



CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES  
QUALITY ASSURANCE  
SURVEILLANCE REPORT

PROJECT NO: 20.06002.01.031

REPORT NO: 2005-1

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**SURVEILLANCE SCOPE:** Development and control of scientific and engineering software

**REFERENCE DOCUMENTS:** TOP-018, Development and Control of Scientific and Engineering Software

**STARTING DATE:** December 16, 2004

**ENDING DATE:** January 6, 2005

**QA REPRESENTATIVE:** R. Folck

**PERSONS CONDUCTING TEST/EXAM/ACTIVITY:** B. Dasgupta, N. Franklin, R. Janetzke, G. Adams, S. Painter, B. Winfrey, R. Fedors, D. Gute, S. Gonzalez, O. Povetko, K. Smart, L. Howard, M. Smith, T. Maxwell, S. Mohanty, S. Hsiung

**SATISFACTORY FINDINGS:**

- Software development activities and documentation were found to be in accordance with applicable requirements of TOP-018 for the following software: TPA, Version 5.0.0.e and PCSA Tools, Version 3.0.1, DCM PACKAGE, V.1.0.
- Test cases developed for validation of SAPHIRE, Version 6.8 are within expected range of use and values selected exercise both normal and extreme cases, e.g. boundary conditions.
- Validation reports are complete and on file for software listed in Table 1 attached. The status of software pending validation is presented in Table 2.

**UNSATISFACTORY FINDINGS:** None

**NONCONFORMANCE REPORT NO:** N/A

**ATTACHMENTS:** Tables 1 and 2

**RECOMMENDATIONS/ACTIONS:**

- Continue to encourage software testers to interface with software users to ensure test cases adequately represent expected use of the software.
- To ensure traceability, cross-reference SCR numbers when an SCR is issued to document rework and retesting of a SCR initiated test failure.
- Ensure validation tests cases for new software versions include a comparison to previous validation test cases (e.g. back-to-back testing) to ensure software changes did not adversely affect other portions (e.g., modules) of the software.
- PCSA Tools, Version 3.0.1 includes SAPHIRE, Version 6.8. Since SAPHIRE will be validated as a standalone code, SAPHIRE, Version 6.8 should be placed under TOP-018 configuration control.

APPROVED: \_\_\_\_\_

CENTER DIRECTOR OF QUALITY ASSURANCE

DATE: \_\_\_\_\_

1/17/2005

**DISTRIBUTION:**

ORIGINAL - CENTER QA DIRECTOR/ QA RECORDS

ORIGINATOR - R. Folck

PRICIPAL INVESTIGATORS

ELEMENT MANAGERS

TECHNICAL & ADMINISTRATIVE DIRECTORS

M. Ehnstrom

**Table 1. Validated Software**

| Software                     | Version         | Responsible Staff    | Date of Validation   |
|------------------------------|-----------------|----------------------|--|
| ABAQUS                       | 5.8-16          | G. Ofoegbu           | Validated (ASL)  |
| ABAQUS                       | 6.4             | D. Gute              | Validated (ASL)  |
| ABAQUS                       | 6.3             | D. Gute              | Validated (ASL)  |
| ABAQUS                       | 6.2             | D. Gute              | Validated (ASL)  |
| AMESH                        | 2               | C. Dinwiddie         | Validated 04/16/03   |
| ANYSYS/LS-Dyna(LS-DYNA 960)  | 5.7             | A. Chowdhury/PA Cox  | Validated 12/16/03   |
| AQTESOLV                     | 2.12            | J. Winterle          | Validated 07/7/2002  |
| Arc/Info                     | 7.0.2           | M. Necsoiu           | Validated 09/15/00   |
| ArcView                      | 3.2/3.2a        | D. Waiting/D. Wyrick | Validated 08/6/03  |
| ArcView                      | 3.1             | D. Waiting           | Validated 08/5/03  |
| BREATH                       | 1.2             | R. Fedors            | Validated 05/2/02  |
| DCM Package                  | 1.0             | S. Painter           | Validated 10/15/04. Software needs to be placed under TOP-018 control. |
| DICTRA                       | 21              | Y.-M. Pan            | Validated 02/2/04  |
| EarthVision                  | 5.0.1           | S. Colton            | Validated 09/26/00   |
| EarthVision                  | 7.5             | S. Colton            | Validated 08/20/04   |
| EQ 3/6                       | 7.2 b           | D. Pickett           | Validated 10/1/02  |
| ESP/CSP/ESPCB/StreamAnalyzer | 6.6/2.3/7.0/1.2 | L. Yang              | Validated 12/19/03   |
| EZ-FRISK                     | 6.1             | S. Gonzalez          | Validated 08/13/04   |
| FITEQL                       | 2               | D. Turner            | Validated 06/23/03   |
| Geochemists Work Bench (GWB) | 4.0.2           | R. Pabalan           | Validated 08/22/03   |
| GMS (Modflow96)              | 3.1             | C. Manepally         | Validated 11/25/02   |
| GM-SYS                       | 4.8.45b         | B. Winfrey           | Validated 07/27/04   |
| GMT                          | 3.4.2           | B. Winfrey           | Validated 11/19/03   |
| MELCOR                       | 1.8.5           | R. Benke             | Validated 07/16/02   |
| MINTEQA2/PRODEFA2            | 4.02            | D. Turner            | Validated 05/8/02  |

