CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QUALITY ASSURANCE
SURVEILLANCE REPORT

PROJECT NO: 20.06002.01.031	**REPORT NO:** 2004-11	**PAGE** 1 **OF** 6

SURVEILLANCE SCOPE:

1. Review CNWRA technical products to verify software used to generate data is controlled in accordance with TOP-018.
2. Verify Software Development Plans are up-to-date and implemented for CNWRA-developed software.
3. Provide an update on the status for code validation.

REFERENCE DOCUMENTS: TOP-018, Development and Control of Scientific and Engineering Software
QAP-004, Surveillance Control
QAP-014, Documentation and Verification of Scientific and Engineering Calculations
QAP-002, Review of CNWRA Documents, Reports and Papers

STARTING DATE: June 29, 2004 **ENDING DATE:** July 9, 2004

QA REPRESENTATIVE: R. Folck

PERSONS CONDUCTING TEST/EXAM/ACTIVITY: Y. Pan, V. Jain, L. McKague, N. Franklin, R. Janetzke, G. Adams, R. Fedors, S. Painter, B. Winfrey, J. Winterle, D. Gute, G. Ofoegbu, O. Pensado, B. Dasgupta, S. Hsiung, O. Povetko, B. Morgan

SATISFACTORY FINDINGS: See pages 2 - 6.

UNSATISFACTORY FINDINGS: Nonconformance Report 2004-04 issued March 15, 2004 identified a technical report issued with a reference to software not under TOP-018 configuration control. Of five randomly selected reports reviewed during this surveillance, two reports included a reference to software not under TOP-018 configuration control. See page 2.

NONCONFORMANCE REPORT NO: Corrective Action Request 2004-4

ATTACHMENTS: None

RECOMMENDATIONS/ACTIONS: See page 6.

APPROVED: _____
CENTER DIRECTOR OF QUALITY ASSURANCE

DATE: 7/13/2004

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

SURVEILLANCE RESULTS, Part 1:

1. ***Chemical Specification, Using Thermodynamic Modeling, During a Representative LOCA Event - Draft Report,*** June 29, 2004

   Software used in this technical report included Stream Analyzer, Version 1.2 and Environmental Simulation Program, Version 6.6. Both programs were initially validated December 19, 2003. Use of the code for this report was outside to initial scope of the validation but additional test cases were developed and included in the technical report. Stream Analyzer, Version 1.2 and Environmental Simulation Program, Version 6.6 were placed under TOP-018 configuration control July 8, 2004 after release of the report.

2. ***Drift Scale Thermohydrological Process Modeling In-Drift Heat Transfer and Drift Degradation,*** July 2004

   Software used in this technical report included MULTIFO, Version 2.0. MULTIFO, Version 2.0 was placed under TOP-018 control March 5, 2004. Validation for MULTIFO, Version 2.0 is scheduled for November 2004.

3. ***Final Report on Experiments to Model Normal Faulting in Carbonate Strata Above Salt Domes and 3D Digital Fault Analysis to Estimate Synthetic Fracture Network of Zakum Field,*** June 2003

   Software used in this technical report included FracWorks XP, Version Beta 0.22. FracWorks XP, Version Beta 0.22 is not under TOP-018 control.

4. ***3rd Quarterly Progress Report - Structural Controls on the Edwards Aquifer/Trinity Aquifer Interface, June 25, 2003***

   Software used in this technical report included 3DStress and EarthVision. 3DStress, Version 3.0 was placed under TOP-018 control August 15, 2003, EarthVision, Version 5.0.1, September 27, 2000 and EarthVision, Version 5.1, March 1, 2001. There is no reference to version numbers in report. Additionally, the report was incorrectly dated June 25, 2003 rather than the correct date of June 24, 2004.

5. ***Temperature and relative Humidity Along Heated Drifts with and without Drift Degradation,*** June 2004

   Software used in this technical report included MULTIFLO, Version 1.5.2 and Flow-3D, Version 8.2. MULTIFLO, Version 1.5.2 was placed under TOP-018 control November 12, 2002 and validated February 25, 2003. Flow-3D, Version 8.2 was placed under TOP-018 control March 11, 2004 and is scheduled for validation October 2004.

SURVEILLANCE RESULTS, Part 2:

In accordance with TOP-018, Section 5.4.5, verified currency of Software Development Plans for 3DStress, PCSA Tools, TPA, Multiflow and XFlo.

SURVEILLANCE RESULTS, Part 3:
Software that is likely to be used in regulatory review process and their validation status are listed below in Tables 1 and 2.

