SOFTWARE RELEASE NOTICE

1. SRN Number: 334

2. Project Title: TSPA & Technical Integration Code | Project No. 20.06002.01.354

3. SRN Title: TPA Version 4.1jpdls_beta4

4. Originator/Requestor: Sitakanta Mohanty | Date: 11/17/2004

5. Summary of Actions

- ☐ Release of new software
- ☐ Change of access software
- ■ Release of modified software:
- ☐ Software Retirement
  - ■ Enhancements made
  - ■ Corrections made

6. Validation Status

- ☐ Validated
- ☐ Limited Validation
- ■ Not Validated Explain: A beta version is being sent to satisfy NRC Intermediate Milestone 06002.01.354.5120.

7. Persons Authorized Access

Name	Read Only/Read-Write	Addition/Change/Delete
Sitakanta Mohanty	RW	Bret Leslie (Addition)
Ron Janetzke	RW	Chris Grossman (Deletion)
Keith Compton (NRC)	RW	
Tim McCartin (NRC)	RW	
Chris Grossman (NRC)	RW	
Others (NRC/CNWRA)	RO	

8. Element Manager Approval: Sitakanta Mohanty Date: 11/18/2004

9. Remarks: A CD containing the TPA Version 4.1jpdls_beta4 code executables.

CNWRA Form TOP-6 (09/01)

SOFTWARE SUMMARY FORM

01. Summary Date: 10-22-04	02. Summary prepared by (Name and phone): Ron Janetzke (210) 522-3318	03. Summary Action: Modified
04. Software Date: 10-22-04	05. Short Title: TPA Version 4.1jpdls-beta4	
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: Ronald Janetzke (210) 522-3318

13. Software Application: The TPA Code consists of the following modules: UZFLOW, NFENV, EBSREL, UZFT, SZFT, DCAGW, FAULTO, SEISMO2, VOLCANO, ASHPLUMO, ASHRMVO, DCAGS, SNLLHS, EXEC.

14. Computer Platform: PC	15. Computer Operating System: Windows/XP	16. Programming Language(s): Lahey LF95 V5.71	17. Number of Source Program Statements: Approx. 53,000 lines w/o stand alone codes
18. Computer Memory Requirements: 1.3Gb	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: Ron Janetzke Date: 11-17-04

CNWRA Form TOP-4-1 (05/98)

1. SCR No. (*Software Developer Assigns*): PA-SCR-521	2. Software Title and Version: TPA 4.1jpd	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): uzflow.def, climato2.dat, uz_parms.i, tpa.inp, szft.f, seismo.f, nintv.i, nfenv.f, maxntime.i, exec.f, ebsrel.f, dcags.f, ashplumo.f, ebsfilt.f, failt.f, nefmks.f, releaset.f, zportpc.f, dcagw.f, and SIZES.INC.

The current version of the code is limited to simulations up to 100,000 years. NRC has requested that this limit be extended for longer term simulations. Also, an update to the curium matrix Kds for the unsaturated zone were received.

5. Change Requested by: S. Mohanty	6. Change Authorized by (*Software Developer*): R. Janetzke Date: 10-27-2004

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

See attachment A - original file is on CD:SCR521as *\scr_521_attach_A.doc.*

8. Implemented by: Rob Rice	Date: 10-27-2004

9. Description of Acceptance Tests:

See Attachment B - original file on CD:NEW as *\SCR521\testplan\Test Plan and Test Results SCR521.wpd*

and

See Attachment C - original file on CD:SCR521 as *\tp_scr521.wpd.*

10. Tested by: G. Adams R. Janetzke	Date: 10-29-04 11-17-04

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
→*DEVELOPED OR ACQUIRED TO BE MODIFIED SOFTWARE*←

Software Title/Name: TPA
Version: 4.1 JPDLS_B4
Demonstration workstation: PC A/by
Operating System: Windows XP
Developer: R. Janetzke/R. Rice

Software Requirements Description (SRD) [TOP-018, Section 5.3]

SRD Version: 4.0
SRD Approval Date:

SRD and any changes thereto reviewed in accordance with QAP-002 requirements?

Yes: ☑ No: ☐ N/A: ☐

Is a Software Change Report(s) (SCR) used for minor modifications (i.e., acquired code), problems or changes to a configured version of software?

