SOFTWARE RELEASE NOTICE

1. SRN Number: PA-SRN-229

2. Project Title: TSPA & Technical Integration Code	Project No. 20-01402-762
3. SRN Title: TPA Version 4.1	
4. Originator/Requestor: Bruce Mabrito	Date: 09/27/00

5. Summary of Actions

- ☐ Release of new software
- ■ Release of modified software:
  - ■ Enhancements made
  - ■ Corrections made
- ☐ Change of access software
- ☑ Software Retirement BW 2/12/2007

6. Persons Authorized Access

Name	Read Only/Read-Write	Addition/Change/Delete
Sitakanta Mohanty	RW	
Ron Janetzke	RW	
David Esh (NRC)	RW	
Tim McCartin (NRC)	RW	
James Firth (NRC)	RW	

7. Element Manager Approval: Gordon Wittmeyer Date: 9/27/2000

8. Remarks:

An 8mm tape containing FORTRAN source code for the TPA Version 4.1 code, and 1 data CD containing binary executable files for the PC/Windows NT platform were sent to NRC.

SOFTWARE SUMMARY FORM

01. Summary Date: 09/27/00	02. Summary prepared by (Name and phone): Sitakanta Mohanty (210) 522-5185	03. Summary Action: Modified
04. Software Date: 09/27/00	05. Short Title: TPA Version 4.1	
06. Software Title: TPA - System Performance Assessment Computer Code, Version 4.1		07. Internal Software ID: None

08. Software Type: ☐ Automated Data System ■ Computer Program ☐ Subroutine/Module	09. Processing Mode: ☐ Interactive ■ Batch ☐ Combination	10. Application Area: a. General: ☐ Scientific/Engineering ☐ Auxiliary Analyses ■ Total System PA ☐ Subsystem PA ☐ Other b. Specific:
11. Submitting Organization and Address: CNWRA/SwRI 6220 Culebra Road San Antonio, TX 78228		12. Technical Contact(s) and Phone: Sitakanta Mohanty (210) 522-5185

13. Software Application: The TPA Code consists of the following modules: UZFLOW, NFENV, EBSREL, UZFT, SZFT, DCAGW, FAULTO, SEISMO, VOLCANO, ASHPLUMO, ASHRMVO, DCAGS, LHS, EXEC.

14. Computer Platform: SUN Workstation PC	15. Computer Operating System: UNIX Windows NT	16. Programming Language(s): SUN FORTRAN 5.0 Lahey LF90 V4.5	17. Number of Source Program Statements: Approx. 41000 lines w/o stand alone codes
18. Computer Memory Requirements: 95 Mb	19. Tape Drives: None	20. Disk Units: N/A	21. Graphics: N/A

22. Other Operational Requirements:

Uses system environment variables: TPA_TEST and TPA_DATA.

23. Software Availability: ■ Available ☐ Limited ☐ In-House ONLY	24. Documentation Availability: ☐ Available ☐ Preliminary ■ In-House ONLY

25.

Software Developer: _____ Date: 9/27/2000

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CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
DESIGN VERIFICATION REPORT FOR CNWRA SOFTWARE

DEVELOPED SOFTWARE[1]

Software Title/Name: TOTAL-System Performance Assessment (TPA)

Version: 4.1 (both UNIX and NT)

Demonstration workstation: SPARC STATION 20 - SUN ~~4~~ 9/27/2000 (SOLARIS)

Operating System: Solaris 5.8

Developer: R. JANSTKE and S. Mohanty

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1. Software Requirements Description: TOP-018, Section 5.3

Software Requirements Description (SRD) and any changes thereto reviewed in accordance with QAP-002 requirements?

Yes: ☒ No: ☐ N/A: ☐

SRD Version: TPA Version 4.0

SRD Approval Date: 11/30/99

Notes: N/A

2. Software Development Plan (SDP): TOP-018, Section 5.4

a) The Element Manager has approved the SDP and any changes?

Yes: ☒ No: ☐ N/A: ☐

b) The SDP addresses applicable section of TOP-018, Appendix B, Software Development Plan Template?

Yes: ☒ No: ☐ N/A: ☐

SDP Version: TPA Version 4.0

SDP Approval Date: 2/15/2000

Notes: N/A - From Solaris 5.5.1 to Solaris 5.8, only change in operating system.

[1] See TOP-018, Table 1 for criteria.

DESIGN VERIFICATION REPORT FOR CNWRA SOFTWARE DEVELOPED SOFTWARE

3. Design and Development: TOP-018, Section 5.5.1, 5.5.2

a) Is development and module/subroutine-level testing documented either in scientific notebooks and/or in Software Change Reports (SCR)?

Yes: ☒ No: ☐ N/A: ☐

Scientific Notebook(s): CNWRA S/N 170E

SCR Number(s): PA-SCR-321 Through PA-SCR-326

Notes: Attachments to each SCR document description of activity and Testing.

b) Is development and module/subroutine-level testing sufficiently documented so that an informed reviewer can follow the testing procedures and logic?

Yes: ☒ No: ☐ N/A: ☐

Notes: See SCR Attachments.

c) Is development in accordance with the conventions described in the SDP/SCR, i.e. coding convention?

Yes: ☒ No: ☐ N/A: ☐

Notes: N/A

4. Internal Documentation: TOP-018, Section 5.5.3

Software internally documented to allow a user to understand the function(s) being performed and to follow the flow of execution of individual routines?

Yes: ☒ No: ☐ N/A: ☐

Module(s) Reviewed: TPA V.4.1 Seismo.f

TPA V.4.1 ZpostPC.f

TPA V.4.1 EXEC.f

Notes: Only difference between Unix and PC Versions of TPA V.4.1 are in the ZpostPC.f & ZpostUNX.f files.

5. Output: TOP-018, Section 5.5.4

Software designed so that individual runs are uniquely identified by Date, Time, Name of software and version?

Yes: ☒ No: ☐ N/A: ☐

Date and time of run: Tues Sept 26 19:54:26 2000

Name and version: TPA Version 4.1

Notes:

6. Code Reviews: TOP-018, Section 5.5.5

Are code reviews (if implemented) documented in a scientific notebook or in another format that allows others to understand the code review process and results?

Yes: ☐ No: ☒ N/A: ☐

Scientific Notebook: Code Reviews not yet budgeted.

Notes: Acquired code that is not to be modified is accepted as is. No code reviews required.

7. Medium and Header Documentation: TOP-018, Section 5.5.6

a) Program title block of main program contains required information?

Yes: ☒ No: ☐ N/A: ☐

Program Title: TOTAL-System Performance Assessment Code/TPA

Customer Name: U.S. NRC

Customer Office/Division: NRC Office of Nuclear Material Safety and Safeguards

Customer Contact(s): Tim McCartin

Customer Phone Number: 301-415-6681

Associated Documentation: Professional Information

Disclaimer Notice: Yes, 2 full paragraphs

Notes: N/A

b) Source code module header contains required information provides Program Name, Client Name, Contract Reference, Revision Number, and Revision History?

Yes: ☒ No: ☐ N/A: ☐

Module Reviewed: TPA V. 4.1 ARRAY.F

Module Reviewed: TPA V. 4.1 E65RSL.F

Module Reviewed: TPA V. 4.1 MV.F

Notes:

DESIGN VERIFICATION REPORT FOR CNWRA SOFTWARE
DEVELOPED SOFTWARE

7. Medium and Header Documentation, continued: TOP-018, Section 5.5.6

c) The physical labeling of software medium (tapes, disks, etc.) contain required information?

Yes: ☒ No: ☐ N/A: ☐

Program Name: TPA Version 4.1 (8mm Tape)

Module/Name/Title: TPA Source Code

Module Revision: 4.1 –

File Type (ASCII, OBJ, EXE): TAR - cvf/dev/rmt/0

Recording Date: September 27, 2000

Operating System of Supporting Hardware: SOLARIS 5.8

Notes: Source code used as example, not executable version.

8. User's Manual: TOP-018, Section 5.5.5

a) Is there a Users' Manual for the software?

Yes: ☒ No: ☐ N/A: ☐

User's Manual Version and Date: TPA 4.0 Users Manual, April 2000

Notes: NRC Contract No. NRC-02-97-009

b) Are there basic instructions for the use of the software?

Yes: ☒ No: ☐ N/A: ☐

Location of Instruction: Key STAFF members have a copy.

Notes: Section 21 has basic instructions

9. Acceptance Testing: TOP-018, Section 5.6

a) Does the acceptance testing demonstrate whether or not requirements in the SRD and/or SCR have been fulfilled?

Yes: ☒ No: ☐ N/A: ☐

Location of Test Results: CNWRA QA Records Room holds The

Notes: Acceptance Test Documentation

DESIGN VERIFICATION REPORT FOR CNWRA SOFTWARE DEVELOPED SOFTWARE

9. Acceptance Testing, continued: TOP-018, Section 5.6

b) Has acceptance testing been conducted for each intended computer platform and operating system?

Yes: ☒ No: ☐ N/A: ☐

Platform(s): NT Platforms in SwRI Div 10 & El Paso Consultants Office. Also on Sun platforms.

Operating System(s): Solaris 5.7 and 5.8; Windows NT 4.0

Location of Test Results: In CNWRA QA Records Room.

Notes:

c) Has installation testing been conducted for each intended computer platform and operating system?

Yes: ☒ No: ☐ N/A: ☐

Platform(s): Sun Solaris and Windows NT

Operating System(s): Solaris and NT

Location of Test Results: In The CNWRA Records Room.

Notes:

10. Configuration Control: TOP-018, Section 5.7

a) Is the Software Summary Form completed and signed?

Yes: ☒ No: ☐ N/A: ☐

Software Summary Form Approval Date: 9/27/2000

Notes:

b) Is a software technical description prepared, documenting the essential mathematical and numerical basis?

Yes: ☒ No: ☐ N/A: ☐

Location Technical Description: In The TPA V. 4.0. Users Guide.

Notes:

c) Is the source code available (or, is the executable code available in the case of (acquired/commercial codes)?

Yes: ☒ No: ☐ N/A: ☐

Location of Source Code: In The CNWRA QA Records Room

Notes:

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DESIGN VERIFICATION REPORT FOR CNWRA SOFTWARE DEVELOPED SOFTWARE

11. Configuration Control, continued: TOP-018, Section 5.7

d) Have all the script/make files and executable files been submitted to the Software Custodian?

Yes: ☒ No: ☐ N/A: ☐

Location of Script/Make Files: CNWRA QA Records Room – TPA V. 4.1 Folder

Notes: N/A

12. Software Release: TOP-018, Section 5.9

Upon acceptance of the software as verified above, has a Software release Notice, Form TOP-6 been issued?

Yes: ☐ No: ☐ N/A: ☐

Version number on software (1.0 for 1st issue): TPA Version 4.1

Version number on SRN: PA-SRN-229

Notes: N/A

13. Software Validation: TOP-018, Section 5.10

a) Has a Software Validation Test Plan (SVTP) been prepared for the range of application of the software?

Yes: ☐ No: ☒ N/A: ☐

Version/Date of SVTP: _____

Date reviewed and approved via QAP-002: _____

Notes: To be accomplished in the future.

b) Has a Software Validation Test Report (SVTR) been prepared that documents the results of the validation cases, interpretation of the results, and determination if the software has been validated?

Yes: ☐ No: ☒ N/A: ☐

Version/Date of SVTR: _____

Date reviewed and approved via QAP-002: _____

Notes: To be accomplished in the future.

Additional Remarks: N/A

Ron Janetzke 9-27-00
CNWRA Software Developer/Date

[signature] 9/27/2000
CNWRA Software Custodian/Date

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a tpa41/ 0 tape blocks
a tpa41/CLEANUP 3 tape blocks
a tpa41/array.f 58 tape blocks
a tpa41/ashplumo.f 38 tape blocks
a tpa41/ashrmovo.f 46 tape blocks
a tpa41/condxyzt.f 20 tape blocks
a tpa41/dcags.f 41 tape blocks
a tpa41/dcagw.f 230 tape blocks
a tpa41/ebsfail.f 65 tape blocks
a tpa41/ebsrel.f 100 tape blocks
a tpa41/exec.f 493 tape blocks
a tpa41/execa.i 4 tape blocks
a tpa41/execb.i 1 tape blocks
a tpa41/execc.i 1 tape blocks
a tpa41/faulto.f 17 tape blocks
a tpa41/fileunit.f 13 tape blocks
a tpa41/findelev.f 12 tape blocks
a tpa41/invent.f 87 tape blocks
a tpa41/iareader.f 76 tape blocks
a tpa41/ia.i 3 tape blocks
a tpa41/ia1.i 2 tape blocks
a tpa41/Makefile 2 tape blocks
a tpa41/max500yr.i 1 tape blocks
a tpa41/maxchain.i 1 tape blocks
a tpa41/maxnnucl.i 1 tape blocks
a tpa41/maxnsuba.i 1 tape blocks
a tpa41/maxntime.i 1 tape blocks
a tpa41/mv.f 23 tape blocks
a tpa41/nfenv.f 150 tape blocks
a tpa41/reflux2.i 1 tape blocks
a tpa41/nintv.i 1 tape blocks
a tpa41/notice.i 3 tape blocks
a tpa41/numrecip.f 13 tape blocks
a tpa41/path.i 1 tape blocks
a tpa41/peakfind.f 13 tape blocks
a tpa41/ran.f 91 tape blocks
a tpa41/reader.f 225 tape blocks
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a tpa41/reader2.i 1 tape blocks
a tpa41/reader3.i 1 tape blocks
a tpa41/reader4.i 1 tape blocks
a tpa41/driftsa.i 1 tape blocks
a tpa41/sampler.f 155 tape blocks
a tpa41/seismo.f 80 tape blocks
a tpa41/stop.i 1 tape blocks
a tpa41/subarea.f 72 tape blocks
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a tpa41/tpa.inp 119 tape blocks
a tpa41/tpa.inp.meanvalues 126 tape blocks
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a tpa41/uzflow.f 99 tape blocks
a tpa41/uzft.f 174 tape blocks
a tpa41/volcano.f 28 tape blocks
a tpa41/fu1.i 1 tape blocks
a tpa41/fu2.i 1 tape blocks
a tpa41/inventa.i 1 tape blocks
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a tpa41/inventk.i 1 tape blocks
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a tpa41/uz_flowr.i 2 tape blocks
a tpa41/uz_flowz.i 1 tape blocks
a tpa41/uz_parms.i 6 tape blocks
a tpa41/zportunx.f 23 tape blocks
a tpa41/codes/ 0 tape blocks
a tpa41/codes/Makefile 2 tape blocks
a tpa41/codes/README 1 tape blocks
a tpa41/codes/SIZES.INC 5 tape blocks
a tpa41/codes/SIZES2.INC 1 tape blocks
a tpa41/codes/ashplume.f 187 tape blocks
a tpa41/codes/failt.f 146 tape blocks
a tpa41/codes/nefmks.f 602 tape blocks
a tpa41/codes/releaset.f 239 tape blocks
a tpa41/codes/snllhs.f 385 tape blocks
a tpa41/codes/ebsfilt.f 25 tape blocks
a tpa41/codes/gentpa/ 0 tape blocks
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a tpa41/codes/gentpa/AIRPAR.CMN 3 tape blocks
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a tpa41/codes/gentpa/ANMPAR.CMN 2 tape blocks
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a tpa41/codes/gentpa/DECAY.CMN 1 tape blocks
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a tpa41/codes/gentpa/ORGMAS.CMN 1 tape blocks
a tpa41/codes/gentpa/ORGPAR.CMN 2 tape blocks
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a tpa41/codes/gentpa/anmcal.f 17 tape blocks
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a tpa41/codes/gentpa/crpcal.f 11 tape blocks
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a tpa41/codes/gentpa/edrres.f 6 tape blocks
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a tpa41/codes/gentpa/headng.f 6 tape blocks
a tpa41/codes/gentpa/idnuc.f 5 tape blocks
a tpa41/codes/gentpa/inhcal.f 6 tape blocks
a tpa41/codes/gentpa/initnv.f 5 tape blocks
a tpa41/codes/gentpa/intpol.f 4 tape blocks
a tpa41/codes/gentpa/invmol.f 3 tape blocks
a tpa41/codes/gentpa/makda2.f 2 tape blocks
a tpa41/codes/gentpa/Makefile 4 tape blocks
a tpa41/codes/gentpa/opnfil.f 12 tape blocks
a tpa41/codes/gentpa/order.f 9 tape blocks
a tpa41/codes/gentpa/packag.f 5 tape blocks
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a tpa41/codes/gentpa/xqin.f 11 tape blocks
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a tpa41/codes/itym/makefile 2 tape blocks
a tpa41/codes/itym/src/ 0 tape blocks
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a tpa41/codes/itym/src/array.f 59 tape blocks
a tpa41/codes/itym/src/check_valid.f 31 tape blocks
a tpa41/codes/itym/src/estimator.f 102 tape blocks
a tpa41/codes/itym/src/init_itym.f 8 tape blocks
a tpa41/codes/itym/src/itym.f 12 tape blocks
a tpa41/codes/itym/src/itym.i 17 tape blocks
a tpa41/codes/itym/src/itymutils.f 45 tape blocks
a tpa41/codes/itym/src/path.i 1 tape blocks
a tpa41/codes/itym/src/preuzf.i 1 tape blocks
a tpa41/codes/itym/src/ran.f 84 tape blocks
a tpa41/codes/itym/src/strtokfunc.f 71 tape blocks
a tpa41/codes/itym/src/uncertain.f 80 tape blocks
a tpa41/codes/itym/src/uncertain.i 24 tape blocks
a tpa41/codes/itym/src/unctab.i 1 tape blocks
a tpa41/codes/itym/src/zportunx.f 22 tape blocks
a tpa41/data/ 0 tape blocks
a tpa41/data/multiflo.dat 209 tape blocks
a tpa41/data/strmtube.dat 9 tape blocks
a tpa41/data/climato1.dat 1661 tape blocks
a tpa41/data/climato2.dat 5 tape blocks
a tpa41/data/dilution.dat 4 tape blocks
a tpa41/data/ebsfail.def 11 tape blocks
a tpa41/data/ebsrel.def 9 tape blocks
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a tpa41/data/ia.dat 15 tape blocks
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a tpa41/data/gs_pb_ad.dat 6 tape blocks
a tpa41/data/gs_pb_ci.dat 5 tape blocks
a tpa41/data/tefkti.inp 318 tape blocks
a tpa41/data/tpanames.dbs 144 tape blocks
a tpa41/data/ebsfilt.def 2 tape blocks
a tpa41/data/drythick.dat 1 tape blocks
a tpa41/data/nuclides.dat 9 tape blocks
a tpa41/data/burnup.dat 3 tape blocks
a tpa41/data/wpflow.def 35 tape blocks
a tpa41/data/FILENAME.DAT 2 tape blocks
a tpa41/data/gbioac1.dat 13 tape blocks
a tpa41/data/gdefault.def 7 tape blocks
a tpa41/data/gdosinc2.dat 1 tape blocks
```