Table 1. Validated Software or Scheduled for Validation

Software Name	Version	Target Validation Date	Actual Validation Date	Key Staff
ABAQUS	5.8-16		N/A - ASL	G. Ofoegbu
ABAQUS	6.2		N/A - ASL	D. Gute
AMESH	2.0		04/16/03	C. Dinwiddie
ANSYS/LS-DYNA (LS-DYNA 960)	5.7		12/16/03	A. Chowdhury/P.A. Cox
AQTESOLV	2.12		07/07/02	J. Winterle
Arc/Info	7.0.2		09/15/00	M. Necsoiu
ArcView	3.2/3.2a		08/06/03	D. Waiting/D. Wyrick
BREATH	1.2		5/02/02	R. Fedors
DICTRA	21		02/02/04	Y.-M. Pan
DRIFTVNT	1.0	08/04		S. Painter
Dtherm	1.1	08/04		D. Gute
EarthVision	5.0.1		09/26/00	S. Colton
EarthVision	5.1	07/04		S. Colton
EQ 3/6	7.2 b		10/01/02	D. Pickett
ESP/CSP/ESPCB/ StreamAnalyzer	6.6/2.3/7.0/ 1.2		12/19/03, Updated 06/29/04	L. Yang
HyperMesh	6.0	08/04		D. Gute/T. Maxwell
FITEQL	2.0		6/23/03	D. Turner
FLOW-3D	8.2	10/04		R. Fedors
Geochemists Work Bench (GWB)	4.0.2		08/22/03	R. Pabalan

Table 1. Validated Software or Scheduled for Validation

Software Name	Version	Target Validation Date	Actual Validation Date	Key Staff
GMS (Modflow96)	3.1		11/25/02	C. Manepally
GMS (ModPath3)	3.1		06/04/04	J. Winterle
GMT	3.4.2		11/19/03	B. Winfrey
HYDRUS2D	2.05	10/04		R. Fedors
KINEROS2	1.12wS	08/04		R. Fedors
Mag-Parrellel	1.0	09/04		B. Winfrey
MELCOR	1.8.5		07/16/02	R. Benke
MODFLOW96	3.1		11/25/02	C. Manepally
MINTEQA2/ PRODEFA2	4.02		05/08/02	D. Turner
MULTIFLO	2.0	11/04		S. Painter
MULTIFLO	1.5.2		02/25/03	S. Painter
OASIS MONTAJ	5.1.8	07/04		B. Wingfrey
OLYMPUS DISS	1.0	07/04		M. Necsoiu/ B. Winfrey
PCSA	3.0	11/04		G. Adams
PHREEQC	2.6		05/06/03	D. Turner
PVHA_YM	2.0		08/27/02	B. Hill
RSAC	6.2		03/19/04	G. Adams
RSAC	6.1		10/22/03	R. Benke
RSAC	5.2		01/23/03	R. Benke
SAPHIRE	6.7	08/04		B. Dasgupta
SOLCALC	1.0		01/30/02	R. Pabalan
Stereonet	3.0		08/06/03	D. Waiting/D. Wyrick
StereoStat	1.2		12/22/03	K. Smart

Table 1. Validated Software or Scheduled for Validation				
Software Name	**Version**	**Target Validation Date**	**Actual Validation Date**	**Key Staff**
TPA (NRC)	5.0s		12/05/03	R. Janetzke
TPA	5.0r		12/05/03	R. Janetzke
TPA/GPP	1.01		01/31/03	O. Pensado
THERMOCALC	N		02/02/04	Y.-M. Pan
UDEC	3.1	09/04		S. Hsiung

Table 2. Software to be Scheduled for Validation				
Software Name	**Version**	**Target Validation Date**	**Actual Validation Date**	**Key Staff**
3DStress	3.0			N. Franklin
GENII-S	1.485			P. LaPlante
GM-SYS	4.04.08C			S. Gonzalez
MCNP	5.0			O. Povetko
MULTIFLO/GUI	1.2Beta			S. Painter
ProShake	1.1			G. Ofoegbu/ S. Gonzalez
NRC-WVDP-GIS	1.1			D. Farrell
ORIGEN-ARP	2.0			R. Ness
RESRAD	5.82			P. LaPlante
RESRAD	6.1			TBD
Scale	4.4a			R. Ness
SOIL REUSE TOOL	1.02eta			M. Smith
EZ-FRISK	4.4			A. Ghosh/ S. Gonzalez
THCPROB	1.0			R. Janetzke

Table 2. Software to be Scheduled for Validation				
Software Name	**Version**	**Target Validation Date**	**Actual Validation Date**	**Key Staff**
TPA/GUI	1.0 2			S. Mohanty
Vnet PC 2000	1.0.4			T. Maxwell

Recommendations/Actions:

1. If a technical report expands the scope of validation, either place a copy of the technical report in the software control file or update the existing validation report.
2. For traceability and repeatability, reference versions/releases of software used in technical reports.
3. Place the software control list and a link to applicable validation reports on the QA web site to enhance usability of these references.
4. Update instructions to technical reviewers to (a) verify that referenced software is under TOP-018 control and (b) if the software is validated, verify that the use of the software is within the scope of validation.
5. Merge category I and category II software on the software control list and redefine define categories as follows:

   Category I - Approved for use in regulatory review.

   Category II - Commercial use software not to be used in regulatory review.

   Category III - Retired software not to be used for regulatory review or commercial work.