_{S, \text{Am}} + \gamma_{\text{U}} C_{S, \text{U}}} \quad \text{and similar for Am.}$$

Solubility for Th and Cm are unchanged.

(5) Call RELEASET with the effective solubility limits.

(6) Convert release rate to concentration:

$$C[\text{kg/m}^3] = 2.795\text{e-}9 * \frac{\text{Release}[\text{ci/yr}] * t_{1/2}[\text{yr}]}{Q_{\text{out}}[\text{m}^3/\text{yr}]} * A[\text{AMU}]$$

where A is atomic weight, $Q_{\text{out}} = Q_{\text{in}}$ (for bathtub model, Q_{in} after bathtub fills, 0 before) and $t_{1/2}$ is the half-life

(7) Using concentrations C_j as calculated above, set the "J" species concentrations:

$$C_{J, \text{Pu}} = S_X * \frac{\gamma_{\text{Pu}} \text{Min}(C_{\text{Pu}}, C_{S, \text{Pu}})}{\sum \gamma_j \text{Min}(C_j, C_{S, j})} \quad \text{where sum is over Pu, Am, Th, Cm, and U.}$$

(8) $C_{J, \text{Pu}} = \text{Min}(C_{\text{Pu}}, C_{J, \text{Pu}})$

(9) Dissolved concentration in water leaving waste package is the $C_{\text{Pu}} - C_{J, \text{Pu}}$.

(10) Convert from concentration back to release rate before written to output files.

Notes:


Final dissolved concentrations may be slightly above true solubility limit, but this is relatively unimportant.

At later times, when releases from waste package are limited by dissolution rate, colloids may take all released Pu. This is consistent with Los Alamos sorption experiments that show strong uptake and little desorption of Pu and Am and is not important for performance.

Required TPA modifications are minor.

Work needed on two parameter distributions, but we have distributions for other parameters. Need to look at possible correlations in Kd values.

Entries into Scientific Notebook #612-4e for pages 1 - 79 have been made by Carol S. Scherer. No original text entered into this Scientific Notebook has been removed.

 , manager , August 14, 2009

No Further entries