



# CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES QUALITY ASSURANCE SURVEILLANCE REPORT

PROJECT NO: 20.06002.01.031

REPORT NO: 2003-23

PAGE 1 OF 2

SURVEILLANCE SCOPE: Development and control of scientific and engineering software

REFERENCE DOCUMENTS: TOP-018, Development and Control of Scientific and Engineering Software  
QAP-004, Surveillance Control

STARTING DATE: December 8, 2003

ENDING DATE: December 29, 2003

QA REPRESENTATIVE: R. Folck

PERSONS CONDUCTING TEST/EXAM/ACTIVITY: R. Janetzke, B. Winfrey, N. Franklin, M. Padilla, G. Wittmeyer, G. Adams, K. Smart, S. Painter, M. Ehnstrom, B. Dasgupta

## SATISFACTORY FINDINGS:

1. Verified release of TPA, 5.0r and development of PCSA Tools, 3.0 in accordance with TOP-018. The software development plan for PCSA is being revised.
2. Of the twenty-six Category I codes, seven require validation, 3DStress, Dtherm, Earth Vision, HyperMesh, Olympus DISS, PCSA and Sapphire. Of the forty Category II codes, thirty-one require validation and of those, nineteen require target completion dates to be established. See the attached CNWRA Master Directory of Scientific & Engineering Software for a complete listing.

## UNSATISFACTORY FINDINGS:

Minor documentation discrepancies were corrected/addressed during the course of the surveillance and no further action is required.

NONCONFORMANCE REPORT NO: None

ATTACHMENTS: CNWRA Master Directory of Scientific & Engineering Software

RECOMMENDATIONS/ACTIONS: See page 2 for recommendations associated with the validation of "small" codes, placing a code under TOP-018 control and TPA code commentary and regression testing.

APPROVED:   
CENTER DIRECTOR OF QUALITY ASSURANCE

DATE: 12/31/03

## DISTRIBUTION:

ORIGINAL - CENTER QA DIRECTOR/ QA RECORDS  
ORIGINATOR - R. Folck  
PRICIPAL INVESTIGATORS  
ELEMENT MANAGERS  
TECHNICAL & ADMINISTRATIVE DIRECTORS  
M. Ehnstrom

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Page 2 of 2

**RECOMMENDATIONS/ACTIONS:**

The staff should be reminded of the following:

1. To reduce the overhead associated with the validation of "small" codes, TOP-018, section 5.10.5 permits the merging of the validation report and validation plan into single documented. This single document is then reviewed in accordance with QAP-002 rather than two documents and two reviews.
2. TOP-018, section 5.7.1 requires that code be placed under TOP-018 control prior to use in CNWRA activities. The user/developer should provide to CNWRA QA the following:
  - Installation testing on target software and hardware platform(s) (TOP-018, 5.6.3)
  - CD copy of the code and printed list of files, (TOP-018, 5.5.6)
  - Software Summary Form, (TOP-018, 5.7.2)
  - Software Release Notice, (TOP-018, 5.9)
  - Acceptance testing for developed code, (TOP-018, 5.6)

Once the above items are submitted, CNWRA QA will complete a QA Verification Report, (TOP-018, 5.8), issue a Software Release Notice number and the code will be considered under TOP-018 control.

Concerning the client's request to remove commentary from delivered TPA source code and regression testing of the validated TPA code:

1. For each "major" release (e.g., 5.1, 5.2, 6.0) all code commentary should be removed except for detailed design information. Detailed design information includes basic header information (e.g., point of contact, contract numbers, referenced documents, etc.), variable definitions, module functional definitions, and in-line comments. Viable test code would also remain. This information would allow a knowledgeable reviewer/programmer to understand the functions being performed and follow the flow of execution. This is essential so needed maintenance of the code can be performed. Comments that should be removed include revision history, references to SCRs, programmer notes, and dead code. This comment removal exercise would be for major releases and not for quick bug fixes, etc.
2. TPA, version 5.0p was validated December 5, 2003. Regression testing was performed on versions 5.0q and 5.0r and documented on SCRs. While SCRs provide adequate testing for specific code changes, the overall affect of those changes may not be fully assessed or understood. It may be beneficial to develop a test suite for TPA that would exercise the code end-to-end. Again, this test suite would be run at each major release, at a minimum.