Yes: ☑ No: ☐ N/A: ☐

Comments: SCR 521 - Enable code to calculate long term simulations.

Software Development Plan (SDP) [TOP-018, Section 5.4]

SDP Version: 4.0
SDP (EM) Approval Date:

The SDP addresses applicable sections of TOP-018, Appendix B, SDP Template?

Yes: ☑ No: ☐ N/A: ☐

Is the waiver (if used) in accordance with specified guidelines?

Yes: ☐ No: ☑ N/A: ☐

Comments:

Design and Development [TOP-018, Section 5.5.1 - 5.5.4]

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

Yes: ☑ No: ☐ N/A: ☐

Module(s) Reviewed:

Comments: N/A

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Is code 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:

Comments: Changes to code included additional comments.

Is development of the code and informal module/subroutine-level testing documented in scientific notebook and/or SCR?

Yes: ☑ No: ☐ N/A: ☐

SCR's and/or Scientific Notebook(s) Reviewed:

Comments: SCR #521 Work activities associated with code changes are documented as an attachment to SCR #521.

Software designed so that individual runs are uniquely identified by date, time, name of software and version?

Yes: ☑ No: ☐ N/A: ☐

Date and Time Displayed: Month/Day/Time/year

Name/Version Displayed: 4.1jpd15_beta4

Comments: N/A

Medium and Header Documentation [TOP-018, Section 5.5.6]

A program title block of main program contains: Program Title, Customer Name, Customer Office/Division, Customer Contact(s), Customer Phone Number, Associated Documentation, Software Developer and Phone Number, Date, and Disclaimer Notice?

Yes: ☑ No: ☐ N/A: ☐

Comments: Including associated past SCRs.

Source code module headers contain: Program Name, Client Name, Contract reference, Revision Number, Revision History, and Reference to SRD/SCR requirement(s)?

Yes: ☑ No: ☐ N/A: ☐

Module(s) Reviewed:

Comments: Each file contains this information.

The physical labeling of software medium (tapes, disks, etc.) contains: Program Name, Module/Name/Title, Module Revision, File type (ASCII, OBJ, EXE), Recording Date, and Operating System(s)?

Yes: ☑ No: ☐ N/A: ☐

Comments: Source and EXE are the file types.

Code Reviews [TOP-018, Section 5.5.6]

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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: ☐

Documented in Scientific Notebook No.: _____

Comments:

Acceptance and Installation Testing [TOP-018, Section 5.6]

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

SCR changes were tested with two test plans, with two different testers and showed acceptable results. Yes: ☑ No: ☐ N/A: ☐

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

Yes: ☑ No: ☐ N/A: ☐

Computer Platforms: PC Operating Systems: Windows XP

Location of Acceptance Test Results: SCR 521 Documentation Package

Comments: N/A

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

Yes: ☑ No: ☐ N/A: ☐

Computer Platforms: PC Operating Systems: Windows XP

Location of Acceptance Test Results: N/A

Comments: CD supplied to client was verified as being successfully installed.

User Documentation [TOP-018, Section 5.5.7]

Is there a Users' Manual for the software and is it up-to-date?

Yes: ☐ No: ☑ N/A: ☐

User's Manual Version and Date: Version 4.0 January 2002

Comments: Work continues on Version 5.0.

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Are there basic instructions for the *installation* and *use* of the software?

Yes: ☑ No: ☐ N/A: ☐

Location of Instructions: Users Guide Chapter 21

Comments: None

Configuration Control [TOP-018, Section 5.7, 5.9.3]

Is the Software Summary Form (Form TOP-4-1) completed and signed?

Yes: ☑ No: ☐ N/A: ☐

Date of Approval: 11/17/04

Is the list of files attached to the Software Summary Form complete and accurate?

Yes: ☑ No: ☐ N/A: ☐

Comments: Verified on CD supplied to client.

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: N/A

Comments:

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

Yes: ☑ No: ☐ N/A: ☐

Location of script/make files: CD supplied in QA documentation package.

Comments:

Software Release [TOP-018, Section 5.9]

Upon acceptance of the software as verified above, has a Software Release Notice (SRN), Form TOP-6 been issued and does the version number of the software match the documentation?