```
a tpa41/data/gftrans.def 14 tape blocks
a tpa41/data/ggamen.dat 30 tape blocks
a tpa41/data/ggenii.def 28 tape blocks
a tpa41/data/ggrdf.dat 11 tape blocks
a tpa41/data/gnewdf.dat 20 tape blocks
a tpa41/data/grmdlib.dat 26 tape blocks
a tpa41/data/maidtbl.dat 1844 tape blocks
a tpa41/data/organdf.dat 14 tape blocks
a tpa41/ccdf/ 0 tape blocks
a tpa41/ccdf/tccdf.f 46 tape blocks
a tpa41/ccdf/tccdf.i 1 tape blocks
a tpa41/ccdf/tccdf.inp 2 tape blocks
a tpa41/ccdf/Makefile 1 tape blocks
```

B Mabrito 16/70

TPA V. 4.1 Software folder

CNWRA *A center of excellence in earth sciences and engineering*

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September 28, 2000
Contract No. NRC–02–97–009
Account No. 20.01402.762

U.S. Nuclear Regulatory Commission
ATTN: Mr. James Firth
Office of Nuclear Material Safety and Safeguards
Division of Waste Management
Performance Assessment and High-Level Waste Integration Branch
Mail Stop 7C–18
Washington, DC 20555

Subject: Transmittal of the TPA Version 4.1 Code

Dear Mr. Firth:

The purpose of this letter is to transmit the Total-system Performance Assessment Version 4.1 code which fulfills the newly established Administrative Item 20.01402.762.003. Attached herewith is an 8mm tape containing FORTRAN source code for the SUN workstation and the Intel-based PC running NT4.0 operating system, and a CD containing the binary executable files for the PC platform. This version of the code contains approximately 77,000 lines of code and will execute the delivered *tpa.inp* file (base case with one realization and 10 subareas) in 9 minutes on a SUN SparcStation 20.

This version of the code has the following modifications:

(i) All modules were scanned for inappropriate variable names and much dead code was deleted while reformatting some of the difficult-to-read sections.

(ii) The default volcano model is now the model used in the TPA Version 3.3 code. The so-called "dog-leg" model can be selected as an alternative conceptual model.

(iii) The minimum alluvium leg length that can be sampled has been set to 100 meters to relax time-stepping constraints associated with the *nefmks.f* algorithm.

(iv) The "ArealAverageMeanAnnualInfiltrationAtStart" parameter range has been adjusted upward to a minimum of 4 and maximum of 13 as recommended by the USFIC KTI.

(v) The importance analysis implementation has been restructured to give the user more control over defining which parameters participate in the neutralization of various components, barriers, and subsystems. An additional data file (*ia.dat*) is provided as a means for the user to define the parameters. The *tpa.inp* importance analysis control flags are renamed and reorganized to facilitate the use of the new *ia.dat* file.

(vi) The AML used in the TPA code now closely approximates the reduced value used by the DOE (70,000 MTU per 1165 acres yields an AML of approximately 60 MTU/acre). This modification required the addition of subareas 9 and 10.

(vii) A revised *releaset.f* module was incorporated to handle peak releases that occur between TPA time steps.

(viii) Consumption rates for the critical group were changed to fixed mean values to avoid sampling unrealistic values.

(ix) The user specified time of climate change is now operational for all realizations; instead of just the first one.

This version of the TPA code represents about 7,000 lines of code changes. Most of these lines of code were comments that were removed or added in the code cleanup task. We have made a sincere effort to ensure that no lines were altered unintentionally by having each change reviewed by a second individual. In addition, the results of the modified code were reviewed by a third individual to verify that the output files were not changed as a result of the cleanup task. If any errors are found we will make the corrections and a revised TPA Version 4.1 will be shipped to you promptly.

If you have any questions on the installation and execution of the TPA code, please call Mr. Ron Janetzke at (210) 522-3318. If you questions on the additions and modifications that have been made to the TPA code please contact Dr. Sitakanta Mohanty at (210) 522-5185.

Sincerely yours,

Gordon W. Wittmeyer, Ph.D.
Manager, Performance Assessment

GWW/cw
Enclosure

cc: J. Linehan, D. Esh, W. Patrick, P. LaPlante
letter only D. DeMarco, R. Codell, CNWRA Directors, M. Smith
B. Meehan, C. Lui, CNWRA Element Managers, O. Pensado
J. Greeves, C. McKenney, T. Nagy (SwRI Contracts), S. Mayer
J. Holonich, M. Rahimi, P. Maldonaldo, R. Benke
B. Reamer, R Janetzke
S. Wastler, S. Mohanty
T. McCartin, J. Weldy

SOFTWARE CHANGE REPORT

SOFTWARE CHANGE REPORT (SCR)

SCR No. (*Software Developer Assigns*): PA-SCR-321	**Software Title and Version:** TPA 4.0	**/Project No:** 20-1402-762

Affected Software Module(s), Description of Problem(s):

All modules.

Cleanup code by removing dead code and scanning the code for inappropriate variable names.

Change Requested by: T. McCartin Date: 5-12-00	**Change Authorized by** (*Software Developer*): R. Janetzke Date: 6-12-00 Ron Janetzke

Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

All modules were scanned and modified as necessary.

Marleen Edgar 9-27-00

Implemented by: M. Hidalgo and R. Edgar	**Date:** 9-12-00

Description of Acceptance Tests:

See two Attachments.

Tested by: R. Edgar and M. Hidalgo	**Date:** 9/25/2000

Marleen Edgar 9-26-2000

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SOFTWARE VERIFICATION PLAN FOR TPA 4.0 SOFTWARE CLEANUP

1. Introduction

This document specifies the verification procedure for the TPA 4.0 software cleanup.

2. Scope

This document will not verify the results of the TPA 4.0 software. It is limited to verifying that the results produced by the TPA 4.0 software are unchanged after the files modified in the cleanup have been added to the software.

3. References

"Total-System Performance Assessment (TPA) Version 4.0 Code: Module Descriptions and User's Guide" prepared by Center for Nuclear Waste Regulatory Analyses, San Antonio, Texas, April 2000

4. General Requirements

The tester will need the following material to run this verification plan:

- A copy of the baseline TPA 4.0 files
- A copy of the Fortran files cleaned by Miguel Hidalgo
- A copy of the Fortran files cleaned by Reuben Edgar
- A copy of the Lahey Fortran 90 development system

5. The Verification of the TPA 4.0 Software

The TPA 4.0 software shall be tested to verify that produced output files are unchanged other than time, date, and spelling/spacing corrections. Perform the following procedure:

1. Create a directory called baseline_tpa40.
2. Copy the baseline TPA 4.0 software to the directory.
3. Make the baseline TPA program by executing the make.bat file in the baseline_tpa40 directory.
4. Create a directory called base_out.
5. Copy the tpa.exe and tpa.inp files to the base_out directory.
6. Copy all of the files with the "exe" extension from the baseline_tpa40\codes directory to the base_out directory.
7. Create a directory called base_out\data.
8. Copy the files from baseline_tpa40\data to base_out\data.
9. Set the environment variables tpa_data and tpa_test both to the base_out directory.
10. Execute the base_out\tpa.exe program in the base_out directory.
11. Create a directory called mh_tpa40.
12. Copy the baseline TPA 4.0 software to the directory.
13. Copy the files cleaned by Miguel Hidalgo to the mh_tpa40 directory. NOTE: it may be necessary to copy some of the cleaned files to the mh_tpa40\codes directory as appropriate to replace the associated Fortran files with the cleaned files.

14. Make the modified TPA program by executing the make.bat file in the mh_tpa40 directory.
15. Create a directory called mh_out.
16. Copy the tpa.exe and tpa.inp files to the mh_out directory.
17. Copy all of the files with the "exe" extension from the mh_tpa40\codes directory to the mh_out directory.
18. Create a directory called mh_out\data.
19. Copy the files from baseline_tpa40\data to mh_out\data.
20. Set the environment variables tpa_data and tpa_test both to the mh_out directory.
21. Execute the base_out\tpa.exe program in the mh_out directory.
22. Use a diff utility such as the one in WinXs Version 4.1 to compare the output in the base_out directory with the output in the mh_out directory and save the results in a mh_diffs.txt file.
23. Review the mh_diffs.txt file to verify that the only differences found are due to the date/time the files were produced or any spelling errors or spacing errors that were corrected.
24. If there are no differences other than those noted above, the test passes. Record the test results in Table 1.
25. Create a directory called rwe_tpa40.
26. Copy the baseline TPA 4.0 software to the directory.
27. Copy the files cleaned by Reuben Edgar to the rwe_tpa40 directory. NOTE: it may be necessary to copy some of the cleaned files to the rwe_tpa40\codes directory as appropriate to replace the associated Fortran files with the cleaned files.
28. Make the modified TPA program by executing the make.bat file in the rwe_tpa40 directory.
29. Create a directory called rwe_out.
30. Copy the tpa.exe and tpa.inp files to the rwe_out directory.
31. Copy all of the files with the "exe" extension from the rwe_tpa40\codes directory to the rwe_out directory.
32. Create a directory called rwe_out\data.
33. Copy the files from baseline_tpa40\data to rwe_out\data.
34. Set the environment variables tpa_data and tpa_test both to the rwe_out directory.
35. Execute the base_out\tpa.exe program in the rwe_out directory.
36. Use a diff utility such as the one in WinXs Version 4.1 to compare the output in the base_out directory with the output in the rwe_out directory and save the results in a rwe_diffs.txt file.
37. Review the rwe_diffs.txt file to verify that the only differences found are due to the date/time the files were produced or any spelling errors or spacing errors that were corrected.
38. If there are no differences other than those noted above, the test passes. Record the test results in Table 1.

Table 1 Verification Tests Results

Baseline Output Directory	Tested Output Directory	Diff Output Filename	Pass	Fail
Base_out	Mh_out	Mh_diffs.txt	X	
Base_out	Rwe_out	Rwe_diffs.txt	X	

Test Plan Prepared by: Reuben Edgar Date: 9-7-2000

Test Plan Approved by: Ron Jamieson Date: 9-7-2000

Tested by Reuben Edgar Date: 9-7-2000

Test Results Approved by Ron Jamieson Date: 9-7-2000

Integration/Testing and Validation Procedure

The following tools and equipment were required to conduct the procedure.

- espsun.space.swri.edu Sun Microsystems workstation
- Sun Microsystems Inc. SunOS 5.5.1. Generic May 1996
- Fortran compiler - f77: SC4.0 18 Oct 1995 FORTRAN 77 4.0
- make utility
- "makeallandnotify" script
- "runandconverit" script
- "Windiff" utility by Microsoft
- FTP Software

The Integration/Testing and Validation procedure consist of the following steps:

1. FTP modified files (see figure 1) to the tpa40 source directory ("/we/hidalgo/tpa/origtpacd/tpa40") in espsun.space.swri.edu Sun Microsystems workstation.

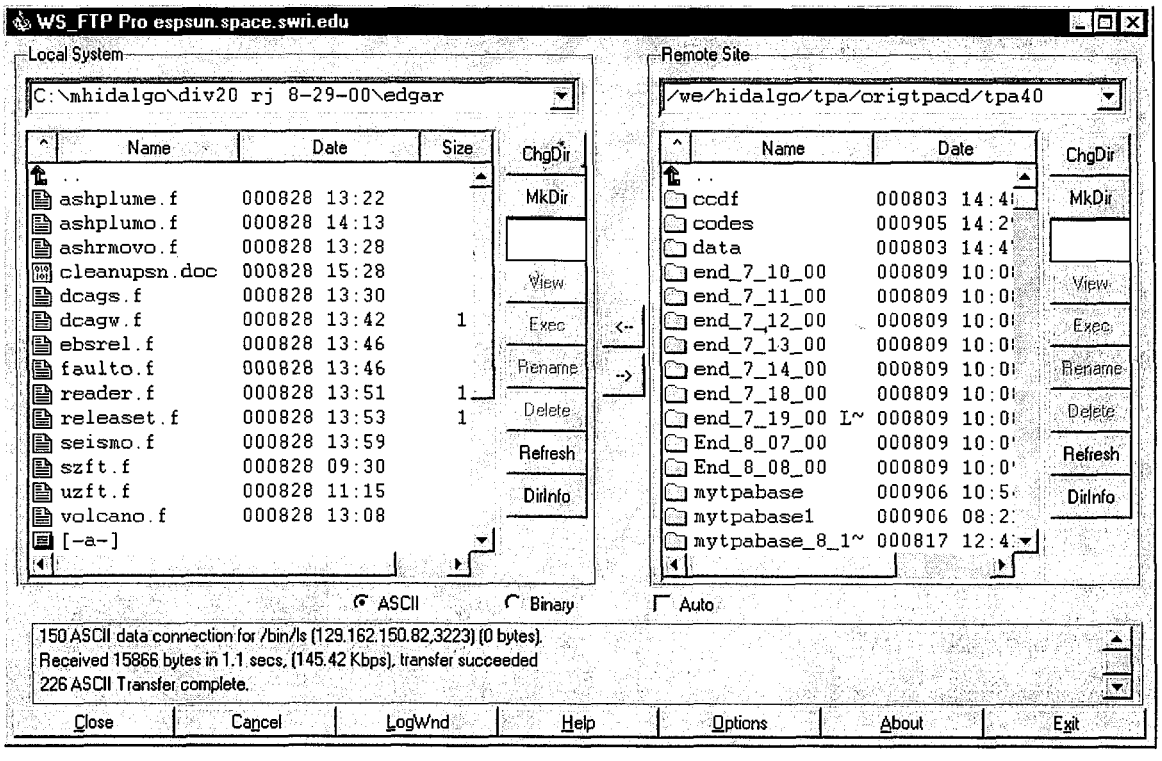

figure 1

The following modified files were FTP:

- faulto.f,
- reader.f,
- releaset.f,
- seismo.f,
- dcagw.f,
- ebsrel.f,
- dcags.f,
- ashrmovo.f,
- volcano.f, a
- shplumo.f

2. Execute the "*makeallandnotify*" script (see Appendix A for scripts) located in the "/we/hidalgo/tpa" directory.

   - The "*makeallandnotify*" scripts executes a make and compiles all code
   - After compilation, the "*makeallandnotify*" script sends e-mail to notify that the compilation process is completed, and calls the "*runitandconvert*".
   - The "*runitandconvert*" script executes the "**tpa.e**", and when the run is completed the output files are moved to "mytpabase" directory. Then, the "*runitandconvert*" sends e-mail to notify that the run is completed.

3. FTP all output files from "mytpabase" directory ("/we/hidalgo/tpa/origtpacd/tpa40/mytpabase") in espsun.space.swri.edu Sun Microsystems workstation to the local PC.

4. Compare the output files in "mytpabase" directory to the output files in the baseline directory "thetpabase" using the "WinDiff" (see figure 2) utility.

Figure 2 contains the list of all output files that differ in content.

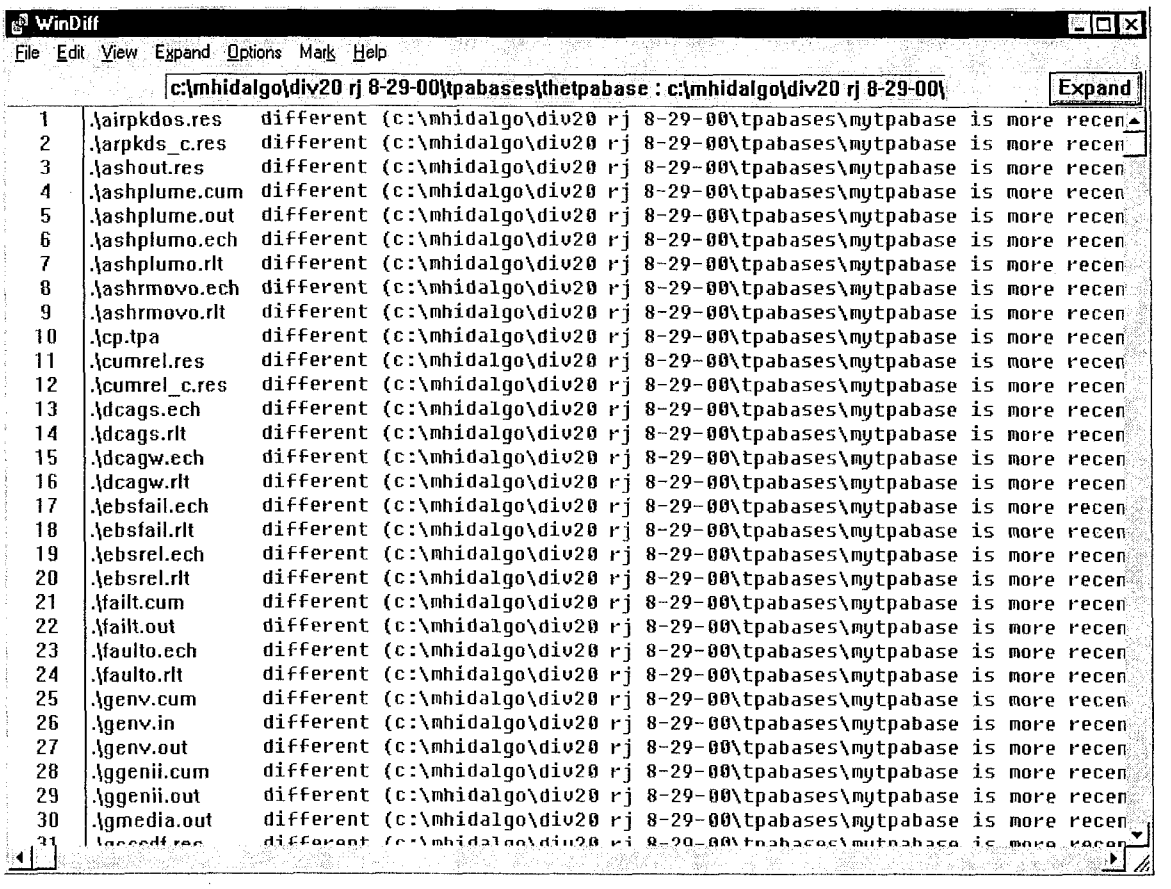

figure 2

5. Double clicking in the first item on the list – airpkdos.res – will cause "WinDiff" to compare the selected item and pinpoint with the "<!" and "!>" symbols, the difference between both files (see figure 3 in next page).

Figure 3 shows that the only difference between both output files is "Job started" date string. Look at the "<!" and "!>" symbols.

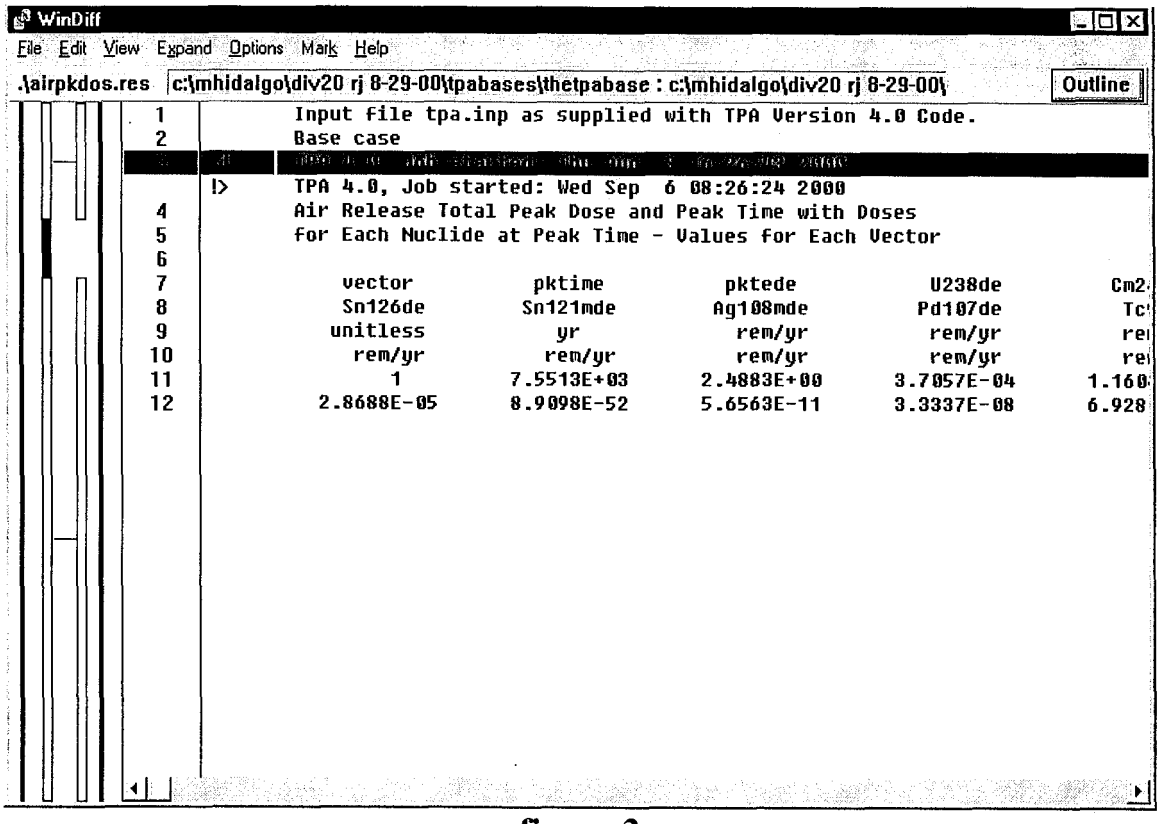

figure 3

The following outcomes can happen from this comparison:

- The data in the files is different
  - ❖ Outputs did not match baseline.
    The validation failed.
- The files differ only in the "Job started" date string
  - ✓ All outputs match baseline.
    The validation was successful

In the comparison in figure 3, the validation for these files was successful.

To complete validation, all files in the list in figure 3 must be compared. Once all files are compared, if the only differences were the "Job started" date string, then **the validation for all output files was successful.**

APPENDIX A

makeallandnotify script