# CNWRA MASTER DIRECTORY OF SCIENTIFIC & ENGINEERING SOFTWARE

December 29, 2003

December 29, 2000

Name	Version	SRN Date	Software Category <sup>1</sup>	Software Validation <sup>3</sup>				Key Staff
				Category <sup>2</sup>	SVTP Due Date	Target Completion Date	SVTR Completion Date	
CATEGORY I SOFTWARE								
3DStress	3.0	08/15/03	D	I	01/04	02/04		N. Franklin
ABAQUS	5.8-16	01/08/99	A/NTBM	I	—	—	N/A - ASL	G. Ofoegbu
ABAQUS	6.2	06/14/02	A/NTBM	I	—	—	N/A - ASL	D. Gute
AMESH	2.0	10/19/01	A/NTBM	I	—	—	04/16/03	C. Dinwiddie
ANSYS/LS-DYNA (LS-DYNA 960)	5.7	05/03/01	A/NTBM	I	—	—	12/16/03	A. Chowdhury/ P.A. Cox
Arc/Info	7.0.2	08/16/00	A/NTBM	I	—	—	09/15/00	M. Necsoiu
ArcView	3.2/3.2a	05/04/01	A/NTBM	I	—	—	08/06/03	D. Waiting/ D. Wyrick
Dtherm	1.1	06/03/02	A/TBM	I	Complete	01/04		D. Gute/ T. Maxwell
EarthVision	5.0.1	09/27/00	A/NTBM	I	—	—	09/26/00*	S. Colton
EarthVision	5.1	03/01/01	A/NTBM	I	TBD	TBD		S. Colton
EQ 3/6	7.2 b	02/08/96	A/TBM	I	—	—	10/01/02*	D. Pickett
HyperMesh	5.0	04/19/02	A/NTBM	I	01/04	01/04		D. Gute/T. Maxwell
MELCOR	1.8.5	08/28/01	A/NTBM	I	—	—	07/16/02	R. Benke

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December 29, 2003

Name	Version	SRN Date	Software Category <sup>1</sup>	Software Validation <sup>3</sup>				Key Staff
				Category <sup>2</sup>	SVTP Due Date	Target Completion Date	SVTR Completion Date	
MINTEQA2/ PRODEFA2	4.02	02/22/02	A/NTBM	I	—	—	05/08/02	D. Turner
MULTIFLO	1.5.2	11/12/02	D	I	—	—	02/25/03	S. Painter
OLYMPUS DISS™	1.0	TBD	D	I	Complete	12/03		M. Necsoiu/ B. Winfrey
PCSA	3.0	TBD	D	I	Complete	12/04		B. Dasgupta
PVHA_YM	2.0	08/27/02	D	I	—	—	08/27/02	B. Hill
RSAC	5.2	09/21/00	A/NTBM	I	—	—	01/23/03	R. Benke
RSAC	6.1	02/04/03	A/NTBM	I	—	—	10/22/03	R. Benke
SAPHIRE	6.7	07/26/02	A/NTBM	I	01/04	01/04		B. Dasgupta
SOLCALC	1.0	07/31/01	A/NTBM	I	—	—	01/30/02	R. Pabalan
STEREONET	3.0	09/20/00	A/NTBM	I	—	—	08/06/03	D. Waiting/ D. Wyrick
STERIOSTAT	1.2	12/08/03	A/NTBM	I	—	—	12/22/03	K. Smart
TPA	5.0r	11/24/03	D	I	—	—	12/05/03	R. Janetzke
TPA/GPP	1.01	03/08/02	D	I	—	—	01/31/03	O. Pensado

