CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QUALITY ASSURANCE
SURVEILLANCE REPORT

PROJECT NO: 20.06002.01.031	REPORT NO: 2004-05	PAGE __1__ OF _3_

SURVEILLANCE SCOPE: See page 2.

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: March 1, 2004   **ENDING DATE:** March 15, 2004

QA REPRESENTATIVE: R. Folck

PERSONS CONDUCTING TEST/EXAM/ACTIVITY: A. Chowdhury, Y. Pan, V. Jain, E. Pearcy, L. McKague, N. Franklin, R. Janetzke, G. Adams, R. Fedors, S. Painter, B. Winfrey, J. Winterle, P. Bertetti, G. Walter, D. Gute

SATISFACTORY FINDINGS:

See pages 2 - 3.

UNSATISFACTORY FINDINGS:

See page 2 - 3.

NONCONFORMANCE REPORT NO: 2004-04

ATTACHMENTS: None

RECOMMENDATIONS/ACTIONS:

See page 2 - 3.

APPROVED: _____
CENTER DIRECTOR OF QUALITY ASSURANCE

DATE: ___3/16/2004___

SURVEILLANCE SCOPE:

1. Review four (4) CNWRA technical reports to determine:
    a. Software used to generate data is controlled in accordance with TOP-018
    b. The use of software is within the scope of the validation for validated software
2. Software Development Plans are up-to-date and implemented for CNWRA-developed software

SURVEILLANCE RESULTS, Part 1:

1. *Effect of Fabrication Processes on Material Stability - Characterization and Corrosion,* IM 06.002.01.081.320, June 16, 2003

    Satisfactory Findings:
    Thermo-Calc, Version N with Ni-Data Version 5 database was placed under TOP-018 control September 5, 2002 and software validation was completed February 2, 2004. Thermo-Calc was used within the scope of validation in that validation test case number one addresses use of solvus temperature modeling and use of the Ni-Data Version 5 database.

    Unsatisfactory Findings:
    None

    Recommendations/Actions:
    The technical report states in-part, "the Ni-Data Version 5 database used in the current calculations has been extensively validated against experimental results reported for multicomponent nickel-base alloys." The basis for this statement is both CNWRA-developed data as well as data generated from outside sources. Reference should be provided to support the claim that the database is extensively validated.

2. *Evaluation of Alternative Concepts for Saturated Zone Flow: Effects of Recharge and Water Table Rise on Flow Paths and Travel Times at Yucca Mountain,* IM 06.002.01.131.320, April 16, 2003

    Satisfactory Findings:
    GMS, Version 3.1, was placed under TOP-018 control July 5, 2002. GMS (Modflow-96), Version 3.1, was validated November 2, 2002. GMS (Modpath), Version 3.1, validation is scheduled for March 2004.

    Unsatisfactory Findings:
    None

    Recommendations/Actions:
    - The Technical Reviewer checked a subset of Modpath calculations to verify reproducibility of results. Input data was not checked as required by QAP-014, 3.2.3(i), review of calculations from controlled software. The reviewer indicated that since the outputs appeared reasonable, there was no need to examine input data. Departure from instructions to technical reviewers should be documented on review sheets.

    - GMS packages Recharge, Block Centered Flow and Drain were used in the report. Validation performed on Modflow-96 included Recharge and Block Centered Flow but not the Drain package. The author indicated the Drain package was used to "calibrate" or set up the model and by simply viewing the model results the package validity can be assessed. Technical reviewers should review the scope of validation for validated software and assess and document the validity of software used.

3. *Mineralogy and Geochemistry of Well Cuttings from Selected Early Warning Drilling Project Wells in Fortymile Wash,* IM 20.06002.01.141.320, July 23, 2003

   Satisfactory Findings:
   JADE, Version 6.15 is a graphics interface program used to display x-ray diffraction patterns. Microsoft Excel 2002 was used for calculations and to generate figures. The use of JADE and Microsoft Excel in this report does not fall under the scope of TOP-018. JADE and Microsoft Excel was used simply to format and display the data graphically and other commercial software is available to do similar functions. Raw data is included in scientific notebooks.

   Unsatisfactory Findings:
   None.

   Recommendations/Actions:
   - The report states in-part, "these codes are not controlled under CNWRA Software Configuration Procedures because they are commercial software packages and only the object codes are available to the CNWRA." Software classified as commercial code is not justification for not placing software under TOP-018 control.

   - The report did not include a reference to which version of JADE was used in development of the report. A reference to the version is needed to ensure reproducibility of report results and simply, to be complete.

   - Instructions to technical reviewers, form QAP-12 indicates that there are no calculations even though the report states that Microsoft Excel 2002 was used for calculations. The Element Manger indicated that since the calculations were straightforward, e.g. simple arithmetic, over checks were not necessary. Rationale for decisions by the Element Manger should be recorded.

4. *Mechfail: A Total-system Performance Assessment Code Module for Evaluating Engineered Barrier Performance Under Mechanical Loading Conditions,* IM 20.06002.01.101.340, April 28, 2003 (Version 1)

   Satisfactory Findings:
   - ABAQUS Version 5.8-16 and ABAQUS Version 6.2 were placed under TOP-018 control January 8, 1999 and June 14, 2002 respectively. Data generated using Microsoft Excel 97, SR-2 and MathCAD 2000 were reviewed in accordance with QAP-014.

   - The development of the Mechfail code is well documented in Scientific Notebook No. 410. Mechfail was incorporated into the TPA, Version 5.0beta as documented in Software Change report No. 414.

   Unsatisfactory Findings:
   Hyper Mesh, Version 3.1 is identified in the report as being under TOP-018 control. Version 3.1 of Hyper Mesh is not under TOP-018 control. Version 4.0 was placed under TOP-018 control November 26, 2001 and Version 5.0 April 19, 2002.

   Recommendations/Actions:
   Review sheets completed by B. Mabrito refer to "attached documentation," however, there was no attached documentation in package. Note that the review sheets were added after the QA QAP-002 review was completed. The discrepancy was corrected during the surveillance.

SURVEILLANCE RESULTS, Part 2:
In accordance with TOP-018, Section 5.4.5, verified implementation and currency of Software Development Plans for 3DStress, PCSA Tools, TPA, and Multiflow.