```
#!csh
cd /we/hidalgo/tpa/origtpacd/tpa40/
make
rm done.txt
echo "SUBJECT:  Finished Make">done.txt
date >>done.txt
mail infoweb@informweb.com <done.txt
mail mhidalgo@swri.org <done.txt
cd /we/hidalgo/tpa/
runitandconvert
```

runitandconvert script

```
#!csh
cd /we/hidalgo/tpa/origtpacd/tpa40/mytpabase
rm *.*
cd /we/hidalgo/tpa/origtpacd/tpa40/
tpa.e
mv *.abb mytpabase
mv *.ash mytpabase
mv *.cum mytpabase
cp *.dat mytpabase
mv *.dbs mytpabase
mv *.dis mytpabase
mv *.ech mytpabase
mv *.in mytpabase
cp *.inp mytpabase
mv *.lgd mytpabase
mv *.nuc mytpabase
mv *.out mytpabase
mv *.res mytpabase
mv *.rlt mytpabase
mv *.src mytpabase
```

```
mv *.tpa mytpabase
mv *.vel mytpabase
mv *.buf mytpabase
mv *.def mytpabase
mv *.hdr mytpabase
mv *.log mytpabase
mv *.rel mytpabase
mv fc mytpabase
rm done.txt
echo "SUBJECT:  Finished RUN">done.txt
date >>done.txt
mail infoweb@informweb.com <done.txt
mail mhidalgo@swri.org <done.txt
```

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SOFTWARE CHANGE REPORT (SCR)

SCR No. (*Software Developer Assigns*): PA-SCR-322	Software Title and Version: TPA 4.0	/Project No: 20-1402-762

Affected Software Module(s), Description of Problem(s):

sampler.f, exec.f, tpa.inp, reader.f, iareader.f, ia1.i, ia.dat, uzft.f, szft.f, seismo.f, nfenv.f, ebsrel.f, ebsfail.f, dcagw.f

The current Importance analysis scheme requires code modification to make minor changes in the importance analysis method. A data file based scheme is desired.

Change Requested by:	**Change Authorized by** (*Software Developer*):
O. Pensado Date: 5-12-00	R. Janetzke Date: 8-24-00 Ron Janetzke

Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

Implementation of Importance Analysis involves work in several areas.
1) create data base handler utilities for the parameters to be controlled during the IA , i.e. iareader.f routines for reading ia.dat and writing ia.ech, and new updateIhs routine in sampler.f and sampler4.i.
2) create new control flag parameters for tpa.inp, and the ia.dat input file format.
3) remove use of the old tpa.inp flags (nfenv.f and iareader.f).
4) remove the use of aiafilter function from all routines (uzft, szft, seismo, nfenv, exec, ebsrel, ebsfail, dcagw)
5) move the location where the cp.tpa and sp.tpa files are written, with an duplicate section added specifically for the PVM case.

File ia.ech should only be produced when IA is selected in the tpa.inp file.

Implemented by:	**Date:**
R. Janetzke Ron Janetzke	8-23-00

Description of Acceptance Tests:

→ see attached sheets for the test plan

Tested by:	**Date:**
R. Rice	9/18/00

Summary of Test Results for SCR-322 - Importance Analysis
TPA Version 4.1

Testing by R. Rice
Date Completed 9/16/00

The following information was extracted from the electronic notebook kept by R. Rice for the period from 7/1/00 - 9/30/00. The information presents the test plan and a summary of the test results. The input, output, and data files are provided with this test results summary on a CD to R. Janetzke.

Received instructions from R. Janetzke to develop a test plan for the Importance Analysis features that were added to version 4.0. The following test plan was developed and faxed to R. Janetzke for his review and approval on 9/1/00. R. Janetzke approved of the test plan, but recommended comparing the *lhs.out* files, in addition to the ones listed. The following test plan includes these changes.

****

TPA Version 4.1 Test Plan: PA-SCR-322

Task Description: Activate importance analysis

Reason for Change: Enable the generation of sub-system, barrier, and component importance analysis

---

Analyst: Robert Rice **Date:** 8/31/00

Controlled Version: **Version 4.0 Released April 3,2000 (see the SCR322\v40 directory)**
Modified Version: **Version 4.1 modified source code for Importance Analysis from R. Janetzke via email attachment on 8/29/00 (see the SCR322\source directory)**

(Note: all tests are conducted for one realization and 201 time steps for 10,000 yr using the basecase *tpa.inp* input file)

Flag 1: ImportanceAnalysisFlag(yes=1,no=0)
Description: This is the master flag to control the importance analysis process. If this flag is zero all importance analysis is skipped regardless of the other component flag values.

Test 1. Run Versions 4.0 and 4.1 with their accompanying *tpa.inp* files with all append files ON, and ImportanceAnalysisFlag(yes=1,no=0) = 0 and all Importance Analysis flags inactive.

Purpose: Because Versions 4.0 and 4.1 should have the same results using their accompanying *tpa.inp* files, this test verifies the modifications introduced in Version 4.1 do not change the output with the importance analysis OFF.

TPA Output Files to Compare:

(use the "fc" DOS command in WINDOWS NT 4.0 with the script file *filecomp.bat*)
- *tpa.inp*
- all **.res* files
- all **.tpa* files
- all append files (**.ech*, **.rlt*, and **.cum*)
- *lhs.out*

Pass/Fail Criteria:

The results in all output files should be the same except for the time and date of the run. See the *filecomp.out* file for the differences between these two runs.

Documentation of Testing:

This test is stored in the SCR322/flag1/test1 directory. The Version 4.0 output is stored in the SCR322/v40 directory. All testing output files are archived on a CD.

Test 2. Run Versions 4.0 and 4.1 with their accompanying tpa.inp files for 10,000 yr with all append files ON, ImportanceAnalysisFlag(yes=1,no=0) = 1 (ON), and all other flags with the barriers inactive.

Purpose: Because Versions 4.0 and 4.1 should have the same results using their accompanying *tpa.inp* files, this test verifies the modifications introduced in Version 4.1 do not change the output. Moreover, with only the importance analysis flag = 1 (ON) and all other importance analysis flags inactive, there should be no difference in the results for Versions 4.0 and 4.1.

TPA Output Files to Compare:

(use the "fc" DOS command in WINDOWS NT 4.0 with the script file *filecomp.bat*)
- *tpa.inp*
- all **.res* files
- all **.tpa* files
- all append files (**.ech*, **.rlt*, and **.cum*)
- *lhs.out*

Pass/Fail Criteria:

The results in all output files should be the same except for the time and date of the run. See the *filecomp.out* file for the differences between these two runs.

Documentation of Testing:

This test is stored in the SCR322/flag1/test2 directory. The Version 4.0 output is stored in the SCR322/v40 directory. All testing output files are archived on a CD.

Test 3. Run versions 4.0 and 4.1 with their accompanying *tpa.inp* files for 10,000 yr with all append files ON, ImportanceAnalysisFlag(yes=1,no=0) = 0 (OFF) but all other importance analysis components active.

Purpose: Because Versions 4.0 and 4.1 should have the same results using their accompanying *tpa.inp* files, this test verifies the modifications introduced in Version 4.1 do not change the output. Moreover, with the importance analysis flag = 0 (OFF) and all other components active, there should be no difference in the results for Versions 4.0 and 4.1.

TPA Output Files to Compare:

(use the "fc" DOS command in WINDOWS NT 4.0 with the script file filecomp.bat)
- tpa.inp
- all *.res files
- all *.tpa files
- all append files (*.ech, *.rlt, and *.cum)
- *lhs.out*

Pass/Fail Criteria:

The results in all output files should be the same except for the time and date of the run. See the *filecomp.out* file for the differences between these two runs.

Documentation of Testing:

This test is stored in the SCR322/flag1/test3 directory. The Version 4.0 output is stored in the SCR322/v40 directory. All testing output files are archived on a CD.

Testing for Flags 2-24

Description: Each of these flags will be examined individually with one test to ensure that the values specified in the *ia.dat* file for each flag is properly transferred from the *tpa.inp* file to the *cp.tpa* file. The following information lists the (1) *ia.dat* file with the parameter values and the flag name and (2) the *tpa.inp* file parameter names that should be modified in the *cp.tpa* file for each of the flags.

Listing of *ia.dat*:

```
TITLE: Importance Analysis data for the TPA code using the IA option.
TITLE: Developed for TPA 4.1 on 8-02-00.
**
  SUBSYSTEM = 'SubsystemNaturalStudy'
**
  BARRIER   = 'BarrierBiosphereStudy'
**
  Component = 'ComponentPrecipitationStudy'
**
  parameter = 'WastePackageFlowMultiplicationFactor'
  value     = 1.11111
```

```
**
  parameter = 'SubAreaWetFraction'
  value     = 2.22222
**
  BARRIER   = 'BarrierUpperUnsaturatedZoneStudy'
**
  Component = 'ComponentTivaCanyonStudy'
**
  parameter = 'ElevationOfGroundSurface[m]'
  value     = 3.33333
**
  parameter = 'MassDensityofYMRock[kg/m^3]'
  value     = 4.44444
**
  parameter = 'SpecificHeatofYMRock[J/(kg-K)]'
  value     = 5.55555
**
  parameter = 'ThermalConductivityofYMRock[W/(m-K)]'
  value     = 6.66666
**
  parameter = 'EmissivityOfDriftWall[-]'
  value     = 7.77777
**
  parameter = 'CritChlorideConcForFirstLayer[mol/L]'
  value     = 8.88888
**
  parameter = 'CritChlorideConcForSecondLayer[mol/L]'
  value     = 9.99999
**
  BARRIER   = 'BarrierLowerUnsaturatedZoneStudy'
**
  Component = 'ComponentTSwStudy'
**
  parameter = 'TSw_Thickness_1SubArea[m]'
  value     = 10.10101
**
  parameter = 'TSw_Thickness_2SubArea[m]'
  value     = 11.11111
**
  parameter = 'TSw_Thickness_3SubArea[m]'
  value     = 12.12121
**
  parameter = 'TSw_Thickness_4SubArea[m]'
  value     = 13.13131
**
  parameter = 'TSw_Thickness_5SubArea[m]'
  value     = 14.14141
**
  parameter = 'TSw_Thickness_6SubArea[m]'
  value     = 15.15151
**
  parameter = 'TSw_Thickness_7SubArea[m]'
  value     = 16.16161
**
```

```
  parameter = 'TSw_Thickness_8SubArea[m]'
  value     = 17.17171
**
  Component = 'ComponentCHnvStudy'
**
  parameter = 'CHnvThickness_1SubArea[m]'
  value     = 18.18181
**
  parameter = 'CHnvThickness_2SubArea[m]'
  value     = 19.19191
**
  parameter = 'CHnvThickness_3SubArea[m]'
  value     = 20.20202
**
  parameter = 'CHnvThickness_4SubArea[m]'
  value     = 21.21212
**
  parameter = 'CHnvThickness_5SubArea[m]'
  value     = 22.22222
**
  parameter = 'CHnvThickness_6SubArea[m]'
  value     = 23.23232
**
  parameter = 'CHnvThickness_7SubArea[m]'
  value     = 24.24242
**
  parameter = 'CHnvThickness_8SubArea[m]'
  value     = 25.25252
**
  Component = 'ComponentCHnzStudy'
**
  parameter = 'CHnzThickness_1SubArea[m]'
  value     = 26.26262
**
  parameter = 'CHnzThickness_2SubArea[m]'
  value     = 27.27272
**
  parameter = 'CHnzThickness_3SubArea[m]'
  value     = 28.28282
**
  parameter = 'CHnzThickness_4SubArea[m]'
  value     = 29.29292
**
  parameter = 'CHnzThickness_5SubArea[m]'
  value     = 30.30303
**
  parameter = 'CHnzThickness_6SubArea[m]'
  value     = 31.31313
**
  parameter = 'CHnzThickness_7SubArea[m]'
  value     = 32.32323
**
  parameter = 'CHnzThickness_8SubArea[m]'
  value     = 33.33333
```

```
**
  Component = 'ComponentPPwStudy'
**
  parameter = 'PPw_Thickness_1SubArea[m]'
  value     = 34.34343
**
  parameter = 'PPw_Thickness_2SubArea[m]'
  value     = 35.35353
**
  parameter = 'PPw_Thickness_3SubArea[m]'
  value     = 36.36363
**
  parameter = 'PPw_Thickness_4SubArea[m]'
  value     = 37.37373
**
  parameter = 'PPw_Thickness_5SubArea[m]'
  value     = 38.38383
**
  parameter = 'PPw_Thickness_6SubArea[m]'
  value     = 39.39393
**
  parameter = 'PPw_Thickness_7SubArea[m]'
  value     = 40.40404
**
  parameter = 'PPw_Thickness_8SubArea[m]'
  value     = 41.41414
**
  Component = 'ComponentUCFStudy'
**
  parameter = 'UCF_Thickness_1SubArea[m]'
  value     = 42.42424
**
  parameter = 'UCF_Thickness_2SubArea[m]'
  value     = 43.43434
**
  parameter = 'UCF_Thickness_3SubArea[m]'
  value     = 44.44444
**
  parameter = 'UCF_Thickness_4SubArea[m]'
  value     = 45.45454
**
  parameter = 'UCF_Thickness_5SubArea[m]'
  value     = 46.46464
**
  parameter = 'UCF_Thickness_6SubArea[m]'
  value     = 47.47474
**
  parameter = 'UCF_Thickness_7SubArea[m]'
  value     = 48.48484
**
  parameter = 'UCF_Thickness_8SubArea[m]'
  value     = 49.49494
**
  Component = 'ComponentBFwStudy'
```

```
**
  parameter = 'BFw_Thickness_1SubArea[m]'
  value     = 50.50505
**
  parameter = 'BFw_Thickness_2SubArea[m]'
  value     = 51.51515
**
  parameter = 'BFw_Thickness_3SubArea[m]'
  value     = 52.52525
**
  parameter = 'BFw_Thickness_4SubArea[m]'
  value     = 53.53535
**
  parameter = 'BFw_Thickness_5SubArea[m]'
  value     = 54.54545
**
  parameter = 'BFw_Thickness_6SubArea[m]'
  value     = 55.55555
**
  parameter = 'BFw_Thickness_7SubArea[m]'
  value     = 56.56565
**
  parameter = 'BFw_Thickness_8SubArea[m]'
  value     = 57.57575
**
  BARRIER   = 'BarrierSaturatedZoneStudy'
**
  Component = 'Component_STFF_SAV_Study'
  parameter = 'DistanceToTuffAlluviumInterface[km]'
  value     = 58.58585
**
  BARRIER   = 'BarrierReceptorGroupStudy'
**
  Component = 'ComponentWellWaterStudy'
**
  parameter = 'WellPumpingRateAtReceptorGroup10km[gal/day]'
  value     = 59.59595
**
  parameter = 'WellPumpingRateAtReceptorGroup20km[gal/day]'
  value     = 60.60606
**
  SUBSYSTEM = 'SubsystemEngineeredStudy'
**
  BARRIER   = 'BarrierDriftStudy'
**
  Component = 'ComponentBackfillStudy'
  parameter = 'EmplacementBackfillThickness[m]'
  value     = 61.61616
**
  Component = 'ComponentDripShieldStudy'
  parameter = 'DripShieldThickness[m]'
  value     = 62.62626
**
  BARRIER   = 'BarrierWastePackageStudy'
```

```
**
  Component = 'ComponentInnerContainerStudy'
  parameter = 'InnerWPThickness[m]'
  value     = 63.63636
**
  Component = 'ComponentOuterContainerStudy'
  parameter = 'OuterWPThickness[m]'
  value     = 64.64646
**
```

Listing of parameter names and values to check for flags 2-24:

Flag 2: SubsystemNaturalStudy

```
  parameter = 'WastePackageFlowMultiplicationFactor'
  value     = 1.11111
  parameter = 'SubAreaWetFraction'
  value     = 2.22222
  parameter = 'ElevationOfGroundSurface[m]'
  value     = 3.33333
  parameter = 'MassDensityofYMRock[kg/m^3]'
  value     = 4.44444
  parameter = 'SpecificHeatofYMRock[J/(kg-K)]'
  value     = 5.55555
  parameter = 'ThermalConductivityofYMRock[W/(m-K)]'
  value     = 6.66666
  parameter = 'EmissivityOfDriftWall[-]'
  value     = 7.77777
  parameter = 'CritChlorideConcForFirstLayer[mol/L]'
  value     = 8.88888
  parameter = 'CritChlorideConcForSecondLayer[mol/L]'
  value     = 9.99999
  parameter = 'TSw_Thickness_1SubArea[m]'
  value     = 10.10101
  parameter = 'TSw_Thickness_2SubArea[m]'
  value     = 11.11111
  parameter = 'TSw_Thickness_3SubArea[m]'
  value     = 12.12121
  parameter = 'TSw_Thickness_4SubArea[m]'
  value     = 13.13131
  parameter = 'TSw_Thickness_5SubArea[m]'
  value     = 14.14141
  parameter = 'TSw_Thickness_6SubArea[m]'
  value     = 15.15151
  parameter = 'TSw_Thickness_7SubArea[m]'
  value     = 16.16161
  parameter = 'TSw_Thickness_8SubArea[m]'
  value     = 17.17171
  parameter = 'CHnvThickness_1SubArea[m]'
  value     = 18.18181
  parameter = 'CHnvThickness_2SubArea[m]'
  value     = 19.19191
  parameter = 'CHnvThickness_3SubArea[m]'
  value     = 20.20202
  parameter = 'CHnvThickness_4SubArea[m]'
```

```
value     = 21.21212
parameter = 'CHnvThickness_5SubArea[m]'
value     = 22.22222
parameter = 'CHnvThickness_6SubArea[m]'
value     = 23.23232
parameter = 'CHnvThickness_7SubArea[m]'
value     = 24.24242
parameter = 'CHnvThickness_8SubArea[m]'
value     = 25.25252
parameter = 'CHnzThickness_1SubArea[m]'
value     = 26.26262
parameter = 'CHnzThickness_2SubArea[m]'
value     = 27.27272
parameter = 'CHnzThickness_3SubArea[m]'
value     = 28.28282
parameter = 'CHnzThickness_4SubArea[m]'
value     = 29.29292
parameter = 'CHnzThickness_5SubArea[m]'
value     = 30.30303
parameter = 'CHnzThickness_6SubArea[m]'
value     = 31.31313
parameter = 'CHnzThickness_7SubArea[m]'
value     = 32.32323
parameter = 'CHnzThickness_8SubArea[m]'
value     = 33.33333
parameter = 'PPw_Thickness_1SubArea[m]'
value     = 34.34343
parameter = 'PPw_Thickness_2SubArea[m]'
value     = 35.35353
parameter = 'PPw_Thickness_3SubArea[m]'
value     = 36.36363
parameter = 'PPw_Thickness_4SubArea[m]'
value     = 37.37373
parameter = 'PPw_Thickness_5SubArea[m]'
value     = 38.38383
parameter = 'PPw_Thickness_6SubArea[m]'
value     = 39.39393
parameter = 'PPw_Thickness_7SubArea[m]'
value     = 40.40404
parameter = 'PPw_Thickness_8SubArea[m]'
value     = 41.41414
parameter = 'UCF_Thickness_1SubArea[m]'
value     = 42.42424
parameter = 'UCF_Thickness_2SubArea[m]'
value     = 43.43434
parameter = 'UCF_Thickness_3SubArea[m]'
value     = 44.44444
parameter = 'UCF_Thickness_4SubArea[m]'
value     = 45.45454
parameter = 'UCF_Thickness_5SubArea[m]'
value     = 46.46464
parameter = 'UCF_Thickness_6SubArea[m]'
value     = 47.47474
parameter = 'UCF_Thickness_7SubArea[m]'
```

```
value     = 48.48484
parameter = 'UCF_Thickness_8SubArea[m]'
value     = 49.49494
parameter = 'BFw_Thickness_1SubArea[m]'
value     = 50.50505
parameter = 'BFw_Thickness_2SubArea[m]'
value     = 51.51515
parameter = 'BFw_Thickness_3SubArea[m]'
value     = 52.52525
parameter = 'BFw_Thickness_4SubArea[m]'
value     = 53.53535
parameter = 'BFw_Thickness_5SubArea[m]'
value     = 54.54545
parameter = 'BFw_Thickness_6SubArea[m]'
value     = 55.55555
parameter = 'BFw_Thickness_7SubArea[m]'
value     = 56.56565
parameter = 'BFw_Thickness_8SubArea[m]'
value     = 57.57575
parameter = 'DistanceToTuffAlluviumInterface[km]'
value     = 58.58585
parameter = 'DistanceToTuffAlluviumInterface[km]'
value     = 58.58585
parameter = 'WellPumpingRateAtReceptorGroup10km[gal/day]'
value     = 59.59595
parameter = 'WellPumpingRateAtReceptorGroup20km[gal/day]'
value     = 60.60606
```

Flag 3: BarrierBiosphereStudy

```
parameter = 'WastePackageFlowMultiplicationFactor'
value     = 1.11111
parameter = 'SubAreaWetFraction'
value     = 2.22222
```

Flag 4: ComponentPrecipitationStudy

```
parameter = 'WastePackageFlowMultiplicationFactor'
value     = 1.11111
parameter = 'SubAreaWetFraction'
value     = 2.22222
```

Flag 5: BarrierUpperUnsaturatedZoneStudy

```
parameter = 'ElevationOfGroundSurface[m]'
value     = 3.33333
parameter = 'MassDensityofYMRock[kg/m^3]'
value     = 4.44444
parameter = 'SpecificHeatofYMRock[J/(kg-K)]'
value     = 5.55555
parameter = 'ThermalConductivityofYMRock[W/(m-K)]'
value     = 6.66666
parameter = 'EmissivityOfDriftWall[-]'
value     = 7.77777
parameter = 'CritChlorideConcForFirstLayer[mol/L]'
value     = 8.88888
```

```
parameter = 'CritChlorideConcForSecondLayer[mol/L]'
value     = 9.99999
```

Flag 6: ComponentTivaCanyonStudy

```
parameter = 'ElevationOfGroundSurface[m]'
value     = 3.33333
parameter = 'MassDensityofYMRock[kg/m^3]'
value     = 4.44444
parameter = 'SpecificHeatofYMRock[J/(kg-K)]'
value     = 5.55555
parameter = 'ThermalConductivityofYMRock[W/(m-K)]'
value     = 6.66666
parameter = 'EmissivityOfDriftWall[-]'
value     = 7.77777
parameter = 'CritChlorideConcForFirstLayer[mol/L]'
value     = 8.88888
parameter = 'CritChlorideConcForSecondLayer[mol/L]'
value     = 9.99999
```

Flag 7: BarrierLowerUnsaturatedZoneStudy

```
parameter = 'TSw_Thickness_1SubArea[m]'
value     = 10.10101
parameter = 'TSw_Thickness_2SubArea[m]'
value     = 11.11111
parameter = 'TSw_Thickness_3SubArea[m]'
value     = 12.12121
parameter = 'TSw_Thickness_4SubArea[m]'
value     = 13.13131
parameter = 'TSw_Thickness_5SubArea[m]'
value     = 14.14141
parameter = 'TSw_Thickness_6SubArea[m]'
value     = 15.15151
parameter = 'TSw_Thickness_7SubArea[m]'
value     = 16.16161
parameter = 'TSw_Thickness_8SubArea[m]'
value     = 17.17171
parameter = 'CHnvThickness_1SubArea[m]'
value     = 18.18181
parameter = 'CHnvThickness_2SubArea[m]'
value     = 19.19191
parameter = 'CHnvThickness_3SubArea[m]'
value     = 20.20202
parameter = 'CHnvThickness_4SubArea[m]'
value     = 21.21212
parameter = 'CHnvThickness_5SubArea[m]'
value     = 22.22222
parameter = 'CHnvThickness_6SubArea[m]'
value     = 23.23232
parameter = 'CHnvThickness_7SubArea[m]'
value     = 24.24242
parameter = 'CHnvThickness_8SubArea[m]'
value     = 25.25252
parameter = 'CHnzThickness_1SubArea[m]'
```