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CATEGORY II SOFTWARE								
AQTESOLV	2.12	03/22/99	A/NTBM	II	—	—	07/07/02	J. Winterle
ASHPLUME-P	1.0	SRD Only	D	II	01/04	01/04		B. Hill/ B. Winfrey
BREATH	1.2	10/02/97	D	II	—	—	5/02/02	R. Fedors
DICTRA	21	09/05/02	A/NTBM	II	02/04	02/04		Y.-M. Pan
DRIFTVNT	1.0	TBD	D	II	Complete	08/04		S. Painter
ESP/CSP/ESPCB /StreamAnalyzer	6.6/2.3/ 7.0/1.2	TBD	A/NTBM	II	—	—	12/19/03	L. Yang
EZ-FRISK	4.4	08/06/99	A/NTBM	II	TBD	TBD		A. Ghosh/ S. Gonzalez
FITEQL	2.0	08/02/96	A	II	—	—	6/23/03	D. Turner
FLAC	4.0	07/01/02	A/NTBM	II	11/04	11/04		S. Hsiung
Geochemists Work Bench (GWB)	4.0.2	TBD	A/NTBM	II	—	—	08/22/03	L. Browning
GENII-S	1.485	07/30/96	E	II	TBD	TBD		P. LaPlante
GMS (Modflow96)	3.1	07/05/02	A/NTBM	II	—	—	11/25/02*	C. Manepally
GMS (ModPath)	3.1	07/05/02	A/NTBM	II	01/04	03/04		J. Winterle

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GM-SYS	4.04.08 C	08/04/99	A/NTBM	II	TBD	TBD		V. Gonzalez
GMT	3.4.2	01/31/03	A/NTBM	II	—	—	11/19/03	B. Winfrey
HYDRUS2D	2.05	01/25/01	A/NTBM	II	12/03	02/04		R. Fedors
KINEROS2	00_04 (1.4)	05/12/00	A/NTBM	II	12/03	12/03		R. Fedors
Mag-Parrellel	1.0	TBD	A/NTBM	II	01/04	01/04		B. Winfrey
MATLAB	6.0/R12	07/07/99	A/NTBM	II	TBD	TBD		R. Fedors/ S. Gonzalez
MCNP	4A	07/30/97	A/NTBM	II	TBD	TBD		O. Povetko
MCNP	5.0	12/08/03	A/NTBM	II	TBD	TBD		O. Povetko
MODFLOW96	3.1	07/05/02	A/NTBM	II	—	—	11/25/02*	C. Manepally
MULTIFLO/GUI	1.2Beta	3/26/02	D	II	TBD	TBD		S. Painter
MULTIFLO	2.0	SRD/SDP	D	II	TBD	TBD		S. Painter
NRC-WVDP-GIS	1.1	07/27/02	D	II	TBD	TBD		D. Farrell
OASIS MONTAJ	5.1.8	TBD	A/NTBM	II	01/04	01/04		B. Wingfrey
ORIGEN-ARP	2.0	1/29/03	A/NTBM	II	TBD	TBD		O. Povetko
PHREEQC	2.6	02/20/03	A/NTBM	II	—	—	05/06/03	D. Turner
ProShake	1.1	11/16/02	A/NTBM	II	11/03	07/04		G. Ofogebu

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RESRAD	5.82	06/08/98	A/NTBM	II	TBD	TBD		P. LaPlante
RESRAD	6.1	06/21/02	A/NTBM	II	TBD	TBD		O. Povetko
Scale	4.4a	1/29/03	A/NTBM	II	TBD	TBD		O. Povetko
Soil Flow	1.0	SRD Only	D	II	05/04	09/04		R. Fedors
SOIL REUSE TOOL	1.0 $\beta$ eta	03/13/03	D	II	TBD	TBD		M. Smith
STELLA	6.0.1	03/06/01	A/NTBM	II	TBD	TBD		O. Povetko
THCPROB	1.0	SRD/SDP	D	II	TBD	TBD		R. Janetzke
THERMOCALC	N	09/05/02	A/NTBM	II	Complete	02/04		Y.-M. Pan
TPA/GUI	1.0 $\beta$	SRD/SDP Only	D	II	TBD	TBD		S. Mohanty
UDEC	3.1	04/19/00	A/NTBM	II	Complete	TBD		S. Hsiung
Vnet PC 2000	1.0.4	4/26/02	A/NTBM	II	TBD	TBD		T. Maxwell