Yes: ☑ No: ☐ N/A: ☐

SRN Number: _____

Comments: None

Software Validation [TOP-018, Section 5.10]

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

Yes: ☐ No: ☑ N/A: ☐

Version and Date of SVTP: N/A

Date Reviewed and Approved via QAP-002: N/A

Comments: These changes contained in SCR #521 will be validated when TPA V5.1 is validated.

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 and Date of SVTR: N/A

Date Reviewed and Approved via QAP-002: N/A

Comments: See above

Additional Comments:

R Janetzke 11-18-04
Software Developer/Date

Mark R. Ehmstrom 11/18/04
Software Custodian/Date

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November 18, 2004
Contract No. NRC–02–02–012
Account No. IM 20.06002.01.354.510

U.S. Nuclear Regulatory Commission
ATTN: Dr. Bret Leslie
Two White Flint North
11545 Rockville Pike
Mail Stop 7J8
Washington, DC 20555

Subject: Transmittal of TPA Version 4.1jpdls_beta4 Code (IM 20.06002.01.354.510)

Dear Dr. Leslie:

The purpose of this letter is to transmit the TPA Version 4.1jpdls_beta4 code. Attached are three compact disks containing the source code and binary executable files for an Intel-based personal computer platform running the XP operating system and using the Lahey LF95 Fortran compiler. This submittal is made in response to TPA Version 4.1j_LSP (Long Simulation Period) Software (IM 20.06002.01.354.510).

In the designation of TPA Version 4.1jpd, 4.1j represents the version of the 4.1 code; *p* represents the personal computer version; and *d* denotes the presence of disclaimer statements. This enhanced version is TPA4.1jpdls_beta4 where *ls* represents long simulation and *beta4* represents the beta version.

This version of the code contains approximately 78,000 lines of code and will execute the delivered *tpa.inp* file (base case with one realization and 10 subareas) in about 25 minutes on a 2.79GHz PC with 512MB of RAM. The virtual memory requirements are 1.5GB at run time.

This version of the code is based on the earlier version 4.1jpd code released in October 2001, and retains most of the operational characteristics and unknown deficiencies of that version. Installation follows procedures described in the TPA 4.0 User's Guide. The TPA Version 4.1jpdls_beta4 code has not been validated, but the new features will be validated when they are brought into the TPA Version 5.0.1 code. The enabling of long time period simulations

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required seven additional sampled parameters in the *tpa.inp* file. Consequently, the number of sampled parameters increased from 330 to 337. This version is a Windows-only version, and has not been tested on the UNIX platform. The attachment to this letter includes a summary of modifications.

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

Sincerely yours,

Sitakanta Mohanty

Sitakanta Mohanty, Ph.D.
Manager, Performance Assessment

SM/rm
Enclosure: Three computer disks containing the TPA Version 4.1jpdls_beta4 code source and executables.

cc: Letter Only
B. Meehan
W. Reamer
D. DeMarco
E. Whitt
E. Collins
L. Kokajko
G. Hatchett
F. Brown
K. Stablein
M. Bailey
J. Guttmann
W. Ford
T. McCartin
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P. Maldonado
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R. Benke
R. Nes
F. Osidele
P. LaPlante
O. Povetko
L. Howard

ATTACHMENT: Enhancements of the TPA code for long simulations

The following is a description of the enhancements, the computer resources required to successfully execute the TPA Version 4.1jpdls_beta4 code, and the limitations as understood at this time.

Previously, the capabilities of the TPA Version 4.1jpd code were a maximum simulation time of 100,000 years using 401 time steps. These capabilities were expanded, two radionuclides added, and additional modifications accomplished to accommodate those expanded capabilities. The specific enhanced capabilities of the TPA4.1jpdls_beta4 code and the basecase *tpa.inp* file values (shown in parentheses) are:

1. Maximum simulation time: 1,000,000 years (basecase: maximum simulation time of 1,000,000 years)

2. Maximum number of time steps: 5001 (basecase: 201 time steps for the first 10,000 years with a ratio of 100.0 for first to last time step and 4800 time steps after 10,000 years with a ratio of 1.0 for first to last time step)

3. The radionuclides U233 and Th229 were added to the *tpa.inp* file as radionuclides tracked in the groundwater. These radionuclides are daughters in the decay chain of Cm245 -> Am241 -> Np237 that is already in the *tpa.inp* file.