```
value     = 26.26262
parameter = 'CHnzThickness_2SubArea[m]'
value     = 27.27272
parameter = 'CHnzThickness_3SubArea[m]'
value     = 28.28282
parameter = 'CHnzThickness_4SubArea[m]'
value     = 29.29292
parameter = 'CHnzThickness_5SubArea[m]'
value     = 30.30303
parameter = 'CHnzThickness_6SubArea[m]'
value     = 31.31313
parameter = 'CHnzThickness_7SubArea[m]'
value     = 32.32323
parameter = 'CHnzThickness_8SubArea[m]'
value     = 33.33333
parameter = 'PPw_Thickness_1SubArea[m]'
value     = 34.34343
parameter = 'PPw_Thickness_2SubArea[m]'
value     = 35.35353
parameter = 'PPw_Thickness_3SubArea[m]'
value     = 36.36363
parameter = 'PPw_Thickness_4SubArea[m]'
value     = 37.37373
parameter = 'PPw_Thickness_5SubArea[m]'
value     = 38.38383
parameter = 'PPw_Thickness_6SubArea[m]'
value     = 39.39393
parameter = 'PPw_Thickness_7SubArea[m]'
value     = 40.40404
parameter = 'PPw_Thickness_8SubArea[m]'
value     = 41.41414
parameter = 'UCF_Thickness_1SubArea[m]'
value     = 42.42424
parameter = 'UCF_Thickness_2SubArea[m]'
value     = 43.43434
parameter = 'UCF_Thickness_3SubArea[m]'
value     = 44.44444
parameter = 'UCF_Thickness_4SubArea[m]'
value     = 45.45454
parameter = 'UCF_Thickness_5SubArea[m]'
value     = 46.46464
parameter = 'UCF_Thickness_6SubArea[m]'
value     = 47.47474
parameter = 'UCF_Thickness_7SubArea[m]'
value     = 48.48484
parameter = 'UCF_Thickness_8SubArea[m]'
value     = 49.49494
parameter = 'BFw_Thickness_1SubArea[m]'
value     = 50.50505
parameter = 'BFw_Thickness_2SubArea[m]'
value     = 51.51515
parameter = 'BFw_Thickness_3SubArea[m]'
value     = 52.52525
parameter = 'BFw_Thickness_4SubArea[m]'
```

```
value     = 53.53535
parameter = 'BFw_Thickness_5SubArea[m]'
value     = 54.54545
parameter = 'BFw_Thickness_6SubArea[m]'
value     = 55.55555
parameter = 'BFw_Thickness_7SubArea[m]'
value     = 56.56565
parameter = 'BFw_Thickness_8SubArea[m]'
value     = 57.57575
```

Flag 8: ComponentTSwStudy

```
parameter = 'TSw_Thickness_1SubArea[m]'
value     = 10.10101
parameter = 'TSw_Thickness_2SubArea[m]'
value     = 11.11111
parameter = 'TSw_Thickness_3SubArea[m]'
value     = 12.12121
parameter = 'TSw_Thickness_4SubArea[m]'
value     = 13.13131
parameter = 'TSw_Thickness_5SubArea[m]'
value     = 14.14141
parameter = 'TSw_Thickness_6SubArea[m]'
value     = 15.15151
parameter = 'TSw_Thickness_7SubArea[m]'
value     = 16.16161
parameter = 'TSw_Thickness_8SubArea[m]'
value     = 17.17171
```

Flag 9: ComponentCHnvStudy

```
parameter = 'CHnvThickness_1SubArea[m]'
value     = 18.18181
parameter = 'CHnvThickness_2SubArea[m]'
value     = 19.19191
parameter = 'CHnvThickness_3SubArea[m]'
value     = 20.20202
parameter = 'CHnvThickness_4SubArea[m]'
value     = 21.21212
parameter = 'CHnvThickness_5SubArea[m]'
value     = 22.22222
parameter = 'CHnvThickness_6SubArea[m]'
value     = 23.23232
parameter = 'CHnvThickness_7SubArea[m]'
value     = 24.24242
parameter = 'CHnvThickness_8SubArea[m]'
value     = 25.25252
```

Flag 10: ComponentCHnzStudy

```
parameter = 'CHnzThickness_1SubArea[m]'
value     = 26.26262
parameter = 'CHnzThickness_2SubArea[m]'
value     = 27.27272
parameter = 'CHnzThickness_3SubArea[m]'
value     = 28.28282
```

```
parameter = 'CHnzThickness_4SubArea[m]'
value     = 29.29292
parameter = 'CHnzThickness_5SubArea[m]'
value     = 30.30303
parameter = 'CHnzThickness_6SubArea[m]'
value     = 31.31313
parameter = 'CHnzThickness_7SubArea[m]'
value     = 32.32323
parameter = 'CHnzThickness_8SubArea[m]'
value     = 33.33333
```

Flag 11: ComponentPPwStudy

```
parameter = 'PPw_Thickness_1SubArea[m]'
value     = 34.34343
parameter = 'PPw_Thickness_2SubArea[m]'
value     = 35.35353
parameter = 'PPw_Thickness_3SubArea[m]'
value     = 36.36363
parameter = 'PPw_Thickness_4SubArea[m]'
value     = 37.37373
parameter = 'PPw_Thickness_5SubArea[m]'
value     = 38.38383
parameter = 'PPw_Thickness_6SubArea[m]'
value     = 39.39393
parameter = 'PPw_Thickness_7SubArea[m]'
value     = 40.40404
parameter = 'PPw_Thickness_8SubArea[m]'
value     = 41.41414
```

Flag 12: ComponentUCFStudy

```
parameter = 'UCF_Thickness_1SubArea[m]'
value     = 42.42424
parameter = 'UCF_Thickness_2SubArea[m]'
value     = 43.43434
parameter = 'UCF_Thickness_3SubArea[m]'
value     = 44.44444
parameter = 'UCF_Thickness_4SubArea[m]'
value     = 45.45454
parameter = 'UCF_Thickness_5SubArea[m]'
value     = 46.46464
parameter = 'UCF_Thickness_6SubArea[m]'
value     = 47.47474
parameter = 'UCF_Thickness_7SubArea[m]'
value     = 48.48484
parameter = 'UCF_Thickness_8SubArea[m]'
value     = 49.49494
```

Flag 13: ComponentBFwStudy

```
parameter = 'BFw_Thickness_1SubArea[m]'
value     = 50.50505
parameter = 'BFw_Thickness_2SubArea[m]'
value     = 51.51515
parameter = 'BFw_Thickness_3SubArea[m]'
```

```
value     = 52.52525
parameter = 'BFw_Thickness_4SubArea[m]'
value     = 53.53535
parameter = 'BFw_Thickness_5SubArea[m]'
value     = 54.54545
parameter = 'BFw_Thickness_6SubArea[m]'
value     = 55.55555
parameter = 'BFw_Thickness_7SubArea[m]'
value     = 56.56565
parameter = 'BFw_Thickness_8SubArea[m]'
value     = 57.57575
```

Flag 14: BarrierSaturatedZoneStudy

```
parameter = 'DistanceToTuffAlluviumInterface[km]'
value     = 58.58585
```

Flag 15: Component_STFF_SAV_Study

```
parameter = 'DistanceToTuffAlluviumInterface[km]'
value     = 58.58585
```

Flag 16: BarrierReceptorGroupStudy

```
parameter = 'WellPumpingRateAtReceptorGroup10km[gal/day]'
value     = 59.59595
parameter = 'WellPumpingRateAtReceptorGroup20km[gal/day]'
value     = 60.60606
```

Flag 17: ComponentWellWaterStudy

```
parameter = 'WellPumpingRateAtReceptorGroup10km[gal/day]'
value     = 59.59595
parameter = 'WellPumpingRateAtReceptorGroup20km[gal/day]'
value     = 60.60606
```

Flag 18: SubsystemEngineeredStudy

```
parameter = 'EmplacementBackfillThickness[m]'
value     = 61.61616
parameter = 'DripShieldThickness[m]'
value     = 62.62626
parameter = 'InnerWPThickness[m]'
value     = 63.63636
parameter = 'OuterWPThickness[m]'
value     = 64.64646
```

Flag 19: BarrierDriftStudy

```
parameter = 'EmplacementBackfillThickness[m]'
value     = 61.61616
parameter = 'DripShieldThickness[m]'
value     = 62.62626
```

Flag 20: ComponentBackfillStudy

```
parameter = 'EmplacementBackfillThickness[m]'
value     = 61.61616
```

Flag 21: ComponentDripShieldStudy

```
parameter = 'DripShieldThickness[m]'
value     = 62.62626
```

Flag 22: BarrierWastePackageStudy

```
parameter = 'InnerWPThickness[m]'
value     = 63.63636
parameter = 'OuterWPThickness[m]'
value     = 64.64646
```

Flag 23: ComponentInnerContainerStudy

```
parameter = 'InnerWPThickness[m]'
value     = 63.63636
```

Flag 24: ComponentOuterContainerStudy

```
parameter = 'OuterWPThickness[m]'
value     = 64.64646
```

Purpose: The values specified in the *tpa.inp* file for the subsystem, barrier, or component should be written to the *cp.tpa* file, since this change should only affect the constant parameters in *cp.tpa*.

TPA Output Files to Compare:

The following files will be checked for flags 2-24.
- *lhs.inp*
- *lhs.out*
- *cp.tpa*

Pass/Fail Criteria:

The *lhs.inp* and *lhs.out* files should be the same for version 4.0 and 4.1. The *cp.tpa* file should contain the above values for each of the parameters listed in each test.

Documentation of Testing:

These tests are stored in the SCR322/flagX subdirectory, where X equals 2 to 24. The Version 4.0 output is stored in the SCR322/v40 directory. All testing output files are archived on a CD.

Flag Combination

Test 1. Run Versions 4.0 and 4.1 with their accompanying tpa.inp files for 10,000 yr with all append files ON, ImportanceAnalysisFlag(yes=1,no=0) = 1 (ON) in both versions, and all other flags with the barriers inactive, except for the following: ComponentOuterContainerStudy, BarrierWastePackageStudy, and ComponentUCFStudy

Purpose: The values specified in the *tpa.inp* file for the subsystem, barrier, or component should be written to the *cp.tpa* file, since this change should only affect the constant parameters in *cp.tpa*.

TPA Output Files to Compare:

The following files will be checked.
- *lhs.inp*
- *lhs.out*
- *cp.tpa*

Pass/Fail Criteria:

The *lhs.inp* and *lhs.out* files should be the same for version 4.0 and 4.1. The *cp.tpa* file should contain the above values for each of the parameters listed in each test.

Documentation of Testing:

These tests are stored in the SCR322/comb/test1 subdirectory. The Version 4.0 output is stored in the SCR322/v40 directory. All testing output files are archived on a CD.

Test 2. Run Versions 4.0 and 4.1 with their accompanying tpa.inp files for 10,000 yr with all append files ON, ImportanceAnalysisFlag(yes=1,no=0) = 1 (ON) in both versions, and all other flags with the barriers inactive, except for the following: BarrierSaturatedZoneStudy, BarrierLowerUnsaturatedZoneStudy, and SubsystemNaturalStudy

Purpose: The values specified in the *tpa.inp* file for the subsystem, barrier, or component should be written to the *cp.tpa* file, since this change should only affect the constant parameters in *cp.tpa*.

TPA Output Files to Compare:

The following files will be checked.
- *lhs.inp*
- *lhs.out*
- *cp.tpa*

Pass/Fail Criteria:

The *lhs.inp* and *lhs.out* files should be the same for version 4.0 and 4.1. The *cp.tpa* file should contain the above values for each of the parameters listed in each test.

Documentation of Testing:

These tests are stored in the SCR322/comb/test2 subdirectory. The Version 4.0 output is stored in the SCR322/v40 directory. All testing output files are archived on a CD.

****

Received the TPA source code and data files via email attachment from R. Janetzke on 8/29/00. These files were either modified or added to the TPA code to conduct Importance Analysis. These files are (note that the "ia" or "i" portion of the file names was dropped for compiling and running the TPA code; also note that the iareader.f file corresponds to the ia.f file in version 4.0):

dcagwia.f
ebsfaili.f
ebsrelia.f
execia.f
ia.dat
ia1.i
iareader.f
nfenvia.f
readeria.f
sampleri.f
seismoia.f
szftia.f
tpaia.inp
uzftia.f

While compiling the version 4.0 code with the above files, there were some compilation errors. From the *exec.f*, *ebsrel.f*, *ebsfail.f*, *sampler.f*, *szft.f*, and *uzft.f* files, lines were commented out that were related to **.log* files and IEEE which were added for the UNIX code development (this was recommended by R. Janetzke). Also, found that in *ia.f*, the following changes were required to compile and run the code and to copy the new data file *ia.dat* to the working directory (the following is a file comparison between the v4.0 and the IA file received from R. Janetzke):

```
Comparing files iareader.f and ..\IA.F
***** iareader.f

      character*60 name
***** ..\IA.F

cc rwr 8/31/00 added to copy ia.f from data
      integer zportsh
      external zportsh
      character*80 command
      include 'path.i'

      character*60 name
*****

***** iareader.f
      external igetunitnumber

***** ..\IA.F
      external igetunitnumber

cc rwr 8/29/00 added to avoid compile errors on the pc
      logical lexist
```

```
*****

***** iareader.f
     if (iaflag .ne. 0) then
       iaunit = igetunitnumber('exec    ')
***** ..\IA.F
     if (iaflag .ne. 0) then

cc rwr 8/31/00 added copy for the ia.f file from data
       call clearchar(80,command)
       command = 'cp ' // dpath // 'data/ia.dat .'
       istatus=zportsh(command)
       if( istatus .ne. 0 ) then
         print *, ' ***>>> Error in ia.f <<<*** '
         print *, ' not able to copy ia.f'
         print *, ' istatus .ne. 0 '
         print *, ' istatus = sh( ', command, ')'
         print *, ' istatus = ', istatus
         stop
       endif

       iaunit = igetunitnumber('exec    ')
*****


***** iareader.f
       cparamvalue = ''
       return
***** ..\IA.F
       cparamvalue = ''
cc rwr 9/11/00 debug    add the following line because clineid is reset for some reason
       clineid = 'VALUE'
       return
*****
```

NOTE: There are three changes in the *ia.f* file: (1) adding copy-related statements which will copy the *ia.dat* file from the data subdirectory to the working directory (requested by R. Janetzke); (2) adding a logical declaration for variable *lexist*; and (3) adding clineid='VALUE' (for some reason the assignment of clineid to 'VALUE' is lost.

In addition to changes in the *ia.f* file, the *sampler.f* file was modified by commenting out the "close" statements (closing *sp.tpa* and *cp.tpa*). These two statements were introduced as part of the Importance Analysis modifications. However, by closing these files, the *exec.f* file is not able to write to these files and an error message is written to the screen during TPA code execution. The comparison file for *sampler.f* follows.