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CATEGORY III SOFTWARE								
3DStress	2.0 Irix/Solaris	09/24/02	D	III				N. Franklin
ArcView	3.1	11/07/00	A/NTBM	III	—	—	08/05/03	D. Waiting
EINVRT	6.0	07/09/99	A/NTBM	III				D. Farrell
GEOINVRT	1.0	SRD Only	D	III				D. Farrell
ISATIS	3.1.3	10/24/98	A/NTBM	III				D. Farrell/ R. Fedors
ORIGEN	2.1	10/10/97	A/NTBM	III				O. Povetko
Slide	4.0	11/14/02	A/NTBM	III				G. Ofoegbu



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CATEGORY IV SOFTWARE								
3DStress	1.3.2	09/08/99	D	IV	Not to be retired per Larry			N. Franklin
3DStress	1.3.3 Irix	09/20/00	D	IV	—	—	11/16/01	N. Franklin
3DStress	1.3.3 Solaris	09/20/00	D	IV	—	—	11/16/01	N. Franklin
Crystal Ball 2000	5.1	04/27/01	A/NTBM	IV	Complete			I. Chichkov
D and D	2.1.0	08/09/01	A/NTBM	IV				M. Smith
DDA-CT	2.0	SRD Only	D	IV				S. Hsiung
ESP/CSP	6.5/2.2	08/17/01	A/NTBM	IV				L. Yang
Geochemists Work Bench (GWB)	3.0	11/11/98	A/NTBM	IV				L. Browning
Geochemists Work Bench (GWB)	3.0.2		A/NTBM	IV				L. Browning
NRC-WVDP-GIS	1.0	08/20/01	D	IV				D. Farrell
MatCad	8.0	09/07/99	A/NTBM	IV				R. Fedors
MATLAB	5.2	07/07/99	A/NTBM	IV				R. Fedors
MCNP	4C2	1/29/03	A/NTBM	IV				O. Povetko
MEPAS	3.2g	08/17/98	A/NTBM	IV				P. LaPlante

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MULTIFLO	1.2.3	12/22/00	D	IV				S. Painter
MULTIFLO	1.5	07/24/01	D	IV				S. Painter
OASIS	4.5	08/06/99	A/NTBM	IV				R. Green
OLI Stream Analyzer	1.1	08/30/02	A/NTBM	IV			11/03	L. Yang
PCSA	2.0	06/25/03	D	IV				B. Dasgupta
PHREEQC	2.4.2	02/25/02	A/NTBM	IV				D. Turner
TPA/GPP	1.0	02/01/02	D	IV				O. Pensado
TPA	4.1j	5/02/01	D	IV	Not to be retired - see e-mail in folder			R. Janetzke
TPA	V.4.0jpd	09/16/2003	D	IV				R. Janetzke
TPA	5.0	02/27/03	D	IV				R. Janetzke
TPA	5.0beta	09/27/02 SRD/SDP	D	IV				R. Janetzke
TPA	5.0d	04/7/03	D	IV				R. Janetzke
TPA	5.0o	07/29/2003	D	IV				R. Janetzke
TPA	5.0p	08/22/03	D	IV	—	—	12/05/03	R. Janetzke