**Table 1. Validated Software**

| <b>Software</b> | <b>Version</b> | <b>Responsible Staff</b> | <b>Date of Validation</b>  |
|-----------------|----------------|--------------------------|--|
| MODPATH         | 3              | J. Winterle              | Validated 06/4/04  |
| MULTIFLO™       | 1.5.2          | S. Painter               | Validated 02/25/03   |
| OASIS MONTAJ    | 5.1.8          | B. Winfrey               | Validated 08/16/04   |
| OLYMPUS DISS™   | 1.0.0          | M. Necsiou/B. Winfrey    | Validated 07/26/04   |
| PCSA TOOL       | 3.0.0          | G. Adams                 | Validated 09/15/04   |
| PHREEQCI        | 2.8            | M. Juckett               | Validated 09/7/04  |
| PVHA_YM         | 2              | B. Hill                  | Validated 08/27/02   |
| RSAC            | 6.2            | G. Adams                 | Validated 3/19/04  |
| Stereonet       | 3              | D. Waiting/D. Wyrick     | Validated 08/6/03  |
| StereoStat      | 1.3            | K. Smart                 | Validated 07/23/04   |
| StereoStat      | 1.2            | K. Smart                 | Validated 12/22/03   |
| Surfer          | 8              | B. Winfrey               | Validated 12/16/04   |
| TEPHRA          | 1.0            | B. Winfrey               | Validated 01/04/05. Software needs to be placed under TOP-018 control. |
| THERMOCALC      | N              | Y.-M. Pan                | Validated 02/2/04  |
| TPA             | 5.0r           | R. Janetzke              | Validated 12/5/03  |
| TPA (NRC)       | 5.0s           | R. Janetzke              | Validated 12/5/03  |

**Table 2. Software Pending Validation**

| <b>Software</b> | <b>Version</b> | <b>Responsible Staff</b> | <b>Status</b>   |
|-----------------|----------------|--------------------------|---|
| 3DStress™       | 3              | N. Franklin              | Combined validation plan and report drafted. Pending decision on additional funding for validation.                     |
| DECOM PA        | 1.0 beta       | P. Laplante              | Software is under evaluation for use.   |
| Dtherm          | 1.1            | D. Gute                  | Validation report needs to be finalized. Code modified and requires release as version 1.2 with SCR.                    |
| EarthVision     | 5.1            | S. Colton                | Validation plan developed. May not be used in licensing.  |
| ENVI            | 4.1            | M. Necsiou/B. Winfrey    | Complete. Report to be issued by January 31, 2005.  |
| ERDAS Imagine   | 8.7            | M. Necsiou               | Scheduled completion by January 31, 2005.   |
| FLOW-3D         | 8.2            | R. Fedors                | TBD pending prioritization of current workload.   |
| FracMan         | 2.606          | K. Smart/N. Franklin     | Test plan approved. Test report in-progress.  |
| HYDRUS2D        | 2.05           | R. Fedors                | Pending prioritization of current workload.   |
| HyperMesh       | 6              | D. Gute/T. Maxwell       | Pending prioritization of current workload.   |
| KINEROS2        | 1.12wS         | R. Fedors                | Plan in review. Scheduled completion 01/31/05   |
| LithoTect       | 1.2.2          | K. Smart                 | Received update from validated version 1.2.0. Reran tests and will document on SRN.                                     |
| MCNP            | 5              | O. Povetko               | In-process to be completed by February 28, 2005   |
| MULTIFLO™       | 2              | S. Painter               | Version 2.0.1 scheduled for validation 01/31/05.  |
| NRC-WVDP-GIS    | 1.1            | R. Green                 | Pending decision on use in licensing and funding.   |
| ORIGEN-ARP      | 2              | O. Povetko               | To be retired when Scale 5.0 is released.   |
| PCSA TOOL       | 3.0.0 BetaN    | G. Adams                 | Version 3.0.1 will be validated and released later 2005.  |
| ProShake        | 1.1            | G. Ofoegbu/S. Gonzalez   | To be validated by January 31, 2005.  |
| RESRAD          | 6.22           | R. Nes                   | NRC endorsed code. See NCR 2004-19  |
| RESRAD          | 6.1            | R. Nes                   | NRC endorsed code. See NCR 2004-19  |
| SAP2000         | 8.3.1          | L. Ibarra                | To be validated by February 28, 2005.   |
| SAPHIRE         | 6.7            | B. Dasgupta              | Version 6.8 is being validated. Report must be finalized and submitted for review. Need to place under TOP-018 control. |
| Scale           | 4.4a           | L. Howard                | Scale, Version 5.0 to be validated by January 31, 2005.   |
| SOIL REUSE TOOL | 1.02eta        | M. Smith                 | Not to be used and no plan for further development.   |

**Table 2. Software Pending Validation**

| <b>Software</b> | <b>Version</b> | <b>Responsible Staff</b> | <b>Status</b>  |
|-----------------|----------------|--------------------------|--|
| TPA/GPP         | 1.01           | O. Pensado               | Version 1.0 validated 01/31/03 but code may not be used. |
| TPA/GUI         | 1.0 2          | S. Mohanty               | Possible release under TPA Version 5.0.1                 |
| UDEC            | 3.1            | S. Hsiung                | Validation under review.                                 |
| Vnet PC 2000    | 1.0.4          | T. Maxwell               | Pending decision on use in licensing.                    |