```
Comparing files sampler.f and ..\SAMPLER.F
***** sampler.f
          call printtitlessp(iunitcp,iunitsp)
          close (iunitcp)
          close (iunitsp)
cc         if(1+1 .eq. 2) STOP
***** ..\SAMPLER.F
          call printtitlessp(iunitcp,iunitsp)
cc rwr debug          close (iunitcp)
cc rwr debug          close (iunitsp)
cc         if(1+1 .eq. 2) STOP
*****
```

Once the above modifications were introduced into the TPA souce code, the testing was conducted according to the test plan listed previously.The test results for flag1 (tests 1-4), flags 2-24, and combinations tests 1 and 2, are located in the directories described in the test plan. A comparison between the test cases and version 4.0 was automatically performed using the "fc" command in a DOS Window with the *filecomp.bat* file. The output file (*filecomp.out*) was examined to verify that the parameters in the *ia.dat* file were correctly written to *sp.tpa*, *lhs.out*, and *cp.tpa*.

The results from all tests show that the values in *ia.dat* for all flags and combinations of flags described in the test plan were correctly written to the *sp.tpa*, *lhs.out*, and *cp.tpa* files (see the *filecomp.out* file in each test subdirectory). Thus, for the tests described in the test plan, the testing results indicate the modifications for Importance Analysis were correctly implemented.

5/10/00

Note to: Dave Esh, Tim McCartin, Sitakanta Mohanty, Ron Janetzke

From: Richard Codell

Subject: Important changes to releaset.f

Several problems came up in some recent runs for tpa4.0 that demand some attention:

1. Dave and Ron showed how a particular vector and subarea caused the releaset model to bog down. I traced the error to a condition of small sampled container volume of 10^{-6} cubic meters, and high flow rate, leading to a short time constant (V/q). The obvious fix is to increase the minimum volume in either the flow thru or bathtub model. I propose 0.01 cubic meters. Figure 1 shows the results with the bad vector for 0.001 and 0.01 cubic meters minimum volume. The 0.01 case runs much faster. The original was very slow, and the 0.001 cubic meter case took about 3 minutes cpu time for one subarea on my Sparc Ultra 10.

2. Dave Esh showed how the release rate of I129 gap fraction only was insensitive to the flow rate through the waste package in the case where there was only the gap fraction. The explanation for this is that the minimum volume in the flow-thru case is set so that there is a minimum of 1/5 volume exchange per year based on the highest flow rate for 10,000 years. If the flowrate is doubled, then the minimum volume is doubled, and the iodine pulse won't come out any faster than 1/5 per year (this minimum volume is irrespective of the 0.01 cubic meters discussed in the previous paragraph. At the time, the minimum was 0.000001 cubic meters). I think this is a reasonable model for release for the following reasons: 1) You need to maintain a minimum volume for numerical stability and economy in the tpa code; 2) Very fast release of all the gap release fraction is unrealistic. The modeled waste package simulates many individual waste packages, which would cause a spread in the release of many years. Cladding will provide substantial barrier to instantaneous release, even in a failed state.

3. Tim commented that for beta emmitters, the bathtub model on average gave a larger peak dose than the flowthru model. This is inconsistent and points to a problem in the releaset code. What I found is that the release rate from the engineered barrier is reported as the derivative of the cumulative release with respect to time. This is OK if releases are slow, but if the release takes place between two time steps, you may miss it entirely. To fix this, I added into the Runge-Kutta integration one additional variable, cumulative release. Interestingly, although the derivative of this was calculated, it was not integrated previously. Now the release rate is calculated as the difference in the cumulative release between time steps. Figure 2 shows the release rate for a single vector, one subarea for I129 bathtub and flowthru models. In this case, the release rate for flowthru increases dramatically, and is about the same quantity as the total for the bathtub model.

4. As I was analyzing the release code, I noticed one other problem. The critical temperature for wetting is set in the tpa.inp file as 999 degrees C, to enhance the possibility that thermal reflux will contact the waste during the reflux period. This never

made any difference as I recall, to the peak doses, and doesn't make much sense for the model with drip shield that would protect juvenile failures from getting wet. What I discovered though, is that irrespective of any flow to the waste packages, the waste form was dissolving into the minimum water volumes specified for the code. For conditions where there is no flow and the waste package temperature is much higher than boiling, this does not make any sense. The high temperatures led to high dissolution rates because the fuel dissolution models are temperature-sensitive. When I put the critical temperature for wetting back to 97 degrees, the release rate fell to about half (Figure 3). This is because there was no fuel leaching until the temperature fell below 97. Remember, 6% of the I129 is in the gap, but 94% is in the matrix.

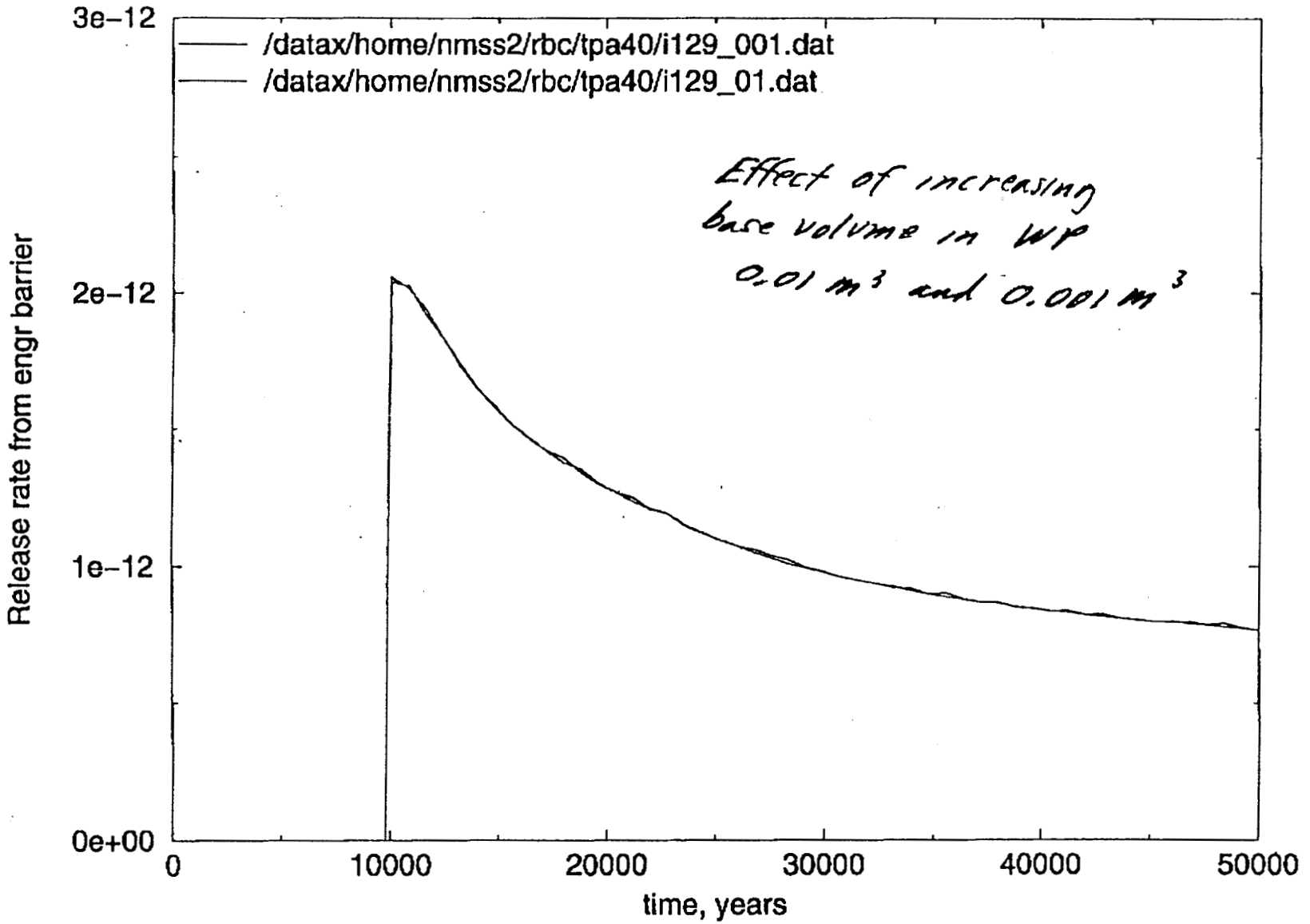
Dick Codell

50/20

Compare min wp volume

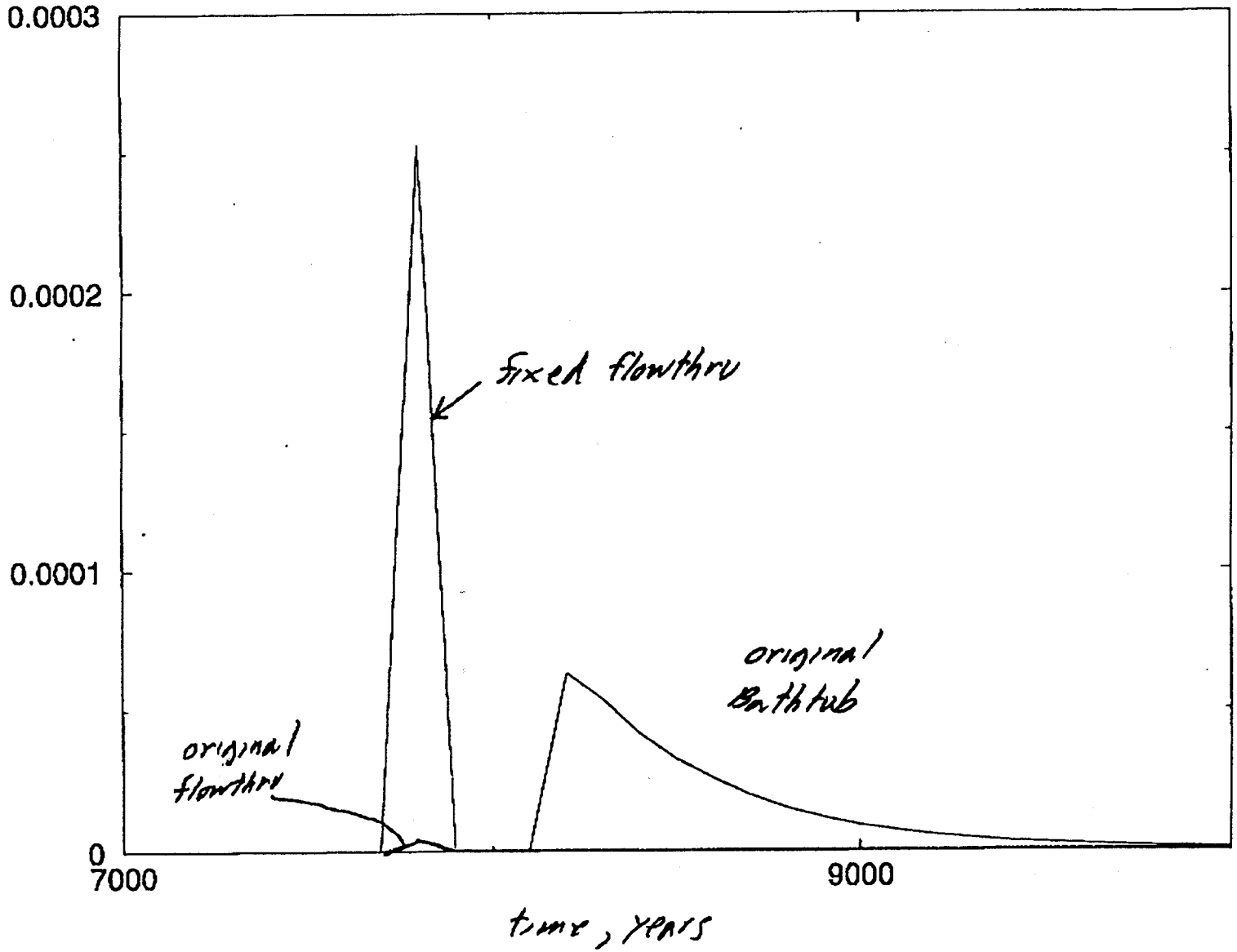
Figure 1

0.001 or 0.01 cubic meters R. Codell 5/8/00



MAY-11-2000 10:08 NRC NMSS

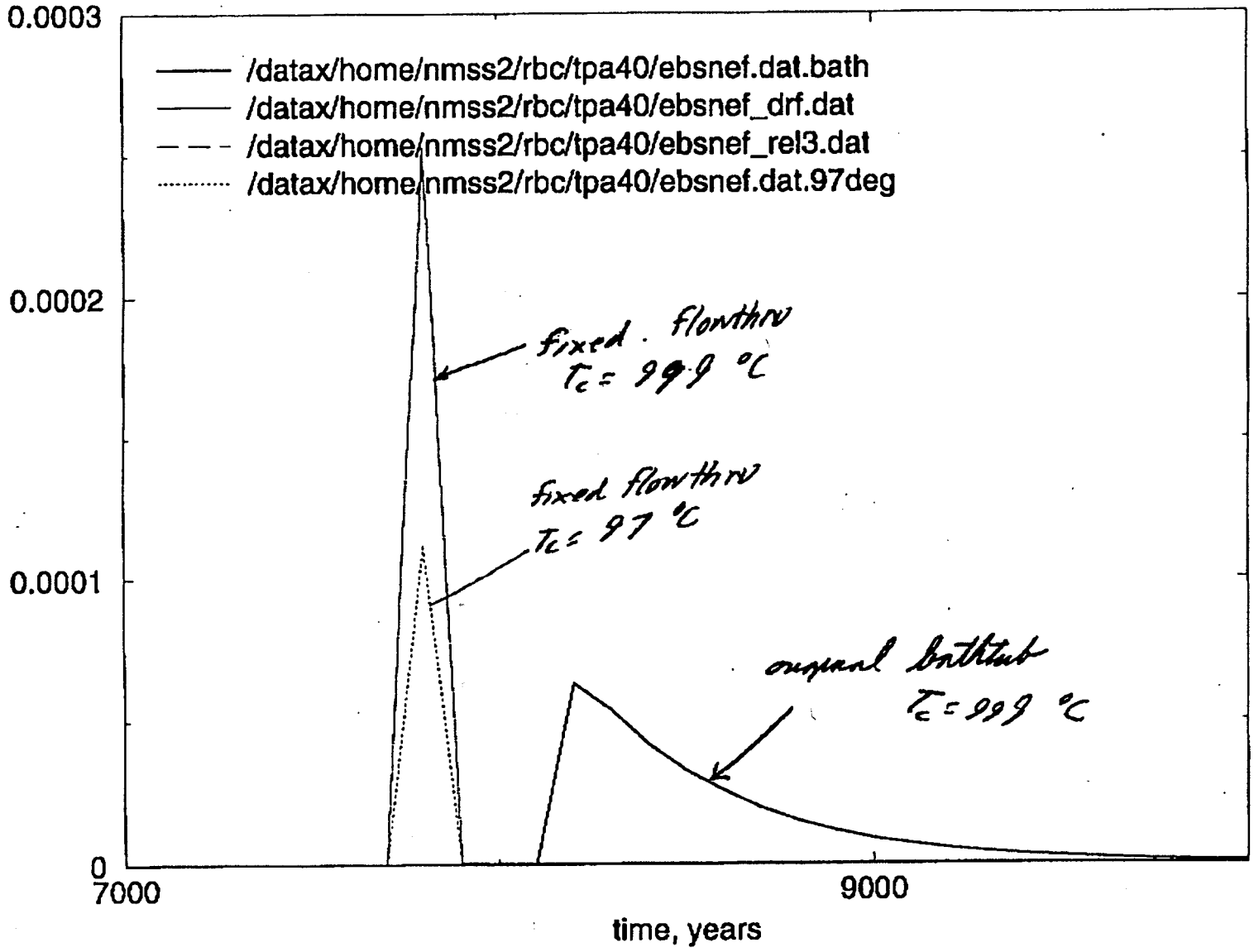
Figure 2



I129 release

Figure 3

5/10/00



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SOFTWARE CHANGE REPORT (SCR)

SCR No. (*Software Developer Assigns*): PA-SCR-323	Software Title and Version: TPA 4.0	/Project No: 20-1402-762

Affected Software Module(s), Description of Problem(s):

releaset.f

Release peaks that occur between two TPA time steps are not correctly represented in the release versus time array.

Change Requested by:	**Change Authorized by** (*Software Developer*):
R. Codell Date: 5-12-00	R. Janetzke Date: 8-24-00 Ron Janetzke

Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

The code should maintain a minimum container volume of 0.01 cubic meters. This assures that there won't be a condition of relatively high flow rate and low volume that gives a very short time constant, and consequently long run times.

Add into the Runge-Kutta integration one additional variable, cumulative release. Interestingly, although the derivative of this was calculated, it was not integrated previously.

Put the critical temperature for wetting back to 97 degrees.

Implemented by:	**Date:**
R. Codell Richard Codell	5-12-00

U.S. NRC

Description of Acceptance Tests:

See attached test plan.

Tested by:	**Date:**
S. Mayer S. Mayer	9/20/2000

Releaset4.f Test Plan - PA-SCR-323

Test name: TPA4.0 - releaset4.f - PA-SCR-323

Anticipated start date: 09-12-00

Anticipated completion date: 09-15-00

Amount of your time available to perform this test: 50%

Percent of testing time to be spent in process level testing and system level testing (e.g. 50/50): 80/20

[*Process level testing tests the subroutine in standalone mode outside of the TPA code, usually with the aid of a special purpose driver of trivial construction. System level testing tests the subroutine in a fully integrated environment with the TPA code.*]

Output files to be checked: relfrac.dat, diagnose.out, totdose.res

Input files to be checked for proper data transfer to the program:

None

Disposition of documentation (storage medium, physical location, and access method):

[*Documentation should include test driver source code, and input, intermediate and output files. Also include any plot files or plot hard copies that are used to display the results.*]

Test work performed on vulcan
Results stored on attached floppy
Summary of test results documented on: Releaset.f Test Result PA-SCR-323
Some results and discussion stored in Scientific Notebook #170 section maintained by Stefan Mayer

Initial comparison tests:

1) What are actual changes between module releaset.f (old) and releaset4.f (new)?
Upon inspection, do these changes appear reasonable to:
- maintain a minimum container volume of 0.01 cubic meters?
- add cumulative release to Runge-Kutta integration?
- set critical temperature for wetting back to 97 degrees?

2) What are the major changes of base case mean value TPA4.0 simulations in output totdose.res when obtained with module releaset.f (old) and releaset4.f (new)?
Do these changes appear reasonable?

Functional test:

The parameter values and/or code changes that significantly influence prediction changes will be identified.

Reasonableness test:

The reasonableness of cause and effect will be discussed.

Final Checklist (completed during testing):

- Did the modification substantially change the results of TPA4.0?
- Is the problem to be addressed by this SCR solved? (Does the modification lead to a better representation of peak release values?)
- Were releaset.f (old) and releaset4.f (new) compared directly?
- Which nuclides were monitored to determine reasonableness of results in terms of dose?

Releaset.f Test Results - PA-SCR-323

(SM 3/20/00)

Details of the test and test results can be read in the appropriate section (pages ~~35 to 41~~ 49 to 55) of inclusion to scientific notebook #170E maintained by Stefan Mayer. Some details of the notebook entry are printed and attached.
The input files and code generated output files that were used for this test are documented in attached floppy disk.

Initial comparison tests:

1) What are actual changes between module releaset.f (old) and releaset4.f (new)?

Only a few lines of code were changed or added. See scientific notebook for details.

Upon inspection, do these changes appear reasonable to:

- maintain a minimum container volume of 0.01 cubic meters? YES / PASSED
- add cumulative release to Runge-Kutta integration? YES / PASSED
- set critical temperature for wetting back to 97 degrees? NO / was already set in module - not needed

See scientific notebook for detailed discussion.

2) What are the major changes of base case mean value TPA4.0 simulations in output totdose.res when obtained with module releaset.f (old) and releaset4.f (new)? MINOR CHANGES

The noted changes were minor for the bathtub model. Note however that maximum release times for certain radionuclides were significantly changed. This does not seem to affect totdose.res significantly.

Do these changes appear reasonable? YES / PASSED

See attached scientific notebook excerpts.

Functional test:

The parameter values and/or code changes that significantly influence prediction changes will be identified.

The code changes are small and reasonable to achieve the stated goals for the SCR. The resulting prediction changes for a mean case scenario simulation are small and appear reasonable, as the changes were only meant to improve estimates of peak release rates, and do not include substantial change in model or model implementation.
The changes of peak release rate estimates for a flowthru model simulation are substantial and reflect the influence of code changes to estimate these rates. The change in the code to better estimate peak relaese rates substantially improves the estimate of TEDE.

PASSED

Reasonableness test:

The reasonableness of cause and effect will be discussed.

The main concern prompting the SCR was that release rates are underestimated for fast release, as can be simulated with a flowthru model. The main modification of the module code lead to a substantial increase in estimates of such a release rate. When compared to the results of the bathtub model under otherwise identical conditions, it appears reasonable that such an increase is computed.

See data in attached scientific notebook excerpts.

PASSED

Final Checklist (completed during testing):

- Did the modification substantially change the results of TPA4.0? YES

For certain input files and the flowthru model, predicted TEDE were substantially changed.

- Is the problem to be addressed by this SCR solved? (Does the modification lead to a better representation of peak release values?) YES

- Were releaset.f (old) and releaset4.f (new) compared directly? YES

- Which nuclides were monitored to determine reasonableness of results in terms of dose?
  All radionuclides for mean case, I129 for bathtub/flowthru model comparison.

Stefan Mayer

57/70
49 - 55 (SM, 9/20/00)

Excerpt of Scientific Notebook # 170 E, pages ~~35 - 44~~ (SM, 9/20/00)

Test pertaining to PA-SCR-323, affected module releaset.f

(SM, 9/20/00)

15 **6.1** Objective

The objective of this part of the TPA project is to test the module releaset.f as part of the PA-SCR-323. A test plan and test results are documented independently. Documentation in this section of the notebook supports the test results report.

(SM, 9/20/00)

15 **6.2** Computers, Computer Codes, and Data Files

The original computer codes to be tested releaset4.f as well as the old version releaset.f are located on the SUN workstation "vulcan" in directory /home/smayer/TPA/Releasettest.dir/Moduletest. The overall TPA4.0 code which integrates the module releaset4.f used to test at the system level is located in /home/smayer/TPA/TPA4.0. The code releaset4.f was compiled as a standalone module using the line command specified in the associated Makefile.

For analysis and comparison purposes, output files generated may be transferred to the PC "lemur". Use of software, for example Excel, may be necessary to assist analysis and to generate graphical output.

Machine Name	Machine Type	Operating System	Compiler	Location
vulcan	SUNW, Ultra-Enterprise; sparc; sun4u	SUNOS 5.6	f77 (SUN); 'Build' in 'workshop'	Building 189

Table 1. Computer, operating system, and compiler used in the tests.

(SM, 9/20/00)

15 **6.3** Actual code lines changed between releaset.f (old) and releaset4.f (new)

Comment lines and blank lines are not listed here.

1) Two new arrays are declared: "real*8 crelwp, yprev"
2) The array size crelwp is set in the common block "cumu" as "crelwp(maxnuc,maxmem)"
3) The array elements of crelwp are initialized to a small value: crelwp(k,i)=1.e-20
4) A nested loop is added to store values of crelwp(i,k) sequentially at the end of vector ystart(j):