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				Category <sup>2</sup>	SVTP Due Date	Target Completion Date	SVTR Completion Date	
RETIRED SOFTWARE								
ASHPLUME	1.0	06/24/97	D	IV	Retired Software			B. Hill
Dtherm	1.0	08/12/01	A/TBM	IV	Retired Software			D. Gute
FLOW-3D	8.0.1	10/18/02	A/NTBM	IV	Retired Software 5/30/03			R. Fedors
GMS	3.0	01/02/01	A/NTBM	IV	Retired Software			C. Manepally
HyperMesh	4.0	11/26/01	A/NTBM	IV	Retired Software			D. Gute
MINTEQA2	3.11/3.12	08/02/96	A/NTBM	IV	Retired Software			D. Turner
MULTIFLO	1.5.1	06/21/02	D	IV	Retired Software			S. Painter
PCSA	1.0	07/29/02	D	IV	Retired Software			B. Dasgupta
PCSA	2.0 Beta	11/14/02	D	IV	Retired Software			B. Dasgupta
PHREEQC	1.6	04/15/99	A/NTBM	IV	Retired Software			D. Turner
PPSGS	1.0	07/02/99	A/NTBM	IV	Retired Software			B. Hill
PPSGS	1.1	10/13/00	A/NTBM	IV	Retired Software			B. Hill
PVHVIEW	1.0	02/17/00	D	IV	Retired Software			B. Hill
RESRAD	6.0	08/09/01	A/NTBM	IV	Retired Software			P. LaPlante
S-PLUS	3.4	11/07/97	A	IV	Retired Software			S. Mohanty

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TECTRAN	1.0	09/05/02	D	IV	Retired Software 8/5/03			N. Sridhar
TPA	3.2 PP β	11/25/98	D	IV	Retired Software			S. Mohanty / H. Thomas
TPA	3.3	11/29/99	D	IV	Retired Software			S. Mohanty / R. Janetzke
TPA	3.2.3	07/19/99	D	IV	Retired Software			R. Janetzke
TPA	4.0	03/30/00	D	IV	Retired Software			S. Mohanty
TPA	4.1	09/27/00	D	IV	Retired Software			S. Mohanty
TPA	4.1e	01/31/01	D	IV	Retired Software			R. Janetzke

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CATEGORY TO BE DETERMINED								
FLOW-3D	8.1.1		A/NTBM	TBD				R. Fedors
NIMHIT	1.0	SRD Only	D	TBD				A.Ghosh
MCUTIL	1.0	SRD Only	D	TBD				M. Silliman G. Adams
PFC2D/3D	3.0/2.0	04/28/03	A	TBD				A. Ghosh
SHOCK	None Provided	SRD Only	D	TBD				B. Hill

NOTES:

- (1) A (Acquired): Software developed by an individual or organization other than the CNWRA or by such individual or organization while not employed by or under contract to the CNWRA. Acquired software is controlled in accordance with the pertinent provisions of TOP-018 (Table 1).
- D (Developed): Software that has been developed or modified by the CNWRA or by an individual or organization employed by or under contract to the CNWRA. Developed software is controlled in accordance with the pertinent provisions of TOP-018 (Table 1).
- E (Existing): Software that has been acquired or developed by the CNWRA outside of the controls provided by TOP-018. Typically, codes in this category were acquired or developed before the procedure was implemented and have since been superseded by other codes or later versions of the same code. The CNWRA management has made a decision that Existing software will not be brought into compliance with the provisions of TOP-018 (Table 1). Such codes cannot be used in support of NRC licensing actions or regulatory reviews.
- NTBM (Not To Be Modified): This term applies only to Acquired software, and affects the provisions of TOP-018 that are pertinent to the code (Table 1).
- TBM (To Be Modified): This term applies only to Acquired software, and affects the provisions of TOP-018 that are pertinent to the code (Table 1).
- (2) Validation Category I: Highly likely that these will be used in regulatory review—validate in FY 2002 and FY 2003  
Validation Category II: Likely that these will be used in regulatory review—validate in FY 2004.  
Validation Category III: Commercial use software but will not be used in regulatory reviews—decide when validation is needed.  
Validation Category IV: Will not be used for regulatory reviews or commercial work—do not validate.
- (3) In all case the validation plan and report should be reviewed to determine the scope of the validation, including approved hardware and operating system platforms, prior to use of the software.
- \* **The scope of validation for this software is limited. Review validation report.**

11/11