Modifications accomplished to accommodate these expanded capabilities include:

1. Array dimensions specified in module and standalone code source files and also specified in "include" files were increased to allow for the long simulation time and larger number of time steps.

2. The data file climato2.dat, which provides data in 100,000 year cycles and is used to determine the unsaturated zone infiltration, was modified to provide a constant value from the initial peak at 40,000 years through 1,000,000 years.

3. Lahey 95 Release 5.71 was used to compile the TPA4.1jpdls_beta4 code, instead of Lahey 90 Version 4.5, which was used in the original TPA 4.1jpd code.

4. In the UZFT module, the mapping of the flow rates in water contacting the waste package to 500 year time steps was removed and replaced with flow rates at TPA times. These flow rates are used in the UZFT module and, depending on the time stepping scheme, caused instabilities in the UZFT release rates. Removing the interpolation from TPA times to 500 year time steps helped to stabilize the UZFT results. Also, the sampled distributions of Cm matrix K_ds for all UZFT hydrostratigraphic units were made the same as Am. This is consistent with recent summaries of the Cm and Am chemical behavior (e.g., Rundle, 2000). An additional benefit is that these new values markedly reduced the runtime of certain UZFT realizations.

5. The TPA Version 4.1jpd near-field module set the end of the reflux period at 10,000 years in both the REFLUX2 and REFLUX3 models. This module was modified to end the reflux period at 20,000 years, which is consistent with TPA 4.1j results (see Figure 3-3 in the March 2004 Sensitivity Analysis Report for the TPA Version 4.1 code).

6. As identified during its development, the TPA4.1jpdls_beta4 code includes some of the enhancements made subsequent to finalization of the TPA Version 4.1jpd code in October 2001 through the current TPA Version 5.0 code that are appropriate for long simulations. It should be noted that these enhancements do not involve new models or new input data.

7. One software modification involved revisions to DCAGW module to recognize the UserDefinedDilutionVolume parameter as specified in the *tpa.inp* file. This parameter now has a fixed value of 2,676,394 gal/d (3,000 acre-ft/yr). In conjunction with this change, the user-defined plume capture model was activated and the plume capture fraction set to a user-defined constant value of 1.0.

Because of the enhanced capability to perform long simulations, the TPA4.1jpdls_beta4 code has increased computer resource requirements. The recommended system requirements for a dedicated computer are (inclusive): (1) XEON or Athlon processor with a speed of 2.0 mHZ or higher; (2) 2.0 GB or higher of RAM; and (3) 1.0 GB of virtual memory. The TPA4.1jpdls_beta4 code was successfully executed during development on computers with these dedicated resources. However, simultaneous execution of more than one TPA simulation, even on a computer with the recommended system requirements, may result in TPA code execution failure.

Approximately, 0.75 GB of disk space may be required for a complete 331 realization run (about 90 MB for the first realization and then 2.0 MB for each subsequent realization). If the APPEND option is selected to generate intermediate results, up to 50 GB of disk space may be needed. Multiple processors, faster processors, and more RAM improve performance. However, the TPA code will not successfully complete execution, even with higher-end processors, if the memory is insufficient. Applications running in the background or concurrently with a TPA code simulation could degrade the performance of this version of the TPA code or even cause TPA code execution failure. To complete a TPA code run faster (and successfully), it is recommended that background applications closed and avoided, especially if the computer resources are below the recommended levels. Minimum computer resources required to successfully execute the TPA4.1jpdls_beta4 code identified during development are a 1.2 GHz processor, 512 MB RAM, and 1.5 GB of virtual memory; however, using these minimum requirements, the execution is slow and may stop depending on background applications.

The simulation run time using the recommended computer resources and the basecase maximum simulation time and number of time steps (i.e., 1,000,000 years and 5,001 time steps) is about 7 minutes per realization or about 40 hours for a 331 realization run. With a computer system having the minimum requirements and assuming there is no execution failure, the run time could degrade to less than 1 realization per hour.

REFERENCE:

Rundle, W. "The Chemical Interactions of Actinides in the Environment". In Challenges in Plutonium Science. Vol II. pp 392–411. Los Alamos Science, No. 26. LA-UR-00-4100. Los Alamos, New Mexico: Los Alamos National Laboratory. 2000.