```
      do 5430 k=1,nchns
            do 5425 i=1,ni(k)
             j=j+1
             ystart(j)=crelwp(i,k)
5425  continue
5430  continue
```

5) The average release rate over an integration time interval is now computed based on an overall difference:

```
            yprev=crelwp(k,i)
            drf(k,i)=-(yprev-ystart(j))/(tstop-tstart)
            crelwp(k,i)=ystart(j)
```

It was set to: drf(k,i)=dydx(j) in the old version.
6) The variable vfullflow used for the flow through model is forced to a minimum value of 10 liters:

```
      if (vfullflow.lt.0.01) vfullflow = 0.01
```

7) The volume vwnow is set to: vwnow=y(1)+0.01.
It was set to vwnow=y(1) in the old version.

Note that while the PA-SCR-323 report sheet lists the setting of critical temperature to 97 degrees in the description of changes, inspection and comparison of old and new versions of module releaset.f show that this was already set to 97 degrees in the old version.

(SM, 9/20/00)

15 6.4 Estimated influence of code changes, by inspection

The vector ystart contains all starting values for the intergration of the ODE, which in the new version of releaset.f includes the sequential elements of crelwp(i,k) (see item 5) above). Upon exit of subroutine odeint, ystart contains the updated dependent values, including updated cumulative release crelwp(i,k). This updated set of values is used to directly compute the average release rate drf(k,i) during time interval (tstop-tstart) (see item 6) above). This release rate was previously directly estimated using the gradient dydx(j) returned from odeint.

The array crelwp only serves as intermediate storage for the current time step cumulative release from waste packages. Upon inspection, it does not appear to affect other variables (other than its intermediate storage place in ystart).

The rate of release drf value is passed to the release rates of the nuclides rlrate1, etc. These in turn are used to compute rlmass, which is passed to fracre. fracre is used for writing and the value is passed to xlarge, which is used to test and update maxrel and associated timrel. The variable maxrel is stored in relfrac.out, and serves as measure of the maximum release rate (release peak) for each radionuclide during the simulation time.

The variable vfullflow is used for the flow through model. Its value is passed to vwnow (current water volume in waste package) if flow through model is considered. Given that vwnow is always >= 0.01, the test on concn (lines 1910 to 1915) will assign the lesser value of (amassl(ielem)/vwnow) or sol(ielem) to concn. The variable concn is used with fracn to calculate radionuclide concentration in waste package water ccfr. Ccfr is used with qout to calculate the mass rate of radionuclide release due to advective flux, adflux.

Inspection of code changes suggest that changes were implemented correctly. However, given the chain of variables that are affected to some extent by the changes, no final statement can be made. Output of the code will be compared between old and new version, both in module stand alone mode, and as part of TPA.

(SM, 9/20/00)

15 6.5 Comparison of sample output files from old and new version releaset.f

The maximum fractional release over the first 50,000 years obtained from a mean input data file for each radionuclide is stored in relfrac.dat. These output files from old and new version code are shown in Table 2 for direct comparison.

The most significant differences are the shift of time of occurrence of the maximum point for certain radionuclides, such as (from old to new version) from 40E+3 [yrs] to 47E+3[yrs] for TH230, and from 40E+3 [yrs] to 45E+3[yrs] for NB94. The actual calculated maximum fractional release rates vary less than 1% between code versions. The new version calculations for release peaks yield either identical, or slightly lower values than obtained with the old version.

releaset4.f (new module version)			releaset.f (old module version)		
CM246	0.2040E+05	0.3961E-07	CM246	0.2040E+05	0.3994E-07
U238	0.5000E+05	0.3017E-09	U238	0.5000E+05	0.3017E-09
CM245	0.2040E+05	0.1389E-06	CM245	0.2040E+05	0.1399E-06
AM241	0.2040E+05	0.2522E-10	AM241	0.2040E+05	0.2529E-10
NP237	0.4124E+05	0.5573E-06	NP237	0.4042E+05	0.5573E-06
AM243	0.3698E+05	0.3385E-07	AM243	0.3698E+05	0.3385E-07
PU239	0.5000E+05	0.8491E-09	PU239	0.5000E+05	0.8492E-09
PU240	0.2040E+05	0.1646E-09	PU240	0.2040E+05	0.1651E-09
U234	0.2654E+05	0.2779E-09	U234	0.2654E+05	0.2779E-09
TH230	0.4702E+05	0.1336E-04	TH230	0.4042E+05	0.1336E-04
RA226	0.5000E+05	0.3297E-03	RA226	0.5000E+05	0.3330E-03
PB210	0.5000E+05	0.3516E-03	PB210	0.5000E+05	0.3536E-03
CS135	0.2040E+05	0.4783E-05	CS135	0.2040E+05	0.4830E-05
I129	0.2040E+05	0.4807E-05	I129	0.2040E+05	0.4854E-05
TC99	0.2040E+05	0.1278E-05	TC99	0.2040E+05	0.1289E-05
NI59	0.2057E+05	0.5679E-06	NI59	0.2040E+05	0.5712E-06
C14	0.2040E+05	0.7317E-06	C14	0.2040E+05	0.7403E-06
SE79	0.2040E+05	0.4753E-05	SE79	0.2040E+05	0.4800E-05
NB94	0.4515E+05	0.6330E-08	NB94	0.4042E+05	0.6330E-08
CL36	0.2040E+05	0.8561E-05	CL36	0.2040E+05	0.8649E-05

Table 2: Maximum fractional release rates from new (left) and old (right) module.

The respective output files diagnose.out were compared to each other using the workshop tool filemerge. Relative differences in estimated dose were on the order of 1% or less for all time steps.

In conclusion, direct comparison of module level test outputs suggests that release peaks are now computed in a different manner, as intended and as shown in item 5) in section 6.3. The actual changes of output values are small for the sample mean data set used in this test.

(SM, 9/20/00)

156.6 Comparison of output files totdose.res obtained from TPA4.0 runs using either old or new version releaset.f

A TPA version 4.0 run was performed using mean value input files and using alternatively the old and new version of module releaset.f. The simulations were performed on Vulcan in /home/smayer/TPA/TPA40O. After completion of the first simulation using the old module, a few output files, including totdose.res (renamed here oldtotdose.res), were stored in /home/smayer/TPA/Releasettest.dir/Systemtest/oldversion. Modules were swapped in /home/smayer/TPA/TPA40O/codes and TPA was executed again with the new module, and the same output files (totdose.res now renamed newtotdose.res) were stored in /home/smayer/TPA/Releasettest.dir/Systemtest/newversion. Using the UNIX utility "diff", both total dose calculation results were compared to each other. They show minor differences in estimation of total dose. During those time steps when total dose approaches [mrem] values, the relative differences are very small, typically less than 1%.

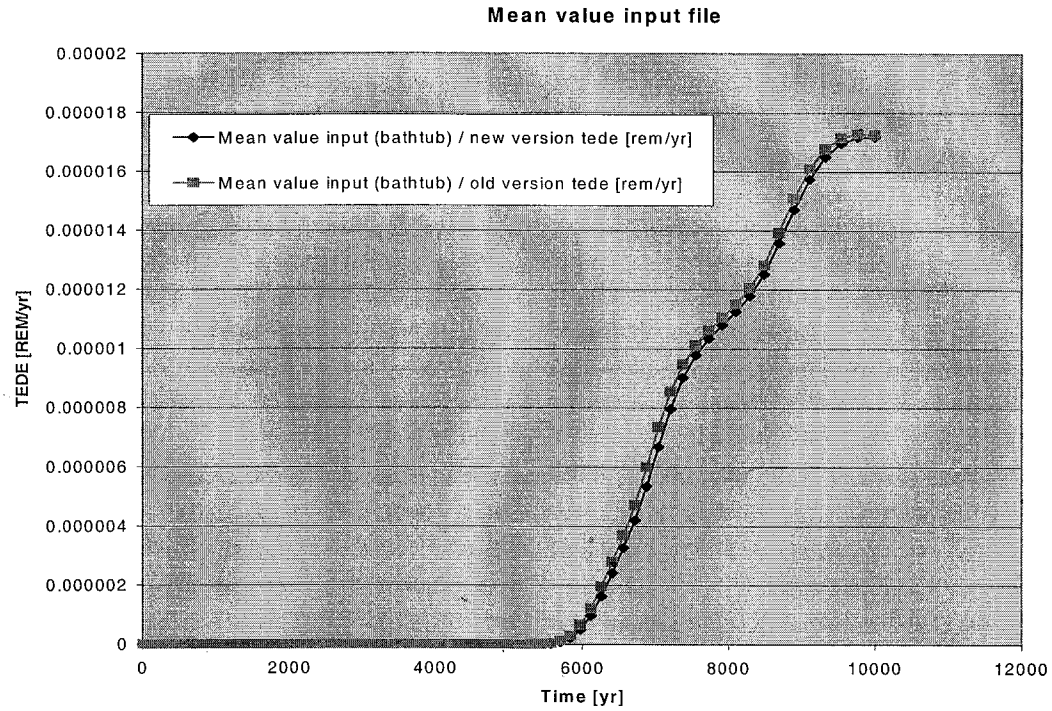
The output files relfrac.out obtained during the entire TPA run were compared to each other. These files are identical to what was produced in stand alone module mode, as expected. The differences between old and new version were also identical as documented in section 6.5. The same result was observed when comparing the diagnose.out files.

The output in totdose.res was also compared and is shown in Figure 1. Only a very small change in prediction of TEDE is seen for this input file.

Therefore, when using a mean value input, which in this case implements the bathtub model, observed changes are minor, which suggests that the modifications in the releaset.f module do not substantially influence this type of scenario.

Figure 1: Total effective dose equivalent for mean input file, bathtub model, old and new releaset.f versions.

Improvements from the better estimate of peak release rates are expected only when release is relatively fast, which could happen with the flowthru model. In the next step, estimates of maximum release are compared when using bathtub and flowthru model, as well as old and new version releaset.f module.



(SN, 3/20/00)

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15 8.7 Comparison of peak release rates

Four TPA runs were performed for subarea 1, modeling only the radionuclide I129, using latin hypercube to sample the distributions of input parameters, turning all disruptive events off (no seismic activity,...), and setting the release modes to either bathtub model (run 1 and 2), or flowthru model (run 3 and 4), and using either the new (run 1 and 3) or the old (run 2 and 4) version of releaset.f.
The two used versions of the tpa.inp file are stored on vulcan as /home/smayer/TPA/Releasettest.dir/Systest/Bathtub/tpa.inp.bathtub and /home/smayer/TPA/Releasettest.dir/Systest/Flowthru/tpa.inp.flowthru. The corresponding used versions of the module are stored in each of the subdirectories.
Results of computed maximum fractional release rates for I129, and time of occurrence, are shown in Table 3. The most significant change is for the flowthru model, where estimates of maximum release rate are increased by nearly a factor of sixty for the given input file. Since the bathtub model for otherwise identical input yields higher maximum release rates than the flowthru model for the old version, an increase in the estimate seems reasonable.

```
Run1:Bathtub model, new releaset.f        Run2:Bathtub model, old releaset.f

I129     0.8300E+04  0.1195E-06           I129     0.8200E+04  0.1366E-06

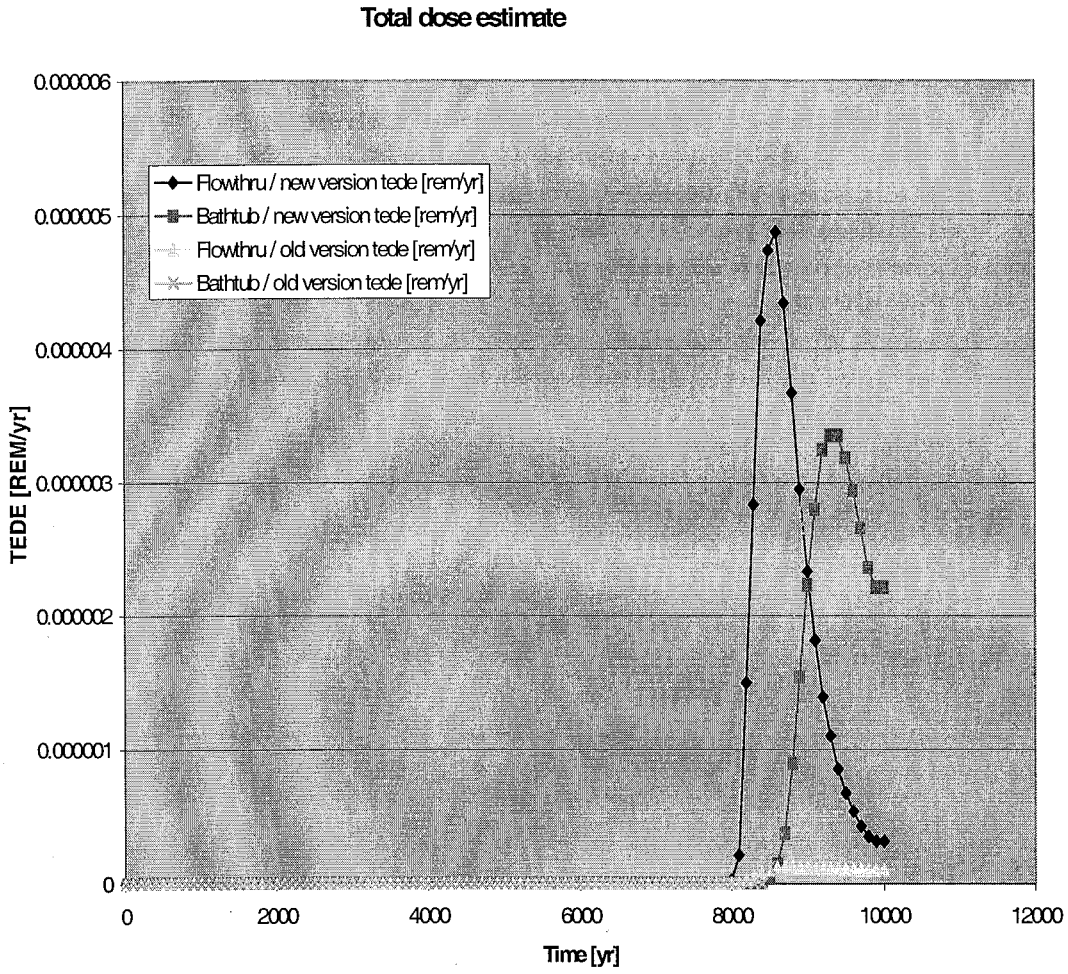
Run3:Flowthru model, new releaset.f       Run4:Flowthru model, old releaset.f

I129     0.7800E+04  0.6021E-06           I129     0.7800E+04  0.1013E-07
```

Table 3: Maximum fractional release rates for bathtub and flowthru models.

The corresponding estimates of total effective dose are shown in Figure 2. They show a decrease in peak estimates for the bathtub model between old and new version of module releaset.f. More significantly, they show a substantial change of the flowthru calculated TEDE curve. Based on this comparison, it is apparent that the old version significantly underpredicted TEDE, while the new one is similar, and slightly higher, to the predictions of the bathtub model.

Figure 2: Total effective dose equivalent in subarea 1 from I129 only, for different models.



(SCR, 9/20/00)

6.8 Conclusion

Tests were performed by inspection of code, in stand alone execution of the module, and in system execution within TPA. The mean value input file tpa.inp was used, as well as a special input file comparing extreme cases of bathtub and flowthru model results.
The changes appear reasonable. By inspection, the minimum volume is set to 0.01 cubic meters, as described in the SCR. No significant influence on TEDE or other observed output files was observed that could be related to this change. The critical temperature was found to be already set to 97 degrees.
The minor influence on overall estimated total dose documents that the changes have only a very small influence on the mean case TPA run.
Note however that some of the time estimates for peak release were changed. It is not clear why this is the case. However, comparison suggests that the influence on calculated TEDE is small.
The simulations for subarea 1 comparing estimates of TEDE from I129 show that the flowthru model in the old version significantly underpredicted release, and that the changes made to the code yield predictions that appear reasonable when compared to a similar bathtub model simulation.

[Stefan Mayer, September 20, 2000]

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SOFTWARE CHANGE REPORT (SCR)

SCR No. (*Software Developer Assigns*): PA-SCR-324	**Software Title and Version:** TPA 4.0	**/Project No:** 20-1402-762

Affected Software Module(s), Description of Problem(s):

dcagw.f

Bug fix. Initialize variable dkGvalue.

Change Requested by: J. Weldy Date: 5-12-00	**Change Authorized by** (*Software Developer*): R. Janetzke Date: 8-24-00 Ron Janetzke

Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

Put an initializing statement before line 800:

dkGvalue = 100.0d0

Declare the variable PLUV as integer.

Implemented by: R. Janetzke Ron Janetzke	**Date:** 9-15-00

Description of Acceptance Tests:

1. Change pluvial pumping rate to a very small number so it is obvious when climate change occurs and run both versions of the code. The switch to pluvial conditions should vary in time from realization to realization (as seen in the output file sgwsr.tpa) in the old version without the initializing statement. The new version should keep the time of the switch to pluvial conditions constant from realization to realization. The test was completed successfully and the code seems to be performing properly.

Tested by: J. Weldy James L. Weldy	**Date:** 9-20-00

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SOFTWARE CHANGE REPORT (SCR)

SCR No. (*Software Developer Assigns*): PA-SCR-325	Software Title and Version: TPA 4.0	Project No: 20-1402-762

Affected Software Module(s), Description of Problem(s):

ashrmovo.f, dcagw.f

Bug fix to the algorithms that use the ash blanket or soil leaching factor in order to reflect current knowledge.

Change Requested by:	Change Authorized by (*Software Developer*):
J. Weldy Date:8-1-00	R. Janetzke Date: 8-24-00 Ron Janetzke

Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

The formula used to calculate the leaching factor in ASHRMOVO and DCAGW is based on the formula in Napier et al., 1988, which is taken from Baes and Sharp, 1981. However, in 1983, Baes and Sharp published a paper which documented the calculation of the leaching factor that resulted in a slightly different formula than in Baes and Sharp, 1981. The difference in the formulae is that the 1981 paper used the infiltration rate of the water to compare the rate of movement of the contaminant whereas the 1983 paper used the more appropriate velocity of water in the subsurface. As such, the TPA code will be modified to utilize the formula developed in Baes and Sharp, 1983. This will be done by dividing the water infiltration rate by the soil volumetric water content when calculating the leaching factor in ASHRMOVO and DCAGW.

Implemented by:	Date:
J. Weldy Jon L. Weldy	9-12-00

Description of Acceptance Tests:

See two attachments.

Tested by:	Date:
M. Smith Michael G. Smith	9-22-00
P. LaPlante	9-25-00

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CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TWINBROOK METRO PLAZA, #210
12300 TWINBROOK PARKWAY
ROCKVILLE, MD 20852-1606

FAX/TELECOPIER NO: (301) 881-0294

FAX (TELECOPY) COVER SHEET

DATE: 9/25/00

NO. OF PAGES (INCLUDING COVER PAGE): 2

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IF ALL PAGES NOT RECEIVED, CALL: (301) 881-0289 Brenda Roberson or Speed No. 298

TO: Ron Janetzke

COMPANY: CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

FROM: ~~[redacted]~~ P. LaPlante

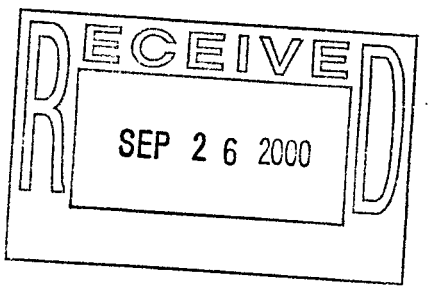
COMPANY: CNWRA – WASHINGTON OFFICE

TELEPHONE: (301) 881-0289

MESSAGE:

Signed SCR.

Pat



Attachment 2 PA-SCR-325 TPA Test Plan

DCAGW Test 1: Perform hand calculations of leaching factor to ensure the code leach factor calculation is performed as expected. Test criteria is that TPA results should be within 5% of hand calculations to account for rounding errors.
Anticipated start date: 9/21/00
Anticipated completion date: 9/25/00
Amount of your time available to perform this test: 8 h
Percent of your time to be spent in process level testing and system level testing: 100/0
Output files to be checked: gftrans.inp, gftrans.def
Input files to be checked for proper data transfer to the program: tpa.inp
Disposition of documentation (storage medium, physical location, and access method): floppy disk attached, related information can be found in scientific notebook # 170E by P. LaPlante.
Functional Test Descriptions:

-Hand Calculations: Calculate leach factors in a spreadsheet using the same (updated) equation as used in TPA 4.0g.

-Process-level tests: Run TPA 4.0g with the same input parameters for the leach factor hand calculation as in the spreadsheet and compare results.

-System-level tests: none

Reasonableness Test Description: none
Final Checklist (completed during testing):

-Did the modification substantially change the results? The leaching factors increased by a factor of approximately 2.7 from previous values. The effect of this change on dose results was not checked but is expected to be small.

-Were TPA 4.0 and TPA 4.1 compared using corresponding mean values in tpa.inp? Dose results were not checked for this test, but 4.0 and 4.1 leach factor differences were checked (see above).

-Which nuclides were monitored to determine reasonableness of results in terms of dose? Not applicable, testing calculation of leach rate.

TEST 1 RESULTS: Pass. All TPA 4.1 leach rate calculations were within 2 % of the hand calculations, well within the 5% criteria set to account for rounding errors (leaccalc41.fin.xls).

Attachment 1 PA-SCR-325 TPA Test Plan

ASHRMOVO Test 1: Perform hand calculations to confirm code calculation of leach rate, dll(i), is performed as expected. Test criteria is that TPA results should be within 1% of hand calculations (1% criteria allows for rounding errors).
Anticipated start date: 9/21/00
Anticipated completion date: 9/22/00
Amount of your time available to perform this test: 4 h
Percent of your time to be spent in process level testing and system level testing: 100/0
Output files to be checked: ashrmovotest.dat
Input files to be checked for proper data transfer to the program: tpa.inp
Disposition of documentation (storage medium, physical location, and access method): 250 Mb zip disk #mas2, stored with scientific notebook # 377, with files stored in /testtpa41beta/testashrmovo/test1.
Functional Test Descriptions:

-Hand Calculations: postprocessing in ashrmovotest.xls to compare TPA leach rate calculations to hand calculations.

-Process-level tests: Write ashrmovo.f parameter values to new file called ashrmovotest.dat to confirm values are processed correctly. These stored values are also used to confirm calculations by hand. Stored parameters are: dll(i), precip, fpe, fpsat, dirr, fie, fisat, depthsoil, theta, rhosoil, and dkd(i). Test was run using the default tpa.inp input file with the following modifications: (i) RelativeRateofBlanketRemoval changed from 0.0007 to 0.0 to eliminate effect of soil erosion, (ii) OutputMode = 2 and SelectAppendFiles = 12 to turn on ASHRMOVO-related append files, and (iii) VolcanismDisruptiveScenarioFlag turned on (= 1) and TimeOfNextVolcanicEventinRegionOfInterest changed to a constant = 100.0.

-System-level tests: none

Reasonableness Test Description: none
Final Checklist (completed during testing):

-Did the modification substantially change the results? Not checked for this test.

-Were TPA 4.0 and TPA 4.1 compared using corresponding mean values in tpa.inp? Not checked for this test.

-Which nuclides were monitored to determine reasonableness of results in terms of dose? Not applicable, testing calculation of leach rate.

TEST 1 RESULTS: Pass. All TPA 4.1 leach rate calculations were within 0.3 % of the hand calculations, well within the 1% criteria set to account for rounding errors (ashrmovotest.xls).

Attachment 1 PA-SCR-325 TPA Test Plan (cont'd)

ASHRMOVO Test 2: Compare results between TPA 4.0 and TPA 4.1 for reasonableness. The areal radionuclide density is expected to decrease slightly over time compared to previous TPA 4.0 results, so reasonableness will be tested graphically to show that the change is not excessive.
Anticipated start date: 9/21/00
Anticipated completion date: 9/22/00
Amount of your time available to perform this test: 4 h
Percent of your time to be spent in process level testing and system level testing: 0/100
Output files to be checked: ashrmovo.ech, ashrmovo.rlt
Input files to be checked for proper data transfer to the program: tpa.inp
Disposition of documentation (storage medium, physical location, and access method): 250 Mb zip disk #mas2, stored with scientific notebook # 377, with files stored in /testtpa41beta/testashrmovo/test2.
Functional Test Descriptions:

- **-Hand Calculations:** none
- **-Process-level tests:** none
- **-System-level tests:** Using the same tpa.inp file used in Test1, run TPA 4.0 and TPA 4.1 leach factor calculations to compare results produced in ashrmovo.rlt for reasonableness. For this test, the leach rate calculation in ashrmovo.f from TPA 4.1 was returned to the form used in TPA 4.0.
- **Reasonableness Test Description:** Areal radionuclide densities vs time reported in ashrmovo.rlt were compared graphically from both runs. Data and plots are in ashrmovo.xls.

Final Checklist (completed during testing):

- **-Did the modification substantially change the results?** No. As expected, the leach rate increased slightly which reduced the areal radionuclide density reported in ashrmovo.rlt.
- **-Were TPA 4.0 and TPA 4.1 compared using corresponding mean values in tpa.inp?** Yes, identical tpa.inp files were used.
- **-Which nuclides were monitored to determine reasonableness of results in terms of dose?** All base case radionuclides.

TEST 2 RESULTS: Pass. Results based on TPA 4.0 and TPA 4.1 leach rate equations were graphically shown to be reasonable (ashrmovo.xls). As expected, the leach rate increased slightly with the TPA 4.1 leach rate equation which reduced the areal radionuclide density reported in ashrmovo.rlt.

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SOFTWARE CHANGE REPORT (SCR)

SCR No. (*Software Developer Assigns*): PA-SCR-326	Software Title and Version: TPA 4.0	/Project No: 20-1402-762

Affected Software Module(s), Description of Problem(s):
condxyzt.f
Improve the Gauss Legendre integration by inhibiting NaN numerical error for the '**tbump2**' variable, divide by zero in function tempgl().

Change Requested by: R. Codell Date:8-3-00	**Change Authorized by** (*Software Developer*): R. Janetzke Date: 8-24-00 Ron Janetzke

Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):
An error was traced to line 133 in subroutine cond3dxyzt, which is an 'if' statement:

if (tend.lt.bftime) then

This allowed a call to the gauss legendre integration routine between two times that were identical; i.e., tend = 50 and bftime = 50. The routine then returned a value for tbump2 = NaN.
This can be solved by changing the if statement from "lt" to "le". This takes care of the case when both values are equal.

Implemented by: R. Codell Richard Codell U.S. NRC	**Date:** 8-3-00

Description of Acceptance Tests:
A single input file was prepared with the backfill time equal to the simulation end time.

Test A: This is a run with the original cond3dxyzt routine and demonstrates the error in the output files contained in the attached CD in subdirectory scr325a. Error messages are written to tpa.out. The run was terminated with a Control-C to avoid excessive file size.

Test B: This is a run with the modified cond3dxyzt routine and demonstrates the absence of the error when using the same input file. This run ran to completion successfully and passed the test. Output from this test in subdirectory scr326b.

Tested by: R. Janetzke Ron Janetzke	**Date:** 9-19-00

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